Supporting Information

Tertiary arsine ligands for Stille coupling reaction

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Contents:

1. NMR Spectra

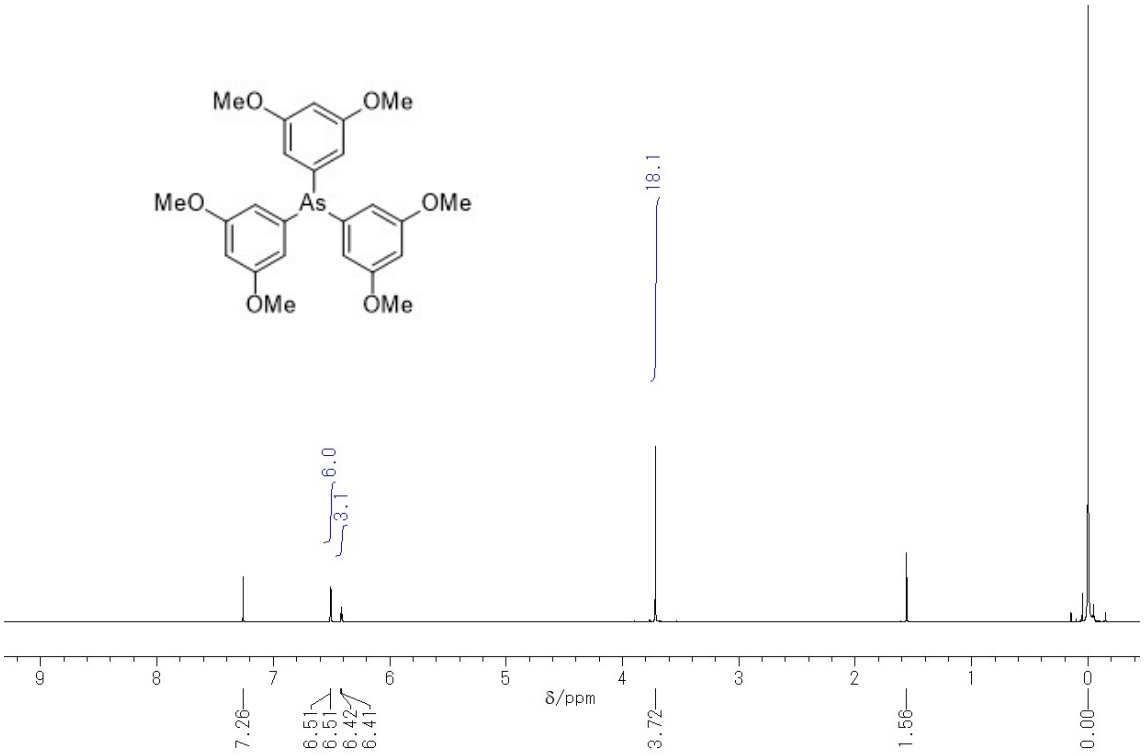


Figure S1. ^{1}H-NMR (400 MHz) spectrum for **1k** in $CDCl_3$.

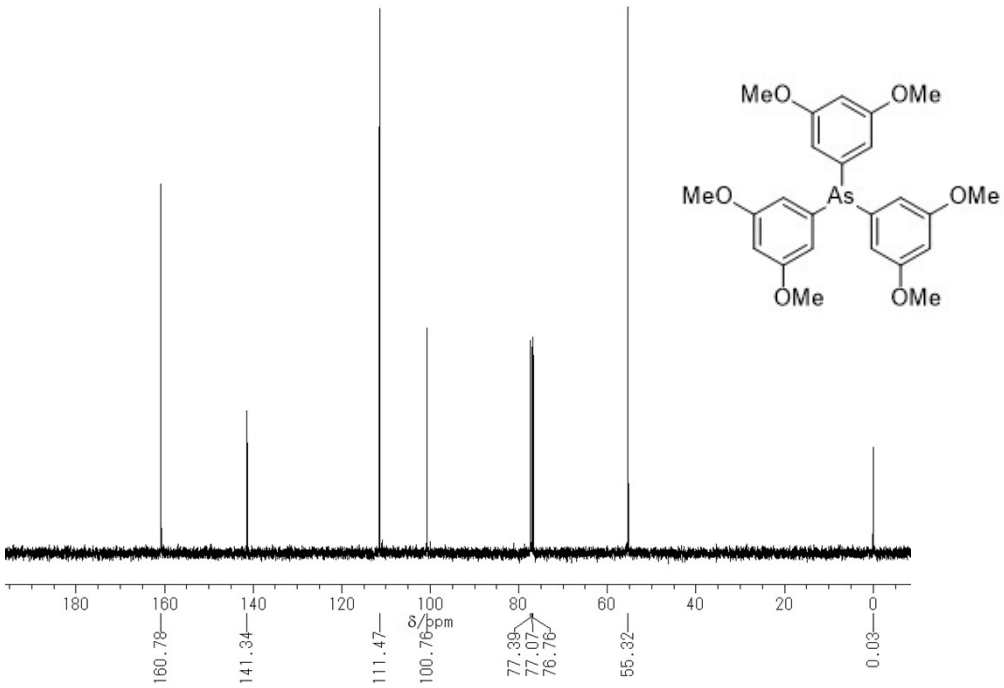


Figure S2. ^{13}C-NMR (100 MHz) spectrum for **1k** in $CDCl_3$.

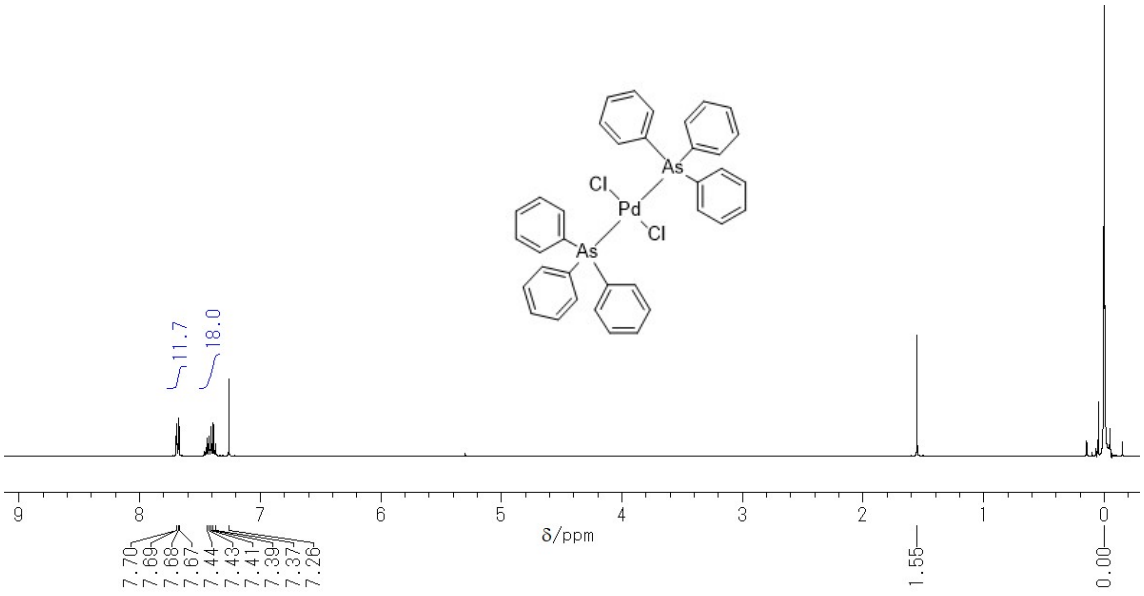


Figure S3. ^{1}H-NMR (400 MHz) spectrum for $[PdCl_2(AsPh_3)_2]$ in $CDCl_3$.

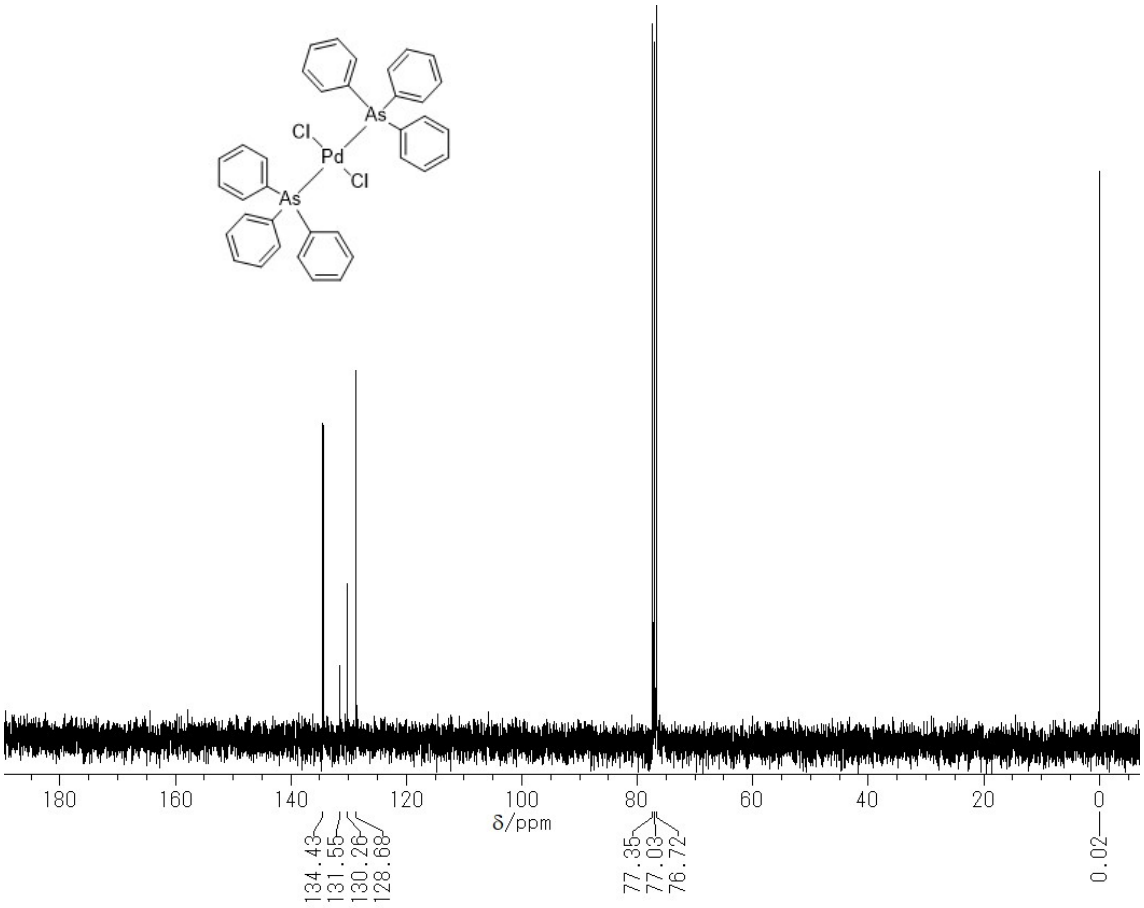


Figure S4. ^{13}C-NMR (100 MHz) spectrum for $[PdCl_2(AsPh_3)_2]$ in $CDCl_3$.

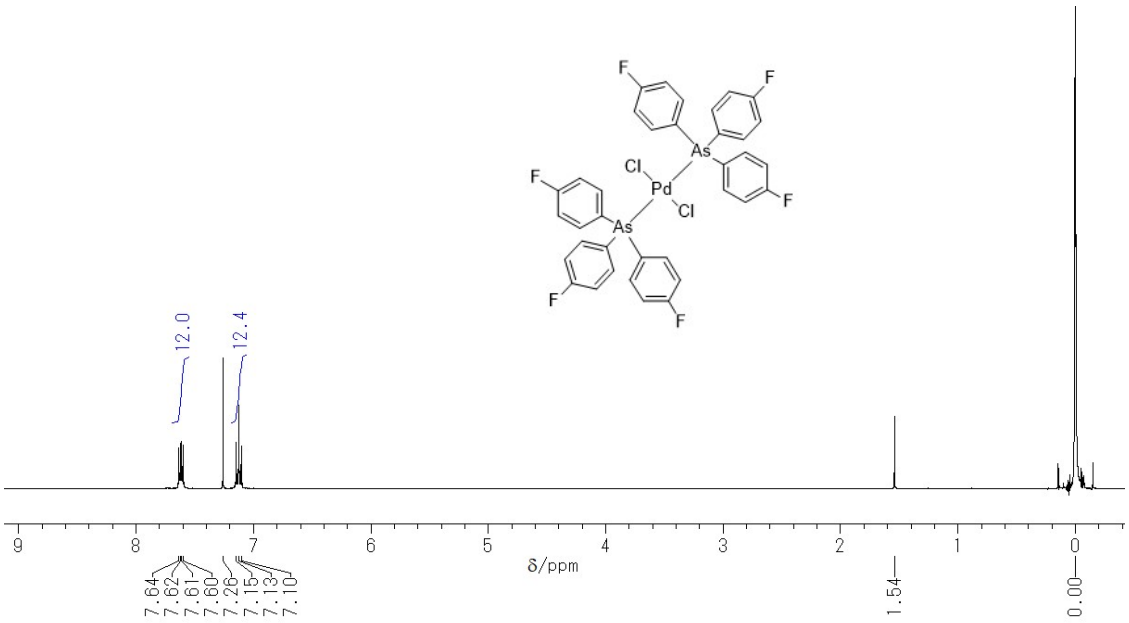


Figure S5. ^{1}H-NMR (400 MHz) spectrum for [$PdCl_2$(**1a**)$_2$] in $CDCl_3$.

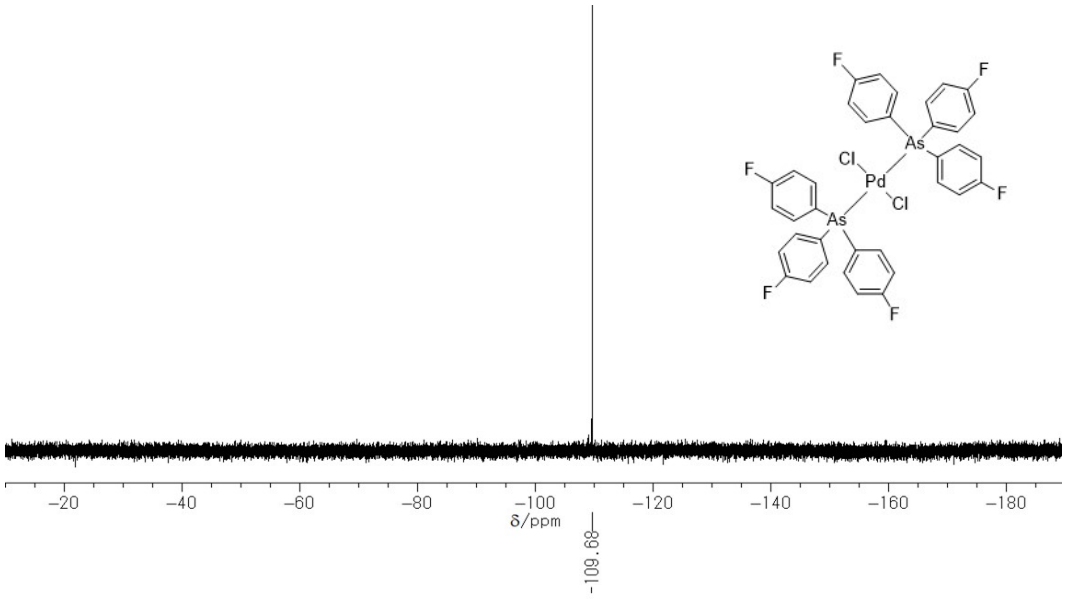


Figure S6. ^{19}F-NMR (376 MHz) spectrum for [$PdCl_2$(**1a**)$_2$] in $CDCl_3$.

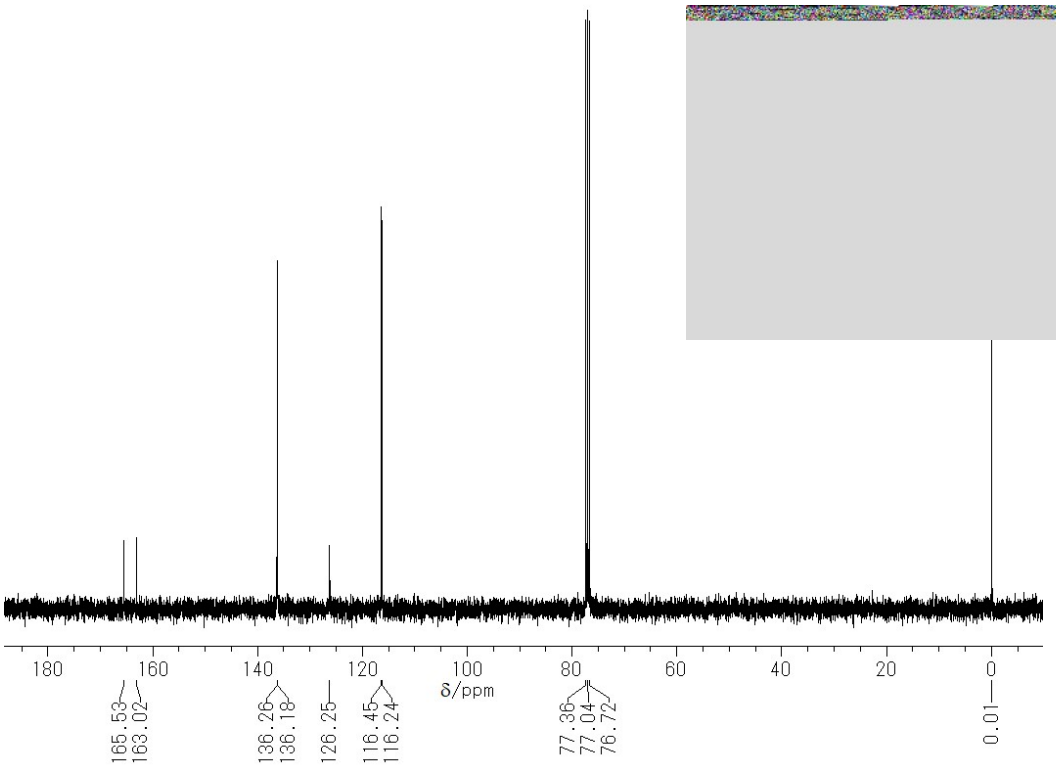


Figure S7 ^{13}C-NMR (100 MHz) spectrum for [$PdCl_2$(**1a**)$_2$] in $CDCl_3$.

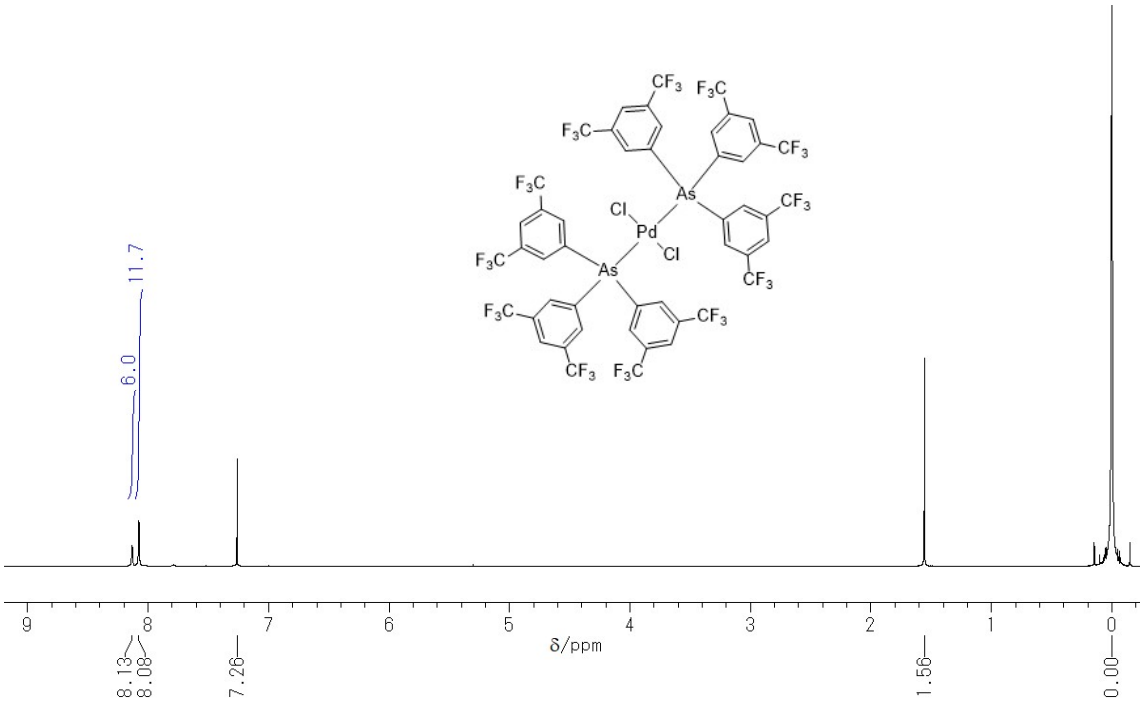


Figure S8. ^{1}H-NMR (400 MHz) spectrum for [$PdCl_2$(**1d**)$_2$] in $CDCl_3$.

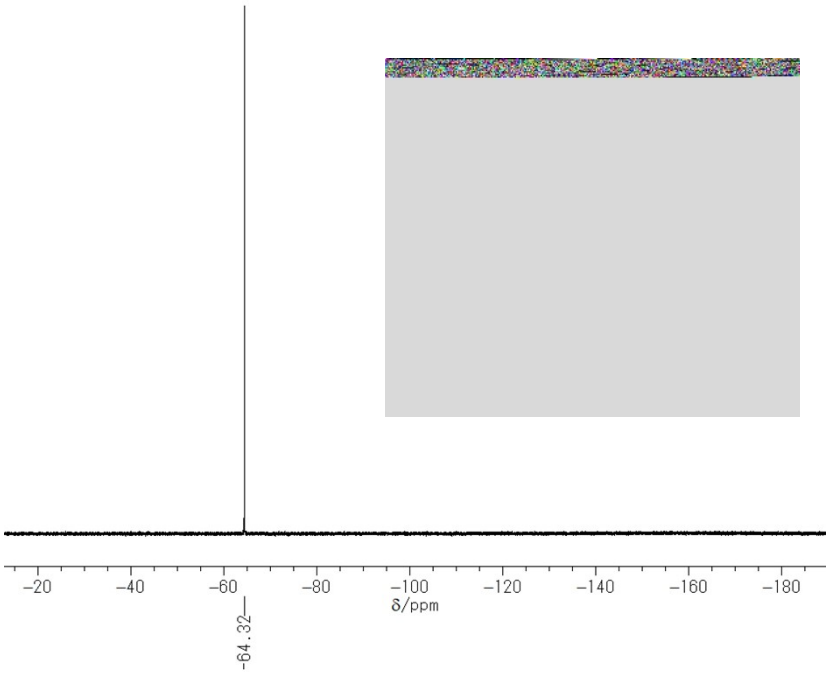


Figure S9. ^{19}F-NMR (376 MHz) spectrum for [$PdCl_2$(**1d**)$_2$] in $CDCl_3$.

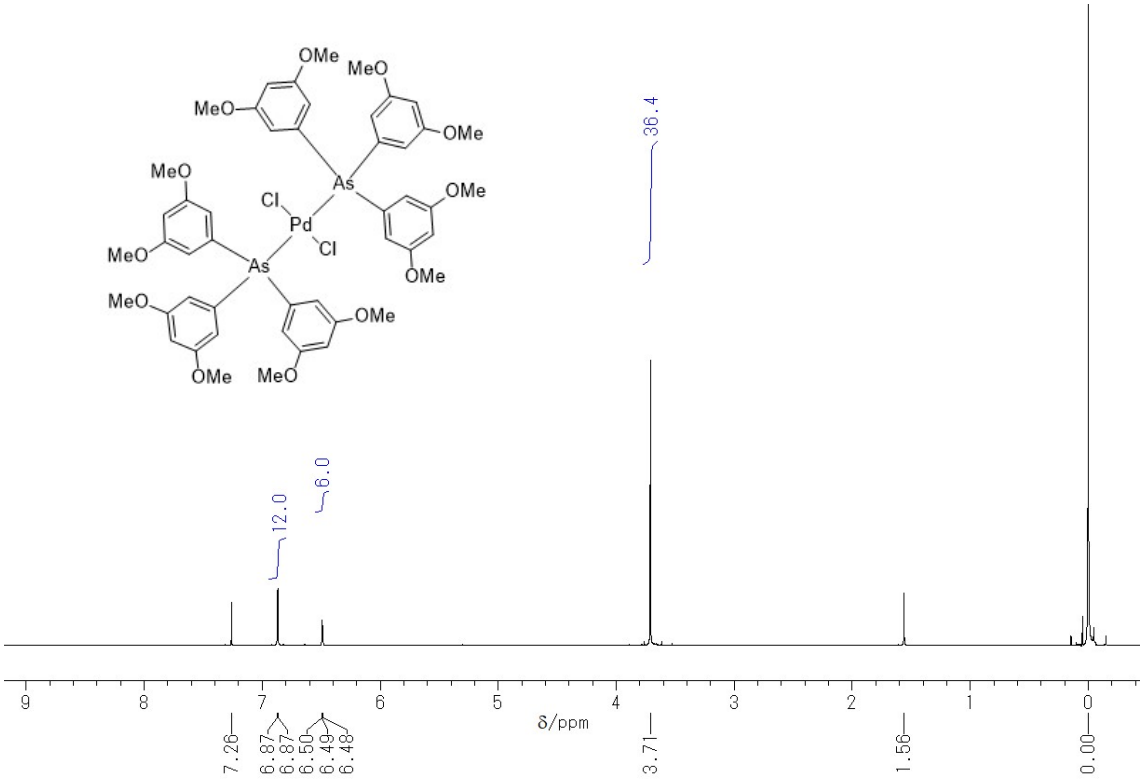


Figure S10. ^{1}H-NMR (400 MHz) spectrum for [$PdCl_2$(**1k**)$_2$] in $CDCl_3$.

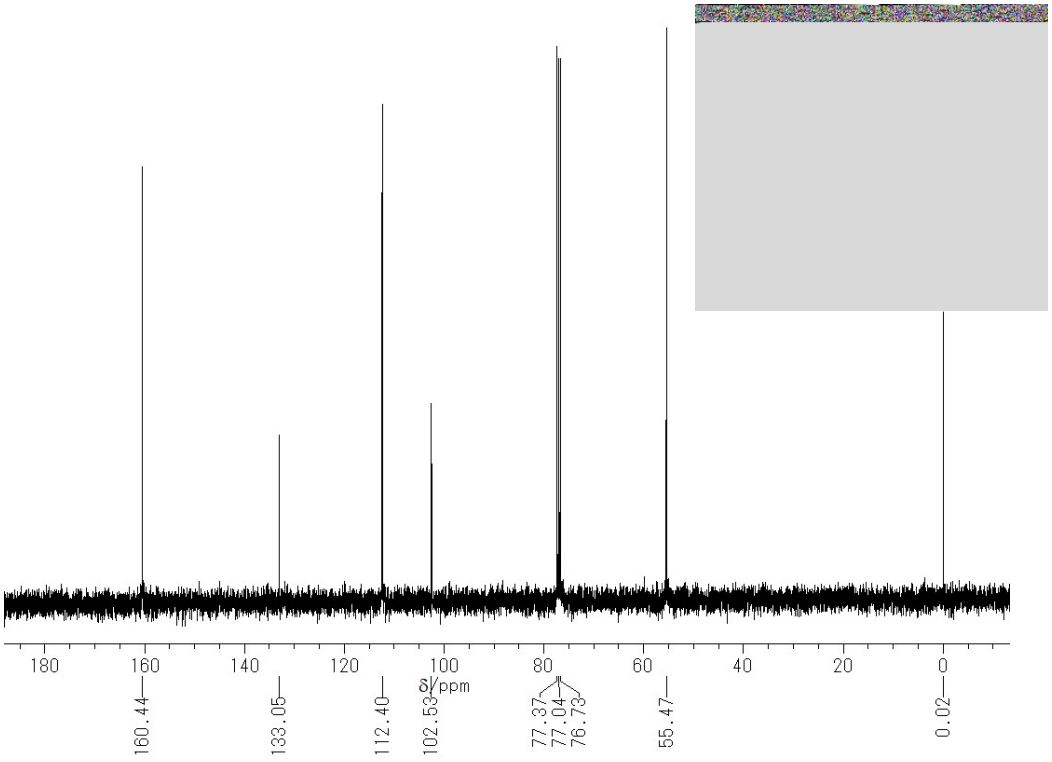


Figure S11 ^{13}C-NMR (100 MHz) spectrum for $[PdCl_2(\mathbf{1k})_2]$ in $CDCl_3$.

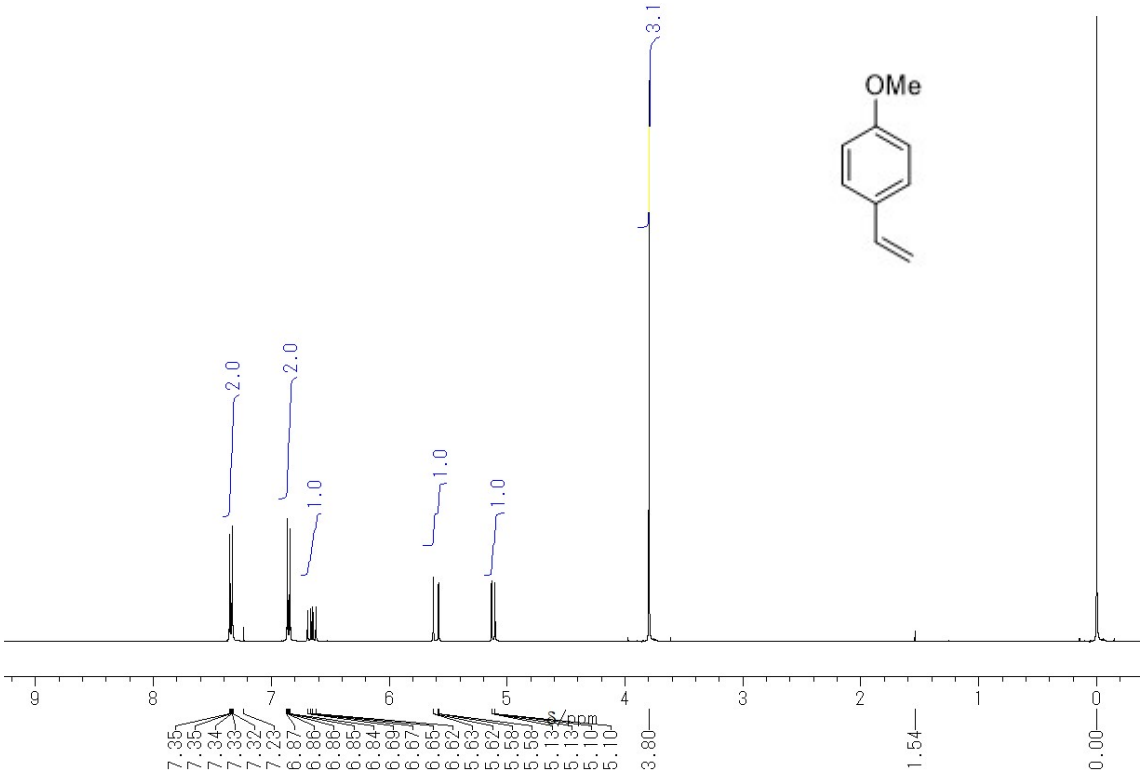


Figure S12. ^{1}H-NMR (400 MHz) spectrum for **4-Methoxystyrene** in $CDCl_3$.

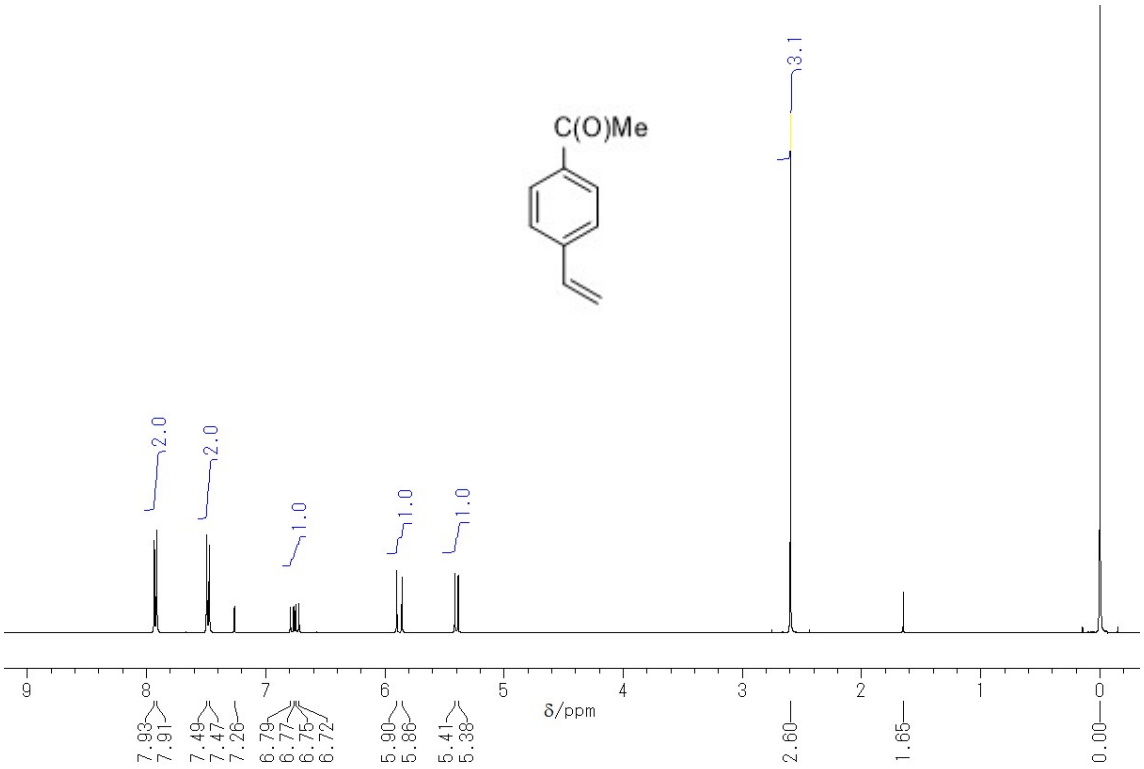


Figure S13. [1]H-NMR (400 MHz) spectrum for **4-Acetylstyrene** in $CDCl_3$.

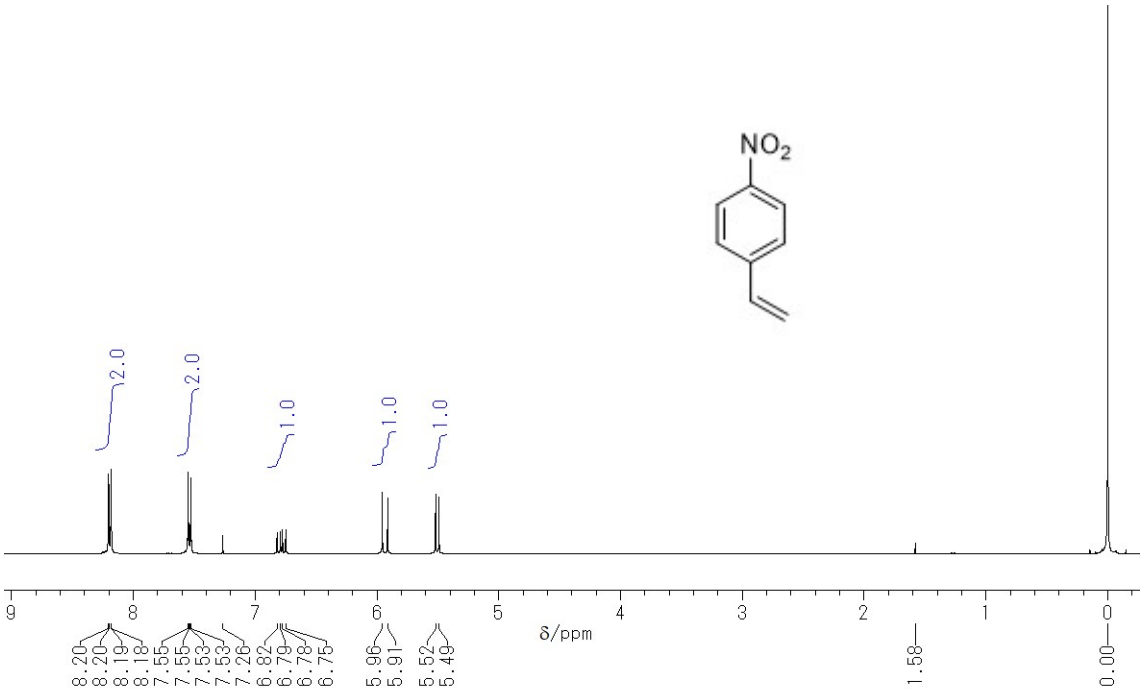


Figure S14. [1]H-NMR (400 MHz) spectrum for **4-Nitrostyrene** in $CDCl_3$.

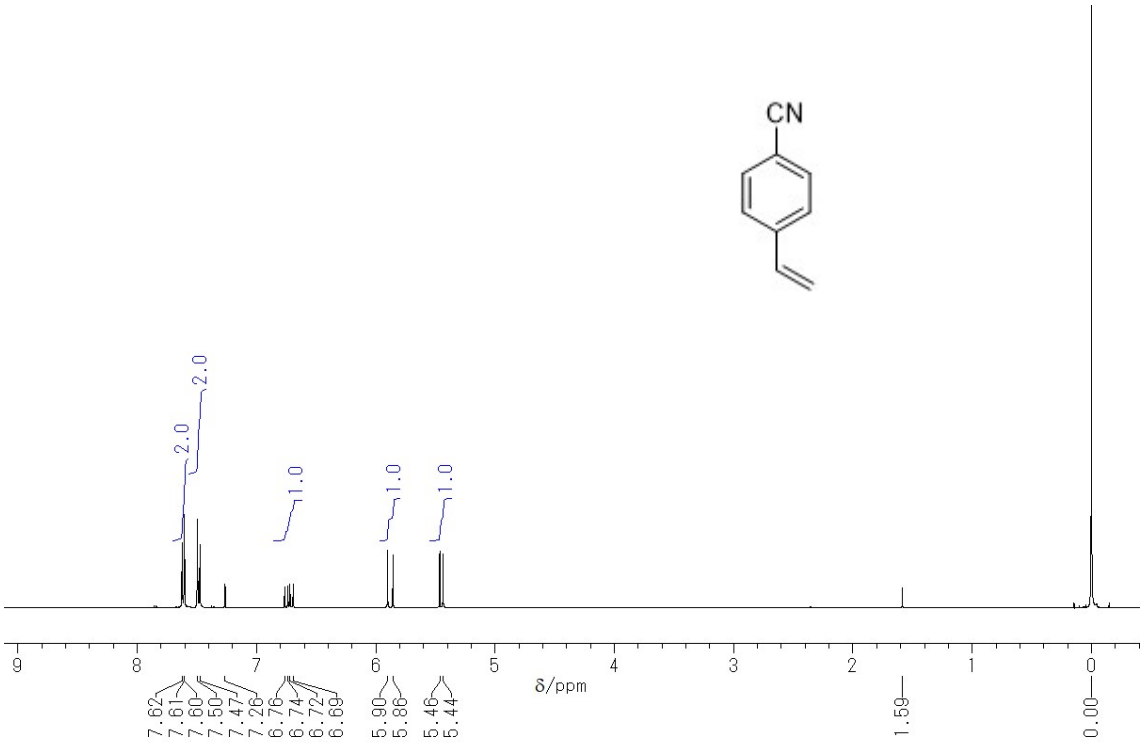


Figure S15. ^{1}H-NMR (400 MHz) spectrum for **4-Cyanostyrene** in $CDCl_3$.

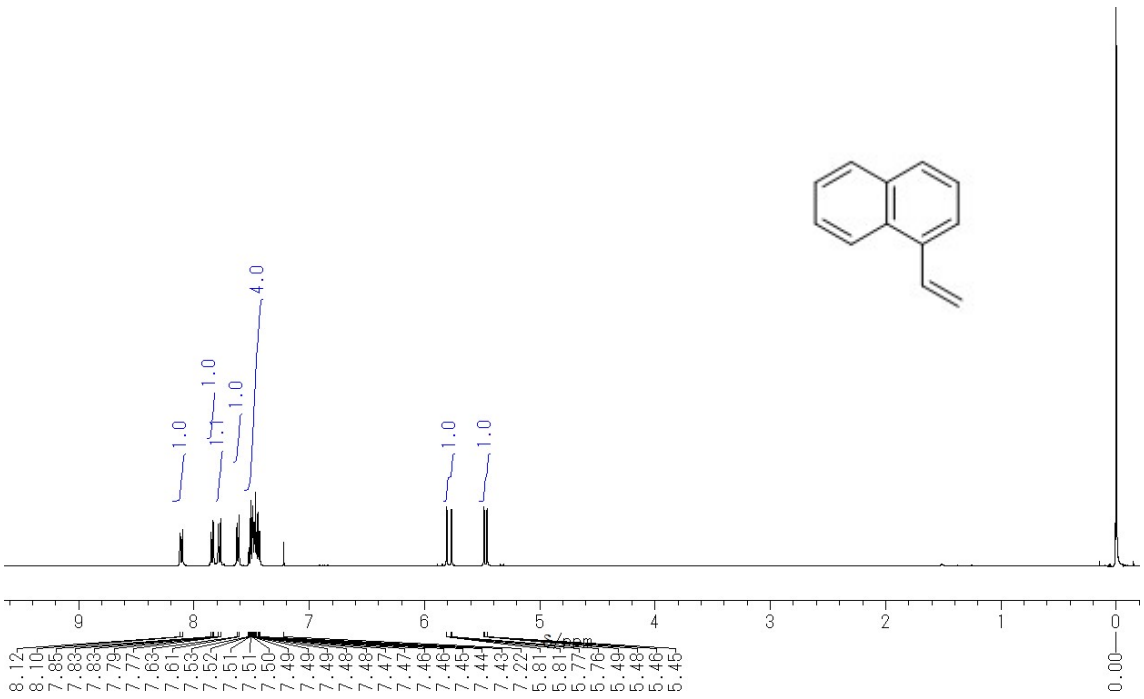


Figure S16. ^{1}H-NMR (400 MHz) spectrum for **1-Vinylnaphthalene** in $CDCl_3$.

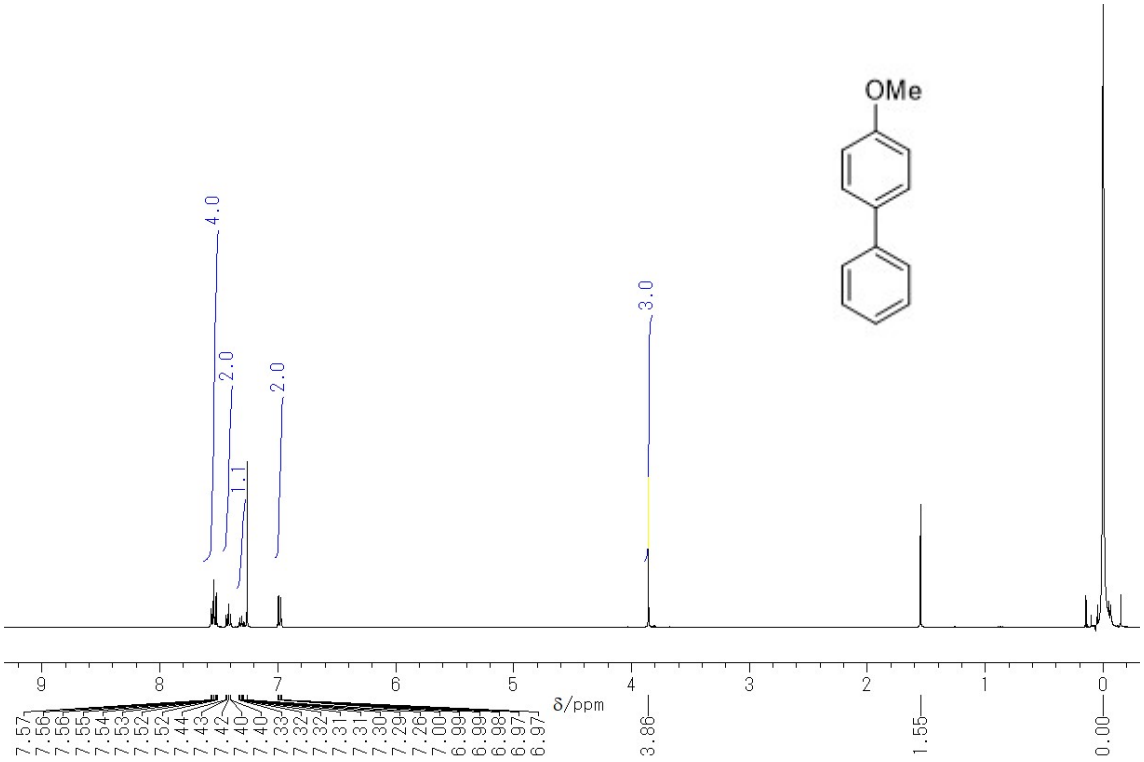


Figure S17. ^{1}H-NMR (400 MHz) spectrum for **4-Methoxybiphenyl** in $CDCl_3$.

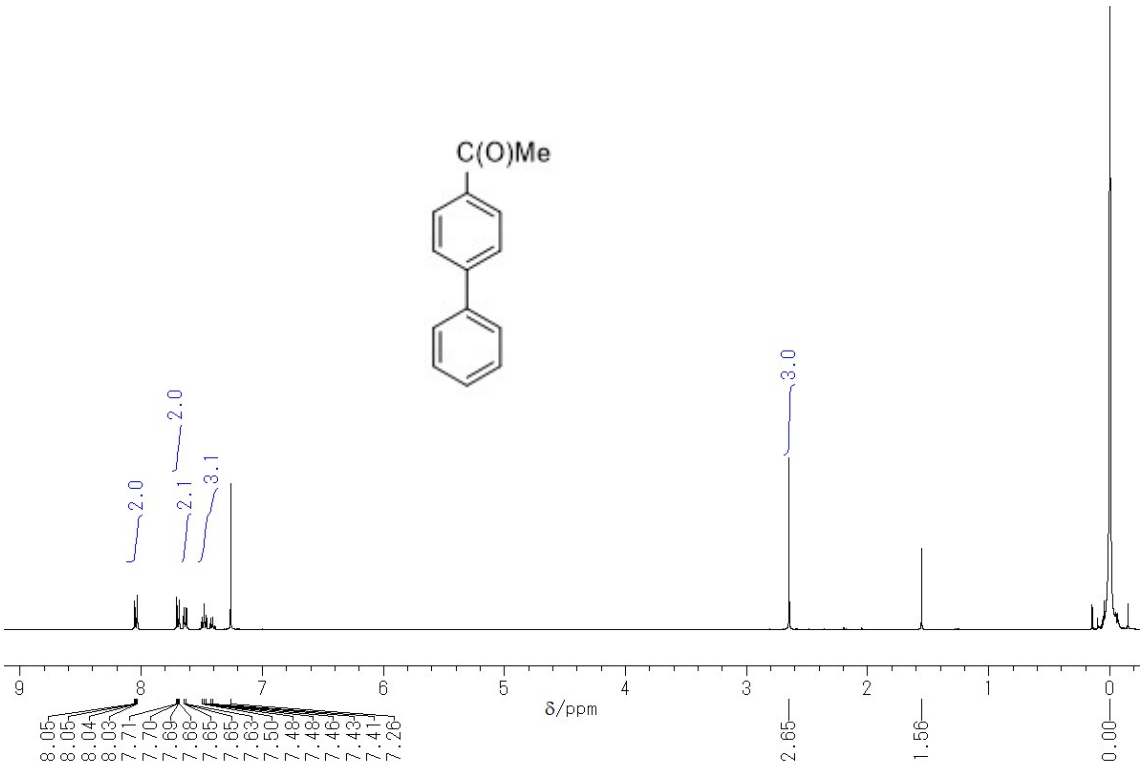


Figure S18. ^{1}H-NMR (400 MHz) spectrum for **4-Acetylbiphenyl** in $CDCl_3$.

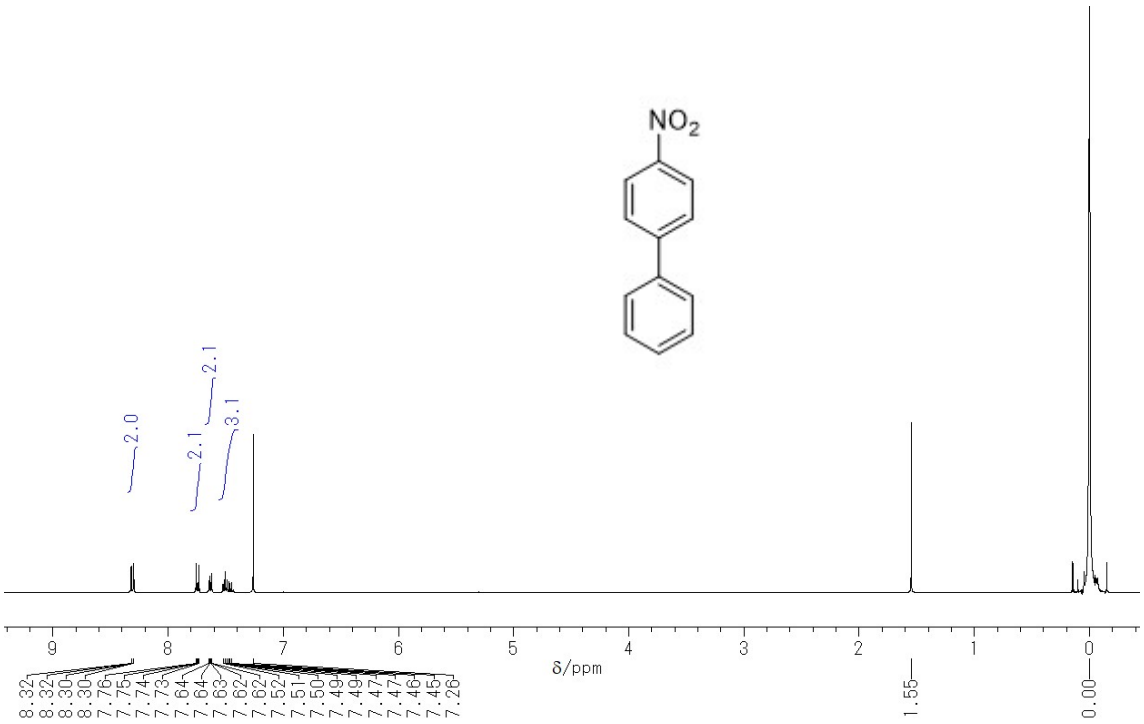


Figure S19. ^{1}H-NMR (400 MHz) spectrum for **4-Nitrobiphenyl** in $CDCl_3$.

2. X-ray crystallographic data for single crystalline products

Table S1. Crystallographic Data of $[PdCl_2(ligand)_2]$ (ligand = $AsPh_3$, **1a**, **1d**).

	$[PdCl_2(AsPh_3)_2]$	$[PdCl_2(\mathbf{1a})_2]$	$[PdCl_2(\mathbf{1d})_2]$
Crystal data			
Empirical Formula	$C_{36}H_{30}As_2Cl_2Pd$	$C_{36}H_{24}As_2Cl_2F_6Pd$	$C_{49}H_{20}As_2Cl_4F_{36}Pd$
Formula Weight	789.74	897.73	1690.69
Crystal Dimension, mm^3	0.4 × 0.1 × 0.08	0.340 × 0.200 × 0.090	0.5 × 0.44 × 0.29
Crystal System	monoclinic	monoclinic	triclinic
Space Group	$P2_1/c$	$C2/c$	P-1
a, Å	15.146(1)	28.18(1)	9.747(4)
b, Å	20.085(2)	8.095(2)	16.203(6)
c, Å	10.528(1)	17.069(7)	20.248(8)
α, deg	-	-	72.26 (2)
β, deg	92.131(9)	115.517(17)	70.60 (1)
γ, deg	90	-	73.96(2)
Volume, $Å^3$	3200.6(5)	3513(2)	2818(2)
D_{calcd}, g cm^{-3}	1.639	1.679	1.993
Z	4	4	2
F(000)	1568.0	1760.00	1636.0
Data Collection			
Temperature, deg	-180.0	25.0	-180.0
2θmax, deg	52.74	55.0	55.012
Tmin/Tmax	0.898/1.000	0.586 / 0.791	0.469/0.603
Refinement			
No. of Observed Data	6539	4002	12805
No. of Parameters	373	214	882
R1[a], wR2[b]	0.0580, 0.0987	0.00511, 0.1478	0.0337, 0.0835
Goodness of Fit Indictor	0.987	1.069	1.029

[a] $R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b] $wR2 = [\ \Sigma\ w\ ((Fo^2-Fc^2)^2 / \Sigma\ w\ (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

CCDC #2087272 ($PdCl_2(AsPh_3)_2$), 2087273 ($PdCl_2(\mathbf{1a})_2$), 2087274 ($PdCl_2(\mathbf{1d})_2$)

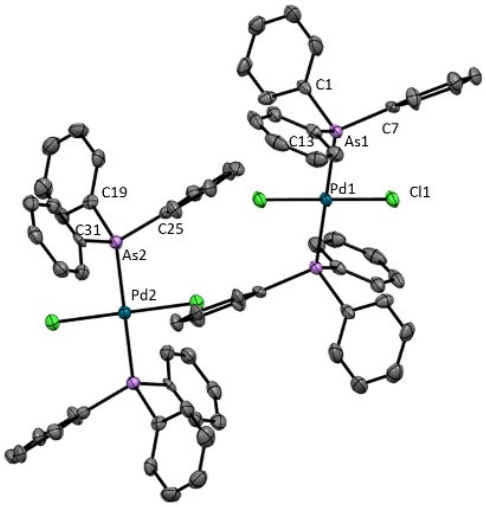
Table S2. Crystallographic Data of $[PdCl_2(ligand)_2]$ (ligand =**1k**, **1m**).

	$[PdCl_2(\mathbf{1k})_2]$	$[PdCl_2(\mathbf{1m})_2]$
Crystal data		
Empirical Formula	$C_{48}H_{54}As_2Cl_2O_{12}Pd$	$C_{36}H_{66}As_2Cl_2Pd$
Formula Weight	1150.10	857.50
Crystal Dimension, mm^3	0.470 × 0.380 × 0.200	0.55 × 0.4 × 0.24
Crystal System	monoclinic	triclinic
Space Group	$P2_1/n$	P-1
a, Å	12.720(2)	9.8187(6)
b, Å	22.095(4)	10.2351(7)
c, Å	18.916(4)	10.768(1)
α, deg	-	112.662(7)
β, deg	100.01(1)	107.773(6)
γ, deg	-	91.967(5)
Volume, $Å^3$	5235(2)	936.6(1)
D_{calcd}, g cm^{-3}	1.459	1.464
Z	4	1
F(000)	2336.00	428.0
Data Collection		
Temperature, deg	25.0	-180.0
2θmax, deg	54.9	52.740
Tmin/Tmax	0.349/0.702	0.399/0.612
Refinement		
No. of Observed Data	11573	3830
No. of Parameters	586	187
R1[a], wR2[b]	0.0587, 0.2223	0.0236, 0.0531
Goodness of Fit Indictor	1.108	1.047

[a] $R1 = \Sigma \, | \, |Fo| - |Fc| \, | \, / \, \Sigma \, |Fo|$ [b] $wR2 = [\, \Sigma \, w \, ((Fo^2-Fc^2)^2 \, / \, \Sigma \, w \, (Fo^2)^2 \,]^{1/2}$ $w = [\, \sigma^2(Fo^2) \,]^{-1}$

CCDC #2087275 ($PdCl_2(\mathbf{1k})_2$), 2087271 ($PdCl_2(\mathbf{1m})_2$)

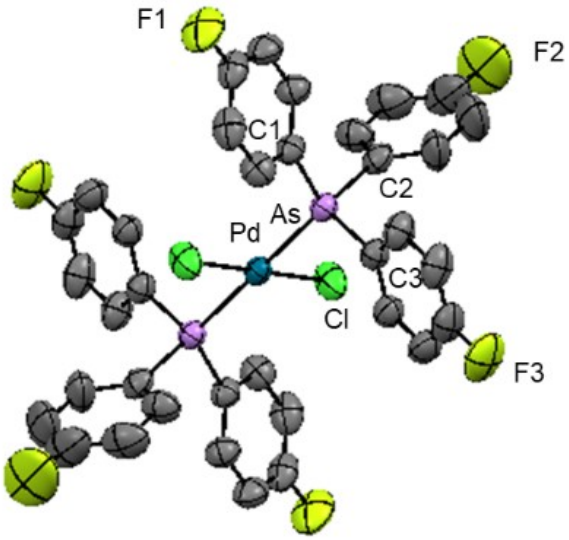
Table S3. ORTEP drawing (ellipsoids at 50% probability), selected distances (Å), and angles (deg) of $[PdCl_2(AsPh_3)_2]$. Hydrogen atoms were omitted for clarity.



A	Bond length (Å)		Angle (deg)
As1-Pd1	2.4272(9)	As1-Pd1-Cl1	86.60(6)
Pd1-Cl1	2.289(2)	C1-As1-C7	104.1(3)
As1-C1	1.927(8)	C7-As1-C13	106.9(3)
As1-C7	1.943(8)	C13-As1-C1	104.1(3)
As1-C13	1.934(7)		

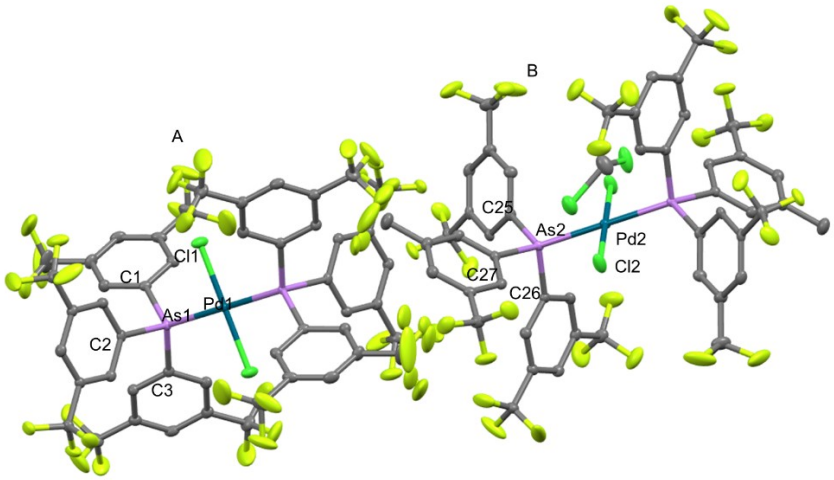
B	Bond length (Å)		Angle (deg)
As2-Pd2	2.4178(8)	As2-Pd2-Cl2	89.10(5)
Pd2-Cl2	2.302(2)	C19-As2-C25	103.2(3)
As2-C19	1.922(8)	C25-As2-C31	101.2(3)
As2-C25	1.954(8)	C31-As2-C19	103.7(3)
As2-C31	1.933(7)		

Table S4. ORTEP drawing (ellipsoids at 50% probability), selected distances (Å), and angles (deg) of [$PdCl_2$(**1a**)$_2$]. Hydrogen atoms were omitted for clarity.



Bond length (Å)			Angle (deg)
As-Pd	2.416(1)	As-Pd-Cl	88.67(5)
Pd-Cl	2.283(2)	C1-As-C2	102.3(2)
As-C1	1.935(5)	C2-As-C3	105.1(2)
As-C2	1.957(5)	C3-As-C1	103.8(2)
As-C3	1.926(5)		

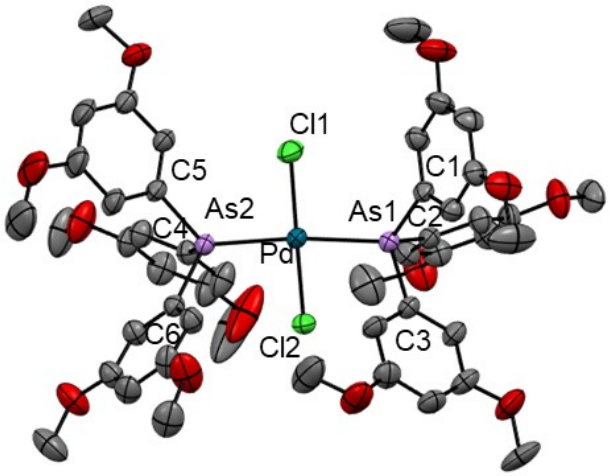
Table S5. ORTEP drawing (ellipsoids at 50% probability), selected distances (Å), and angles (deg) of [$PdCl_2$(**1d**)$_2$]. Hydrogen atoms were omitted for clarity.



A	Bond length (Å)		Angle (deg)
As1-Pd1	2.3989(7)	As1-Pd1-Cl1	92.60(3)
Pd1-Cl1	2.289(1)	C1-As1-C2	104.0(1)
As1-C1	1.946(2)	C2-As1-C3	105.3(1)
As1-C2	1.937(2)	C3-As1-C1	97.4(1)
As1-C3	1.948(3)		

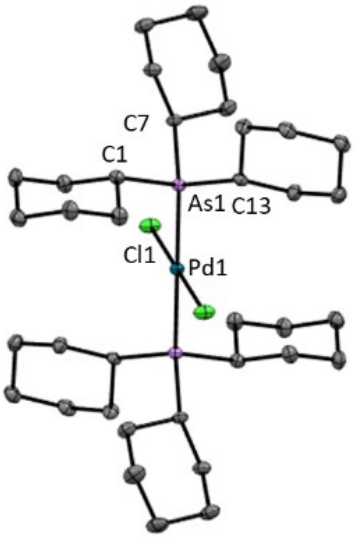
B	Bond length (Å)		Angle (deg)
As2-Pd2	2.4342(7)	As2-Pd2-Cl2	88.87(3)
Pd2-Cl2	2.286(1)	C25-As2-C26	100.3(1)
As2-C25	1.951(2)	C26-As2-C27	103.7(1)
As2-C26	1.950(3)	C27-As2-C25	102.0(1)
As2-C27	1.956 (2)		

Table S6. ORTEP drawing (ellipsoids at 50% probability), selected distances (Å), and angles (deg) of [$PdCl_2$(**1k**)$_2$]. Hydrogen atoms were omitted for clarity.



	Bond length (Å)		Angle (deg)
As1-Pd	2.4282(7)	As1-Pd-Cl1	93.51(4)
Pd-Cl1	2.295(2)	C1-As1-C2	103.5(2)
As1-C1	1.958(5)	C2-As1-C3	104.9(2)
As1-C2	1.944(5)	C3-As1-C1	101.8(2)
As1-C3	1.937(5)	As2-Pd-Cl2	87.41(4)
As2-Pd	2.4248(7)	C4-As2-C5	101.3(2)
Pd-Cl2	2.303(1)	C5-As2-C6	101.8(2)
As2-C4	1.941(6)	C6-As2-C4	103.2(2)
As2-C5	1.947(5)		
As2-C6	1.938(5)		

Table S7. ORTEP drawing (ellipsoids at 50% probability), selected distances (Å), and angles (deg) of [$PdCl_2$(**1m**)$_2$].



	Bond length (Å)		Angle (deg)
As1-Pd1	2.4286(3)	As1-Pd1-Cl1	88.65(2)
Pd1-Cl1	2.3088(5)	C1-As1-C7	103.00(9)
As1-C1	1.970(2)	C7-As1-C13	102.97(9)
As1-C7	1.979(2)	C1-As1-C13	109.93(9)
As1-C13	1.979(2)		

4. DFT calculations

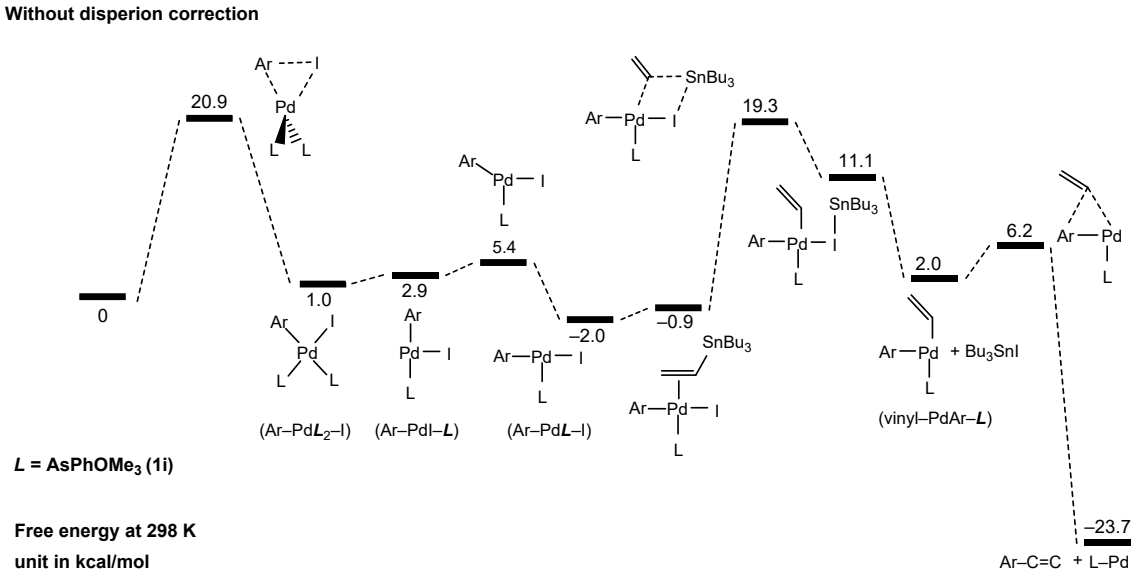


Figure S20. Energy profile for the Stille coupling reactions of *p*-iodoanisole and vinylSnBu$_3$ in the presence of PdL$_2$ (L = AsPhOMe$_3$ (**1i**), ArX = *p*-iodoanisole), obtained from B3LYP calculations without dispersion correction. Changes of Gibbs free energy at 298 K during the reactions are displayed, measured with reference to PdL$_2$, *p*-iodoanisole, and vinylSnBu$_3$. Structures Pd-complexes changed in each step are only given.

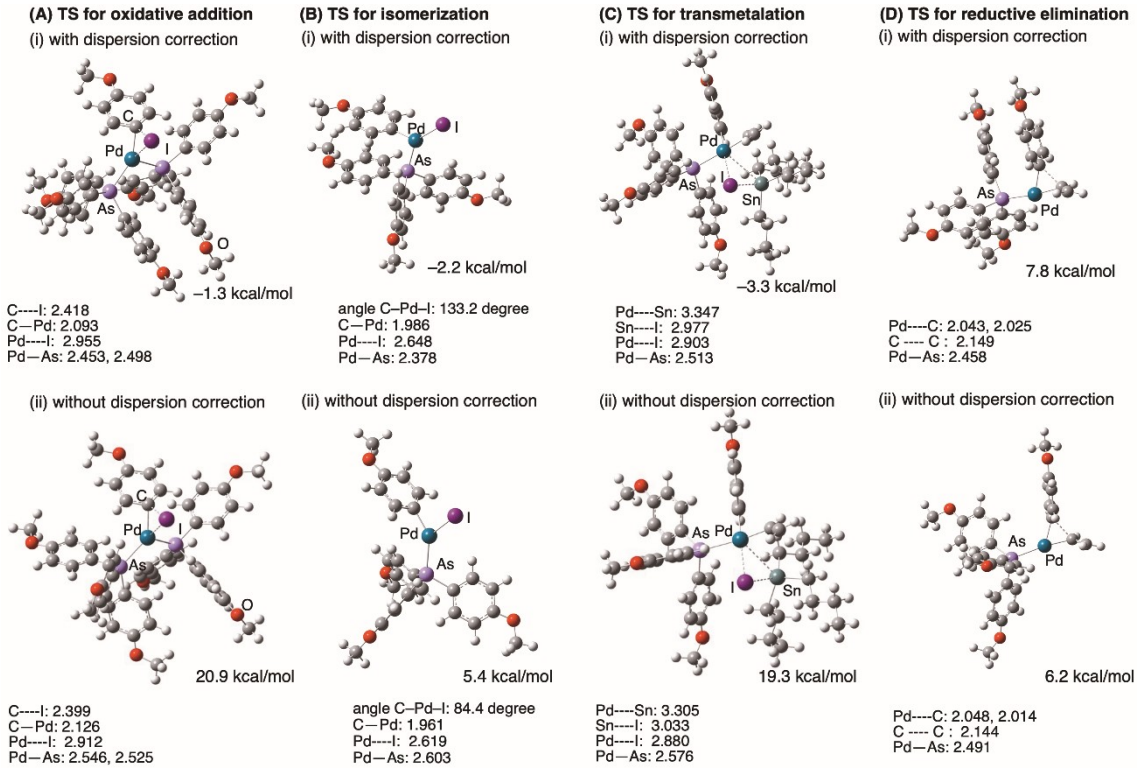


Figure S21. Optimized transition states for the oxidative addition, isomerization, transmetalation, and reductive elimination processes, obtained from B3LYP calculations with and without dispersion corrections, are displayed at the top and bottom, respectively.

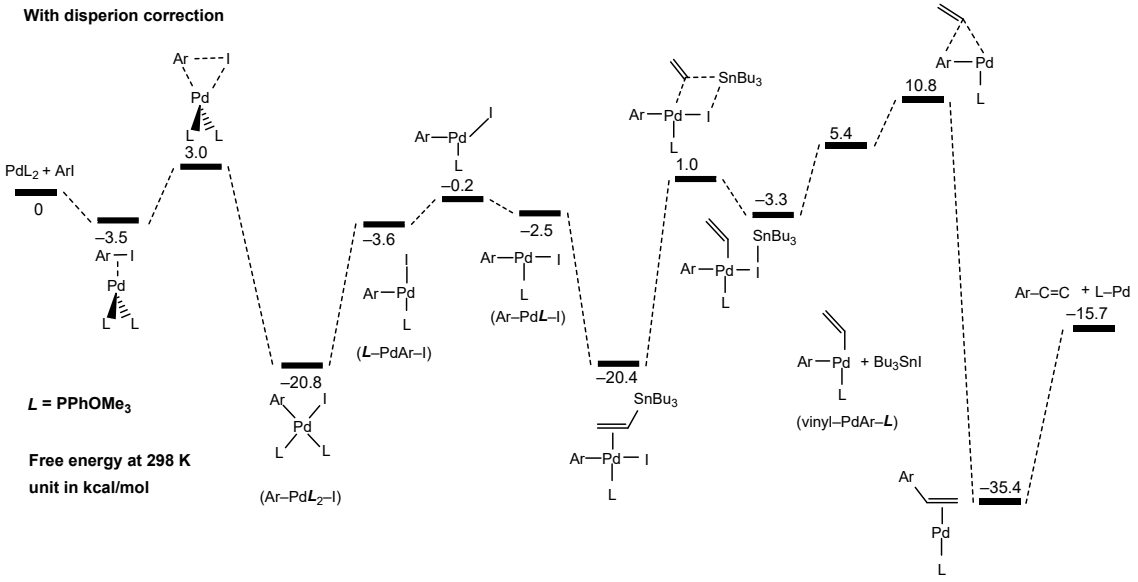


Figure S22. Energy profile for the Stille coupling reactions of *p*-iodoanisole and vinylSnBu$_3$ in the presence of PdL$_2$ (L = PPhOMe$_3$, ArX = *p*-iodoanisole), obtained from dispersion-corrected B3LYP calculations with dispersion correction (B3LYP-GD3). Changes of Gibbs free energy at 298 K during the reactions are displayed, measured with reference to PdL$_2$, *p*-iodoanisole, and vinylSnBu$_3$. Structures Pd-complexes changed in each step are only given.

Cartesian Coordinates of Optimized geometries together with energy values obtained from DFT calculations.

(1) Optimized geometries in Figure 2, obtained from dispersion-corrected B3LYP (B3LYP-GD3) calculations

***L* = As(PhOMe)$_3$ [1i]**

(A) PdL_2

Total energy: -6671.98667117 Hartree

Free energy: -6671.342399 Hartree

Pd	0.00000000	0.00008200	-0.00001800
As	2.38317500	-0.00048500	-0.00056800
C	3.25777400	1.09545500	-1.35749100
C	4.48150400	1.73686900	-1.15530100
C	2.62234800	1.23716500	-2.60242400
C	5.07601800	2.49885200	-2.16619800
H	4.98419800	1.65691200	-0.19590200
C	3.20226900	1.98553300	-3.61739400
H	1.65747900	0.76334500	-2.76609400
C	4.43566200	2.62159400	-3.40528500
H	6.02359500	2.98821900	-1.97430800
H	2.71912200	2.10352400	-4.58192200
C	3.25405200	-1.72518900	-0.27230000
C	2.61458900	-2.87343300	0.22403100
C	4.47906400	-1.87272800	-0.92603600
C	3.19194900	-4.12776800	0.08305700
H	1.64861400	-2.77661600	0.71377200
C	5.07110800	-3.13029400	-1.08068400
H	4.98476400	-1.00242800	-1.33394900
C	4.42681100	-4.26400900	-0.57066900
H	2.70572100	-5.02149700	0.46055000
H	6.01987400	-3.21022500	-1.59804000
C	3.25776600	0.62545100	1.62746300
C	2.62459600	1.63560400	2.37073400
C	4.47970400	0.12688700	2.08352500
C	3.20496400	2.14033100	3.52614000
H	1.66113500	2.01666400	2.04081600

C	5.07462300	0.62120300	3.24872200
H	4.98077600	-0.66586300	1.53582800
C	4.43656900	1.63573600	3.97265400
H	2.72357800	2.91887900	4.10906400
H	6.02080200	0.20812100	3.57783400
As	-2.38317400	0.00054500	0.00055000
C	-3.25775900	-0.62552100	-1.62743400
C	-4.47972600	-0.12703800	-2.08350700
C	-2.62455300	-1.63568700	-2.37065600
C	-5.07463900	-0.62144800	-3.24866700
H	-4.98082600	0.66571900	-1.53584700
C	-3.20491400	-2.14050500	-3.52602600
H	-1.66106900	-2.01668200	-2.04073200
C	-4.43654900	-1.63599200	-3.97255100
H	-6.02084100	-0.20842700	-3.57779000
H	-2.72350000	-2.91906300	-4.10891400
C	-3.25770500	-1.09536100	1.35754600
C	-4.48141400	-1.73683200	1.15541100
C	-2.62225100	-1.23698600	2.60247400
C	-5.07588000	-2.49878900	2.16635600
H	-4.98413000	-1.65694200	0.19601700
C	-3.20212300	-1.98532800	3.61749100
H	-1.65739600	-0.76312200	2.76610200
C	-4.43549600	-2.62144700	3.40543600
H	-6.02344200	-2.98820200	1.97450700
H	-2.71895300	-2.10325400	4.58201500
C	-3.25412600	1.72522400	0.27219800
C	-4.47913800	1.87274300	0.92593900
C	-2.61472000	2.87346900	-0.22420200
C	-5.07123700	3.13029100	1.08052500
H	-4.98479400	1.00244300	1.33390500
C	-3.19213500	4.12778600	-0.08329000
H	-1.64874500	2.77667000	-0.71394800
C	-4.42699700	4.26400800	0.57044100
H	-6.02000100	3.21020700	1.59788600
H	-2.70595000	5.02151700	-0.46083600

O	-4.92035900	-2.19378300	-5.12006200
O	-4.90751000	5.53784100	0.66208800
O	-4.91842100	-3.33700300	4.46220200
O	4.90726800	-5.53786000	-0.66238000
O	4.92038900	2.19344100	5.12020300
O	4.91863600	3.33718300	-4.46200700
C	6.15283700	4.01888400	-4.30387500
H	6.34416100	4.52176800	-5.25332800
H	6.10346800	4.76832500	-3.50259600
H	6.97701200	3.32437700	-4.09198300
C	6.15339100	1.71351800	5.63242400
H	6.34605300	2.28544300	6.54167700
H	6.10144300	0.64542700	5.88268800
H	6.97796700	1.87403700	4.92474400
C	6.14363900	-5.74338100	-1.32733300
H	6.33275700	-6.81748000	-1.28855500
H	6.09897200	-5.42296700	-2.37685200
H	6.96690000	-5.21473400	-0.82805800
C	-6.15259800	-4.01876000	4.30412600
H	-6.10321600	-4.76823700	3.50288200
H	-6.34388500	-4.52160700	5.25360600
H	-6.97680500	-3.32429600	4.09221600
C	-6.15339500	-1.71395300	-5.63228800
H	-6.10150500	-0.64587300	-5.88261500
H	-6.34604500	-2.28594100	-6.54150300
H	-6.97794900	-1.87447100	-4.92458200
C	-6.14388300	5.74334300	1.32704100
H	-6.09919200	5.42298900	2.37657800
H	-6.33305200	6.81743100	1.28820700
H	-6.96712600	5.21463100	0.82780400

(B) Ar−X (p-iodoanisole)

Total energy: -357.597015771 Hartree

Free energy: -357.509312 Hartree

C	-0.18178900	0.07494400	-0.00004200
C	0.42030200	1.33595900	0.00006800

C	0.59028000	-1.08125500	-0.00007200
C	1.80714300	1.42998400	0.00015100
H	-0.18127100	2.23785400	0.00009300
C	1.98613200	-0.98617600	0.00000700
H	0.12322800	-2.05971500	-0.00016300
C	2.59945000	0.27218900	0.00012100
H	2.30092000	2.39599700	0.00024000
H	2.57226600	-1.89712000	-0.00003800
I	-2.33310700	-0.07703900	-0.00014800
O	3.94583800	0.48088100	0.00018500
C	4.80233000	-0.65191200	0.00051000
H	5.82048300	-0.25991100	0.00076800
H	4.65436900	-1.27166800	0.89491100
H	4.65488400	-1.27179300	-0.89389200

(C) the first complex between Ar−X and Pd**L**$_2$

Total energy: -7029.62474316 Hartree

Free energy: -7028.862760 Hartree

Pd	-0.00883300	-1.08973100	-0.60581900
As	1.89898100	0.26590400	0.14111000
C	1.93393400	0.61030000	2.06295800
C	3.08011300	1.02866900	2.74475000
C	0.75091900	0.42826900	2.79819300
C	3.05384900	1.28752500	4.11808300
H	4.01763200	1.14211600	2.20795600
C	0.70580200	0.68449400	4.16229300
H	-0.14332700	0.06961000	2.30112100
C	1.85897000	1.12127400	4.83154100
H	3.96189800	1.60854200	4.61475800
H	-0.20914100	0.54422800	4.72888800
C	1.87458000	2.06785900	-0.61351300
C	1.18068600	2.25456800	-1.82013400
C	2.43840000	3.18240500	0.00962800
C	1.04608600	3.51733000	-2.37946700
H	0.71004900	1.40148200	-2.30177300
C	2.30065200	4.46239100	-0.53349700

H	2.96748800	3.07067800	0.95110500
C	1.59165600	4.63247200	-1.72926200
H	0.48740800	3.67306400	-3.29593300
H	2.72713600	5.31030300	-0.01103200
C	3.74922600	-0.27513100	-0.15319100
C	4.25121900	-1.38304000	0.55083300
C	4.55860600	0.32220700	-1.11938900
C	5.52191000	-1.87625000	0.29465200
H	3.64028300	-1.86125900	1.31201600
C	5.83888300	-0.16817000	-1.39603900
H	4.19443100	1.18173600	-1.67441500
C	6.32377400	-1.27419600	-0.68848200
H	5.91936000	-2.72982900	0.83417400
As	-2.04627600	0.22136600	-0.28123800
C	-3.59937100	-0.15834100	-1.40097000
C	-4.90690400	0.16030200	-1.02587100
C	-3.39066300	-0.78945100	-2.63686900
C	-5.99070000	-0.13756700	-1.85470900
H	-5.09602600	0.63846300	-0.06912400
C	-4.45700400	-1.08835500	-3.47645500
H	-2.37911600	-1.05360200	-2.93461700
C	-5.76572700	-0.76413200	-3.08875500
H	-6.99301900	0.11802100	-1.53186800
H	-4.30679000	-1.57623300	-4.43410400
C	-2.75405400	-0.07198800	1.51573500
C	-2.48307300	-1.30182800	2.12425200
C	-3.48660600	0.88337400	2.23691300
C	-2.92962400	-1.59402600	3.41416100
H	-1.89536300	-2.04388200	1.59559900
C	-3.93547800	0.61045500	3.52396500
H	-3.68718200	1.85718600	1.80006600
C	-3.66183000	-0.63075400	4.12108000
H	-2.69066300	-2.55967800	3.84344500
H	-4.49532100	1.34397800	4.09532500
C	-1.98269000	2.17128200	-0.34589200
C	-2.54548400	2.90296100	-1.39199900

C	-1.21472700	2.85507800	0.61341600
C	-2.33596700	4.28165400	-1.50711300
H	-3.14753500	2.39997000	-2.14321400
C	-1.01473400	4.22337300	0.52203500
H	-0.75314300	2.31206600	1.43253800
C	-1.55925000	4.94377200	-0.55114500
H	-2.77091900	4.81599500	-2.34323900
H	-0.40707800	4.75281000	1.24745100
C	0.72118600	-3.14281400	-0.97069100
C	-0.66253500	-3.19793500	-1.31901000
C	1.14391200	-3.73682800	0.26047000
C	-1.59181900	-3.82486800	-0.43151700
H	-0.97355600	-3.01887800	-2.34221600
C	0.22049400	-4.27920500	1.12269700
H	2.19777900	-3.73168000	0.51529300
C	-1.16072000	-4.31792900	0.78301900
H	-2.63216300	-3.86313000	-0.73039200
H	0.52356400	-4.68626700	2.08199600
O	-1.26542700	6.27874800	-0.57472500
O	-4.14324300	-0.79651900	5.38553100
O	-6.74424400	-1.10205800	-3.97618500
O	-1.97334200	-4.84945500	1.75369000
O	1.71705500	1.34449000	6.16986100
O	1.36401700	5.83739000	-2.33177300
C	-8.09103600	-0.80489300	-3.64023400
H	-8.24850500	0.27398700	-3.50896000
H	-8.69529800	-1.15554500	-4.47844600
H	-8.40610600	-1.32555000	-2.72611600
C	-3.86292100	-2.01840100	6.05316300
H	-2.78286500	-2.17719500	6.17024200
H	-4.32353300	-1.93611700	7.03889800
H	-4.29420600	-2.87846300	5.52387400
C	-1.64225400	7.02005300	-1.72701400
H	-2.73218700	7.04936500	-1.85432400
H	-1.27828300	8.03581300	-1.56236300
H	-1.17234100	6.60811700	-2.62804300

C	2.85143600	1.77917700	6.90331700
H	2.51717600	1.89583100	7.93558000
H	3.66474100	1.04193700	6.86912600
H	3.22832400	2.74310100	6.53583300
C	1.75424600	7.01337100	-1.63565500
H	1.44895200	7.85009700	-2.26660100
H	1.24320800	7.08232100	-0.66800100
H	2.84111600	7.05758900	-1.48823400
C	-3.36797400	-4.87796800	1.49335300
H	-3.60523200	-5.50019200	0.61985000
H	-3.83393300	-5.31325400	2.37948900
H	-3.76688600	-3.86703500	1.33448800
I	2.22245800	-3.11207800	-2.60431800
H	6.44008000	0.31864000	-2.15479900
O	7.55486800	-1.83544700	-0.86858900
C	8.39332300	-1.30093200	-1.88035100
H	7.92632300	-1.36899400	-2.87197900
H	8.65522900	-0.25285200	-1.68095300
H	9.30256600	-1.90444100	-1.86975000

(D)The transition state for the oxidative addition by Pd$\mathbf{L}_2$

imaginary mode 91.77 i cm^{-1}

Total energy: -7029.61510355 Hartree

Free energy: -7028.853721 Hartree

Pd	0.06928800	-1.13773500	-0.60576500
As	1.80860600	0.50833000	0.10690100
C	1.95140400	0.85893900	2.02252400
C	3.03756700	1.50982700	2.61527600
C	0.89795000	0.43652900	2.84910300
C	3.07195400	1.75854900	3.99032600
H	3.88357000	1.81645700	2.00699800
C	0.91161600	0.68106300	4.21595800
H	0.06007100	-0.09911700	2.41841000
C	2.00043700	1.34903200	4.79602000
H	3.93139400	2.26254100	4.41650000
H	0.09381200	0.35639700	4.85127000

C	1.40995800	2.27877600	-0.62325500
C	0.61399500	2.34151400	-1.77875800
C	1.82099300	3.47417500	-0.03110300
C	0.23372700	3.56337100	-2.31684300
H	0.26639100	1.42225400	-2.24185900
C	1.43561800	4.71101200	-0.55341100
H	2.42366100	3.45765900	0.87150000
C	0.62890500	4.75622000	-1.69734500
H	-0.40093900	3.61912600	-3.19468000
H	1.75019400	5.61985200	-0.05454100
C	3.68945400	0.30853600	-0.37446800
C	4.52663500	-0.53384100	0.37815300
C	4.18826700	0.85236900	-1.56047000
C	5.82067100	-0.81396800	-0.03967600
H	4.16008200	-0.97794200	1.29921900
C	5.48642300	0.57358400	-1.99853000
H	3.56036000	1.50261400	-2.16279000
C	6.30895700	-0.26452000	-1.23588800
H	6.47470200	-1.46002600	0.53717300
As	-2.10811800	-0.24949600	0.09269200
C	-3.68276500	-0.86764000	-0.87558000
C	-4.97959700	-0.72881700	-0.37471500
C	-3.50416200	-1.46587000	-2.13295200
C	-6.08589100	-1.17358700	-1.10129300
H	-5.14124800	-0.27802900	0.60019600
C	-4.59623100	-1.90731900	-2.87058400
H	-2.50094500	-1.58673300	-2.53399500
C	-5.89428900	-1.76433200	-2.35849100
H	-7.07860800	-1.05749100	-0.68276600
H	-4.47077100	-2.37017700	-3.84400100
C	-2.56656600	-0.61542900	1.95326700
C	-2.02518900	-1.75989600	2.54702200
C	-3.36086400	0.23468900	2.73862400
C	-2.26130600	-2.06382000	3.88996700
H	-1.38297500	-2.41351600	1.96054700
C	-3.60542600	-0.05332600	4.07531900

H	-3.77008500	1.14398400	2.30885700
C	-3.05599200	-1.20478100	4.66094400
H	-1.81697200	-2.95370900	4.31940300
H	-4.21062800	0.60090700	4.69455900
C	-2.34545400	1.68577600	0.01949100
C	-3.10063100	2.29995300	-0.98004800
C	-1.62368100	2.49904500	0.91064400
C	-3.12777300	3.69199300	-1.11515200
H	-3.67011100	1.69436100	-1.67883500
C	-1.65631000	3.88019100	0.79936300
H	-1.01738900	2.05066700	1.69180000
C	-2.39543500	4.48604000	-0.22703400
H	-3.70819200	4.13529000	-1.91531300
H	-1.08606100	4.51227700	1.47089400
C	1.16684900	-2.74545300	-1.37364600
C	0.24483900	-3.71071100	-0.92790400
C	2.54626800	-2.90117000	-1.11654200
C	0.68624100	-4.74563500	-0.07588600
H	-0.78052500	-3.70646500	-1.27895600
C	2.96507500	-3.92573200	-0.29116300
H	3.25728100	-2.18832700	-1.51482600
C	2.03656200	-4.84422900	0.24920600
H	-0.03444600	-5.47588800	0.27274000
H	4.01281500	-4.03435200	-0.02934900
O	-2.32678400	5.85037700	-0.27739100
O	-3.34619900	-1.39047300	5.97982000
O	-6.89774800	-2.23204800	-3.15492300
O	2.58071000	-5.81026000	1.05111800
O	1.92661900	1.54046100	6.14456200
O	0.16506100	5.90485400	-2.27432400
C	-8.23423400	-2.12006400	-2.69102800
H	-8.52299500	-1.07241900	-2.53195000
H	-8.86216500	-2.54943200	-3.47344200
H	-8.38892200	-2.67836600	-1.75804900
C	-2.78579600	-2.51598800	6.63962500
H	-1.68811300	-2.48898700	6.62452300

H	-3.13188000	-2.46279700	7.67306500
H	-3.12668600	-3.45974600	6.19357100
C	-2.92352700	6.50388100	-1.38951000
H	-4.00967000	6.34779500	-1.41873000
H	-2.72262700	7.56818400	-1.25460900
H	-2.47197100	6.16693100	-2.33003600
C	3.00106000	2.20648600	6.78959300
H	2.73553800	2.25426600	7.84699100
H	3.94516100	1.65625200	6.67974000
H	3.13600400	3.22659500	6.40580700
C	0.40459000	7.13158100	-1.59831800
H	-0.07894300	7.90426900	-2.19887300
H	-0.03933500	7.11838600	-0.59568300
H	1.47705700	7.35526600	-1.52828000
C	1.70707300	-6.76876100	1.62106700
H	1.20466500	-7.37083900	0.85143100
H	2.32990000	-7.42170600	2.23526800
H	0.94369000	-6.29651500	2.25526500
I	0.57171800	-1.68853300	-3.46543000
H	5.83821000	1.01300400	-2.92431100
O	7.58909600	-0.60621400	-1.56224100
C	8.12555000	-0.11079700	-2.77932900
H	7.54127000	-0.44626200	-3.64643300
H	8.17487400	0.98643500	-2.78523500
H	9.13690200	-0.51462600	-2.85011600

(E) Ar−Pd**L**$_2$−I

Total energy: -7029.66142412 Hartree

Free energy: -7028.892342 Hartree

Pd	-0.62869200	1.33991600	0.00821400
As	1.83778500	0.72910200	-0.11188700
C	2.39474100	-0.59850400	1.20944700
C	3.20875200	-1.70010500	0.93701000
C	1.89432900	-0.44478000	2.51321700
C	3.48967900	-2.65566400	1.91881800
H	3.60422400	-1.85100400	-0.06172600

C	2.18099100	-1.37323400	3.50433300
H	1.25221000	0.39840300	2.74871400
C	2.96150500	-2.49812300	3.20569200
H	4.10502100	-3.51064100	1.66485600
H	1.77861800	-1.27120500	4.50559700
C	3.24429100	2.05967900	0.08785300
C	3.24295800	3.17297200	-0.76936500
C	4.26818400	1.93353700	1.02567500
C	4.24797700	4.12434900	-0.69361000
H	2.44192800	3.30455900	-1.48942100
C	5.28254700	2.89265800	1.12054100
H	4.29016300	1.08364800	1.70014300
C	5.27456600	3.99227200	0.25588900
H	4.25491000	4.99091900	-1.34619500
H	6.06122800	2.76776100	1.86342400
C	2.36977300	-0.03589500	-1.82216300
C	1.39587200	-0.31030500	-2.79408500
C	3.70665900	-0.31618300	-2.11984200
C	1.74062100	-0.89616000	-4.00399000
H	0.35571800	-0.07678900	-2.59398200
C	4.06945700	-0.92007700	-3.32644500
H	4.48504900	-0.05508000	-1.40832700
C	3.07738200	-1.22719600	-4.26778100
H	0.99085000	-1.13402200	-4.74998000
As	-1.48009600	-0.97858400	-0.01063500
C	-1.26080200	-1.68183700	1.78689700
C	-0.96325700	-3.01962000	2.05470700
C	-1.37068200	-0.78788300	2.86641600
C	-0.71735200	-3.45633200	3.35845600
H	-0.88967700	-3.73462000	1.24195000
C	-1.16491700	-1.21560600	4.16871900
H	-1.57634400	0.26161400	2.68069900
C	-0.80045600	-2.54760200	4.42061100
H	-0.44912300	-4.49168700	3.52975200
H	-1.22618600	-0.52736600	5.00534500
C	-3.37412200	-1.19256700	-0.36815400

C	-3.90269000	-0.61938300	-1.52762400
C	-4.25041500	-1.77256200	0.55876200
C	-5.27547300	-0.58767100	-1.75764500
H	-3.24883100	-0.12443800	-2.23758900
C	-5.62381800	-1.73556500	0.34817700
H	-3.86419900	-2.22151700	1.46847300
C	-6.14574000	-1.11485800	-0.79639900
H	-5.64966000	-0.09261700	-2.64406300
H	-6.31653100	-2.15199000	1.07231400
C	-0.66165700	-2.33135500	-1.15113500
C	0.60210700	-2.83982700	-0.83987400
C	-1.23788800	-2.68493100	-2.38191000
C	1.30880500	-3.63692600	-1.73957900
H	1.06180300	-2.60525800	0.11093000
C	-0.54352800	-3.47346400	-3.28970700
H	-2.23032600	-2.33310800	-2.64310900
C	0.75066300	-3.92601300	-2.98974000
H	2.29641800	-3.98967300	-1.46783900
H	-0.97045100	-3.73305800	-4.25293800
C	-2.57994700	1.94638700	-0.09672600
C	-3.52454600	1.73864400	0.90955200
C	-3.02501600	2.51524600	-1.30166500
C	-4.88499800	2.00458500	0.71051300
H	-3.22806500	1.32631400	1.86871900
C	-4.37565500	2.78657300	-1.51624700
H	-2.31423600	2.74781900	-2.08986300
C	-5.31759200	2.50192300	-0.52030400
H	-5.58531100	1.78689200	1.50810300
H	-4.72253500	3.20730600	-2.45560400
O	1.37725200	-4.62488700	-3.97541600
O	-7.50540900	-1.04538900	-0.87207700
O	-0.52269700	-2.84667500	5.71812800
O	-6.63570800	2.72135300	-0.85314900
O	3.13499500	-3.38587800	4.23103600
O	6.21093000	4.98374400	0.25090200
C	0.09129600	-4.10045400	5.99997600

H	1.02789700	-4.21004700	5.43951000
H	0.30422300	-4.09375200	7.07010700
H	-0.57885300	-4.94061400	5.77566700
C	-8.07494800	-0.34646500	-1.97590400
H	-7.85194100	-0.84870100	-2.92641500
H	-9.15364600	-0.35793000	-1.81143600
H	-7.71877400	0.68993300	-2.01848000
C	2.75945900	-4.90972600	-3.81464400
H	2.93466700	-5.63172100	-3.00570600
H	3.08880100	-5.34569800	-4.75910300
H	3.33258300	-3.99599500	-3.61479500
C	3.92871100	-4.53958900	3.99349500
H	3.94096800	-5.09619000	4.93192500
H	3.49968100	-5.17115600	3.20415400
H	4.95768900	-4.27317200	3.71947500
C	7.24631900	4.93435500	1.21949600
H	7.85862800	5.82218800	1.05296000
H	6.84651000	4.95814000	2.24193500
H	7.87177400	4.03888400	1.10162500
C	-7.61309800	2.47185700	0.14537000
H	-7.44965200	3.09084100	1.03756700
H	-8.57491200	2.73597800	-0.29949400
H	-7.63139600	1.41341200	0.43924000
I	-0.10351800	3.91539600	0.63617000
H	5.11389300	-1.13168700	-3.52260400
O	3.30716200	-1.84652500	-5.46167000
C	4.64661300	-2.15462200	-5.81508300
H	5.10221100	-2.86128800	-5.10772400
H	4.59898600	-2.61847500	-6.80150200
H	5.27044500	-1.25298700	-5.86893300

(F) L

Total energy: -3271.98410261 Hartree

Free energy: -3271.670245 Hartree

As	0.00040000	-0.00046600	-1.76237100
C	-0.27376700	1.70300500	-0.82531300

C	-1.04710000	1.84319200	0.32998100
C	0.33686800	2.85367600	-1.35346200
C	-1.20909400	3.08359000	0.95533400
H	-1.53569400	0.97460200	0.76033500
C	0.19401000	4.09210100	-0.74213500
H	0.93669500	2.78030800	-2.25748900
C	-0.58394500	4.21548000	0.41921900
H	-1.81867000	3.15069300	1.84883900
H	0.66662500	4.98210800	-1.14494200
C	1.61253700	-0.61452800	-0.82489300
C	2.30721700	-1.71503500	-1.35602100
C	2.11715300	-0.01807700	0.33358700
C	3.45124300	-2.21014600	-0.74456800
H	1.94652500	-2.19511300	-2.26258700
C	3.27232800	-0.49771700	0.95923800
H	1.60653600	0.83665700	0.76617800
C	3.94351300	-1.60145400	0.42003800
H	3.98845600	-3.06161500	-1.14969600
H	3.63254600	-0.00601500	1.85529300
C	-1.33790700	-1.08956000	-0.82553800
C	-2.63758400	-1.14239400	-1.35830300
C	-1.07485300	-1.82296600	0.33438900
C	-3.63882200	-1.88520900	-0.74706600
H	-2.87211200	-0.59138600	-2.26594800
C	-2.06823400	-2.58313500	0.95984500
H	-0.07997000	-1.80690900	0.76840900
C	-3.35898600	-2.61397100	0.41900400
H	-4.64427200	-1.92581000	-1.15345200
H	-1.82339500	-3.13953000	1.85702100
O	-0.66902300	5.47345900	0.94177900
O	5.07579500	-2.15629100	0.94240500
O	-4.40592400	-3.31689800	0.94109400
C	5.62767500	-1.57716200	2.11432400
H	6.51583200	-2.16488200	2.35245600
H	5.92054300	-0.53122600	1.95182100
H	4.92778500	-1.62385200	2.95954400

C	-4.18142300	-4.08227300	2.11462800
H	-5.13451300	-4.55772900	2.35233000
H	-3.42137300	-4.85867800	1.95441000
H	-3.87336900	-3.45117700	2.95916600
C	-1.45138400	5.66295200	2.11026800
H	-1.38528800	6.72571700	2.34922900
H	-2.50343000	5.39591000	1.94280800
H	-1.06610200	5.07890800	2.95695400

(G) L−PdAr−I

Total energy: -3757.61221020 Hartree

Free energy: -3757.190095 Hartree

Pd	0.34176400	1.88135000	-0.24528100
As	-0.85644800	-0.21893800	0.02929500
C	-1.98502800	-0.64217600	-1.49024100
C	-3.09190600	-1.48796600	-1.38190100
C	-1.65767300	-0.10931300	-2.74814200
C	-3.86379900	-1.80826200	-2.49956300
H	-3.37110200	-1.89964400	-0.41659800
C	-2.41394800	-0.42385900	-3.86908800
H	-0.80910200	0.56329300	-2.84642700
C	-3.52278200	-1.27708400	-3.75220700
H	-4.71895500	-2.46309800	-2.38381200
H	-2.17464100	-0.01662900	-4.84572300
C	0.24014400	-1.80131100	0.23189900
C	1.01250800	-1.92639900	1.39000200
C	0.43240500	-2.71398400	-0.81425900
C	1.99069300	-2.91081200	1.49979700
H	0.88376900	-1.22526800	2.20861100
C	1.40977500	-3.69761600	-0.71927700
H	-0.16283800	-2.63887700	-1.71928300
C	2.21769100	-3.77940700	0.42460700
H	2.59600400	-2.95632300	2.39582500
H	1.58754200	-4.39664100	-1.52995300
C	-2.04110000	-0.29838800	1.55859100
C	-2.57606600	0.88626400	2.07179200

C	-2.39131900	-1.51767400	2.16191400
C	-3.45505600	0.87176200	3.15611300
H	-2.29956200	1.84177200	1.63298200
C	-3.26388400	-1.54669200	3.24071900
H	-1.96588900	-2.44664000	1.79424700
C	-3.80481800	-0.35175000	3.74389800
H	-3.84850200	1.80806100	3.53249400
H	-3.54151200	-2.47992500	3.71957700
C	2.06264700	0.90569200	-0.06930300
C	2.51213200	0.10475300	-1.11494000
C	2.76557800	0.94471900	1.13870100
C	3.63042800	-0.71898400	-0.94147600
H	1.98177600	0.07469000	-2.06121700
C	3.87998100	0.12405800	1.31261400
H	2.44902900	1.59815100	1.94450000
C	4.29878500	-0.73195000	0.28602800
H	3.93624000	-1.36267200	-1.75691300
H	4.43083500	0.12341000	2.24806500
O	-4.64669600	-0.48976700	4.80217400
O	3.20774600	-4.71562200	0.39093900
O	-4.19986700	-1.52102300	-4.90554500
O	5.35352100	-1.55831300	0.58491800
C	-5.34126300	-2.36680400	-4.85689900
H	-6.12071300	-1.95636600	-4.20194800
H	-5.72060900	-2.41766900	-5.87836100
H	-5.08120500	-3.37790300	-4.51738700
C	4.09809400	-4.78486200	1.50215600
H	3.57228700	-5.08080700	2.41904500
H	4.83202100	-5.55127800	1.24849600
H	4.60644800	-3.82667600	1.66447700
C	-5.21958300	0.68171900	5.36983200
H	-5.83775200	1.22253300	4.64169200
H	-5.84937100	0.33925900	6.19198200
H	-4.44945100	1.35846200	5.76167000
C	5.83700600	-2.40934000	-0.44581400
H	6.17534000	-1.83554300	-1.31843900

H	6.68783800	-2.94453500	-0.01984400
H	5.07532600	-3.13501400	-0.76048100
I	1.34722400	4.27842500	-0.56838300

(H) Transition state for the isomerization

(TS connecting between L−PdAr−I and Ar−PdL−I)

imaginary mode 26.83 i cm^{-1}

Total energy: -3757.60805201 Hartree

Free energy: -3757.184901 Hartree

Pd	-0.36123400	1.80568300	-0.45906100
As	-0.39178100	-0.51052500	0.08250500
C	-1.32556700	-1.51981600	-1.28098500
C	-1.82378700	-2.79708200	-1.00955500
C	-1.48552300	-0.98220200	-2.56772500
C	-2.46679600	-3.54031100	-1.99951600
H	-1.72460900	-3.22277800	-0.01524100
C	-2.12197200	-1.71300900	-3.56178900
H	-1.12274600	0.01863000	-2.78615000
C	-2.61559600	-2.99776700	-3.28496300
H	-2.84633100	-4.52634700	-1.76071800
H	-2.25982500	-1.30896100	-4.55900300
C	1.27693300	-1.46021600	0.31111600
C	2.07170100	-1.15288000	1.41922300
C	1.81153200	-2.26125300	-0.70796200
C	3.39267600	-1.58447600	1.49808100
H	1.67651100	-0.53215200	2.21699600
C	3.12972600	-2.69576200	-0.64202200
H	1.20648300	-2.51941400	-1.57186000
C	3.93998300	-2.32421200	0.44170900
H	3.99199900	-1.29716600	2.35229900
H	3.56716100	-3.29356400	-1.43483300
C	-1.35991700	-0.84580900	1.72247700
C	-2.34875700	0.05382100	2.13261500
C	-1.11358300	-1.99110800	2.49722800
C	-3.09311100	-0.17894500	3.28954300
H	-2.54099300	0.95406300	1.55437100

C	-1.84818700	-2.23213400	3.64981600
H	-0.33451500	-2.68907700	2.20575700
C	-2.84540600	-1.32851300	4.05304100
H	-3.84987900	0.53814600	3.58293800
H	-1.66915500	-3.10996600	4.26184400
C	1.61194600	1.64404900	-0.29903200
C	2.38356100	1.08175200	-1.31593800
C	2.23763900	2.11197200	0.86440900
C	3.76958600	0.95753500	-1.17398500
H	1.91536200	0.69443000	-2.21579400
C	3.61882700	1.98956600	1.01050600
H	1.65517600	2.55737600	1.66586700
C	4.38553600	1.38078200	0.00789600
H	4.33779500	0.49152000	-1.96958900
H	4.11871100	2.33264300	1.91107400
O	-3.50484900	-1.65563600	5.19523400
O	5.24575000	-2.70560700	0.37011700
O	-3.22299800	-3.62951300	-4.32350300
O	5.71778100	1.21379100	0.28872700
C	-3.76472600	-4.92597900	-4.10766000
H	-4.54777200	-4.91356700	-3.33856700
H	-4.20115300	-5.23075000	-5.05973700
H	-2.98778300	-5.64610500	-3.81951800
C	6.12496300	-2.27283900	1.40536700
H	5.84957400	-2.70869400	2.37427100
H	7.11657600	-2.62922600	1.12267300
H	6.13588800	-1.17887700	1.48698600
C	-4.52076300	-0.77801500	5.66639000
H	-5.33648000	-0.67772800	4.93906900
H	-4.90722300	-1.23075800	6.58044200
H	-4.11914100	0.21695700	5.89682700
C	6.53191000	0.61067700	-0.70805000
H	6.53275300	1.19446900	-1.63782200
H	7.54378900	0.59073900	-0.29903300
H	6.20929400	-0.41629400	-0.92619300
I	-1.98238500	3.85013500	-0.91451400

(I) Ar−PdL−X

Total energy: -3757.61240367 Hartree

Free energy: -3757.188408 Hartree

Pd	0.19355000	-1.34120200	-1.53561600
As	0.30845600	0.23006900	0.22202400
C	1.35420100	1.78825700	-0.25270400
C	1.57524200	2.78059600	0.70747600
C	1.89325100	1.94417500	-1.53757100
C	2.31723500	3.92085700	0.40102900
H	1.17030200	2.67410900	1.70969800
C	2.63227800	3.07642500	-1.85376700
H	1.75420100	1.16934900	-2.28447500
C	2.84948900	4.07168900	-0.88852100
H	2.47500300	4.67265700	1.16467200
H	3.06220400	3.20870200	-2.84080700
C	-1.35649100	0.97369800	0.87089100
C	-2.19994900	0.16059700	1.63359200
C	-1.83963800	2.20493500	0.40472300
C	-3.51537400	0.53249700	1.89399900
H	-1.84623700	-0.79803200	1.99885900
C	-3.15184800	2.58653100	0.65651800
H	-1.19805700	2.85553200	-0.18148600
C	-4.00923400	1.73322100	1.36747900
H	-4.15152700	-0.13777100	2.45737100
H	-3.54837000	3.52395500	0.28075100
C	1.14201800	-0.50176100	1.80788700
C	2.08381400	-1.52774000	1.69192000
C	0.85125200	0.02078500	3.07946100
C	2.73593100	-2.02902600	2.81910300
H	2.32123400	-1.94255800	0.71674400
C	1.49438100	-0.47164900	4.20588200
H	0.10967900	0.80527500	3.19323800
C	2.44389400	-1.49973000	4.08355000
H	3.46110600	-2.82400300	2.69570500
H	1.28008000	-0.08117800	5.19523600

C	-1.79172600	-1.27379700	-1.29651300
C	-2.55887100	-0.24870500	-1.85955500
C	-2.44832200	-2.27736900	-0.56405400
C	-3.94668400	-0.20710000	-1.69831500
H	-2.07747300	0.56168700	-2.40022500
C	-3.83178400	-2.24650400	-0.39710800
H	-1.88082300	-3.08004200	-0.09906800
C	-4.58228000	-1.19217600	-0.93507200
H	-4.50303000	0.61638800	-2.12924100
H	-4.34690600	-3.00941700	0.17868900
O	3.01473400	-1.91117300	5.24633500
O	-5.30443800	2.14028000	1.47548600
O	3.58593100	5.13817700	-1.29851000
O	-5.91884800	-1.18847600	-0.62805200
C	3.86329200	6.17204600	-0.36382600
H	4.43185800	5.79696600	0.49702600
H	4.46584600	6.90694900	-0.89937000
H	2.94290200	6.65196200	-0.00594600
C	-6.22676100	1.26697000	2.12245200
H	-5.97375700	1.12918700	3.18150200
H	-7.20031100	1.75374600	2.04841100
H	-6.26533600	0.28911400	1.62647800
C	3.98582100	-2.94949300	5.19295200
H	4.85238500	-2.66050100	4.58479200
H	4.30670800	-3.11270100	6.22268200
H	3.56053400	-3.87945900	4.79447300
C	-6.71842600	-0.14547100	-1.16960800
H	-6.70447500	-0.15354000	-2.26731900
H	-7.73627000	-0.33571400	-0.82413100
H	-6.39272600	0.84079200	-0.81252700
I	2.70304900	-1.90085700	-2.33181200

(J) vinyl$SnBu_3$

Total energy: -554.982388922 Hartree

Free energy: -554.630126 Hartree

C	-4.29773400	-0.13062200	-0.01833800

C	-3.29309400	-1.00791400	-0.12733800
Sn	-1.21311400	-0.43822200	-0.05274700
H	-5.34468100	-0.43345500	-0.05606000
H	-4.12907900	0.93744700	0.11468800
H	-3.55089400	-2.06073000	-0.25811100
C	-1.09789400	1.73425000	0.18849500
H	-1.91834600	2.19128300	-0.37879200
H	-1.28226500	1.97511900	1.24275400
C	-0.17106200	-1.00480000	-1.89427000
H	-0.44016700	-0.27907200	-2.67176300
H	-0.55819500	-1.97358800	-2.23348600
C	-0.18897900	-1.38961900	1.63456300
H	-0.89626000	-1.47095100	2.46871100
H	0.07072100	-2.41680300	1.34934500
C	1.07223800	-0.63373400	2.08538600
H	1.77720700	-0.53978900	1.24738900
H	0.81035600	0.39494000	2.37147500
C	1.79533800	-1.30423900	3.26223800
H	1.09821200	-1.39575000	4.10629600
H	2.06560900	-2.33049500	2.97827000
C	3.04884100	-0.54243200	3.70482200
H	3.54825400	-1.03829500	4.54374900
H	3.77202600	-0.46458600	2.88457600
H	2.79889200	0.47721100	4.02057800
C	1.35738300	-1.07389200	-1.74189800
H	1.62455300	-1.80119500	-0.96200300
H	1.74681600	-0.10692600	-1.39347200
C	2.08117700	-1.45538000	-3.04118500
H	1.70096500	-2.42448900	-3.39211600
H	1.82294700	-0.72678600	-3.82174600
C	3.60321400	-1.52317100	-2.87920500
H	3.88610200	-2.26591800	-2.12411500
H	4.09791000	-1.79617400	-3.81720100
H	4.00801900	-0.55654600	-2.55731300
C	0.24486500	2.33395200	-0.26156400
H	0.43159300	2.08720600	-1.31645800

H	1.07045800	1.87731900	0.30232000
C	0.31785300	3.85802700	-0.09108600
H	-0.50124600	4.32168700	-0.65766200
H	0.13861500	4.10913600	0.96328800
C	1.65862200	4.44599700	-0.54277400
H	1.84559800	4.23193300	-1.60157800
H	1.68823100	5.53278900	-0.41204900
H	2.48912200	4.01802900	0.03077600

(K) Cation−π complex between Ar−PdL−X and vinylSnBu3

Total energy: -4312.65003698 Hartree

Free energy: -4311.851582 Hartree

Pd	-0.17168700	-0.13578000	-0.93598600
As	1.97564600	-0.43151600	0.17223000
C	1.98038700	-1.52886600	1.76791200
C	3.13378900	-2.21632100	2.17311100
C	0.84211000	-1.57881400	2.57229100
C	3.14167600	-2.93634400	3.35970000
H	4.02663500	-2.19952400	1.55538300
C	0.83891100	-2.28978800	3.77331600
H	-0.06460400	-1.07930300	2.25405800
C	1.99449800	-2.97554900	4.16963200
H	4.02115400	-3.48248800	3.68440000
H	-0.06506700	-2.31483900	4.36931200
C	2.95637400	1.12725000	0.79950800
C	3.51588800	2.04256000	-0.10912500
C	3.08340800	1.38055700	2.16713400
C	4.17666100	3.17453700	0.34119400
H	3.42068800	1.88056700	-1.17665200
C	3.73903000	2.52328300	2.63407900
H	2.66764300	0.68765700	2.89089600
C	4.28815800	3.42796000	1.71794400
H	4.59862900	3.89172800	-0.35471400
H	3.81144100	2.69004100	3.70187000
C	3.23280700	-1.29153900	-1.02473800
C	2.75382100	-2.21673300	-1.95792300

C	4.61237400	-1.03768700	-0.96464200
C	3.62561800	-2.88219400	-2.82107400
H	1.69063100	-2.43372400	-2.00884800
C	5.48834500	-1.69345900	-1.81943200
H	5.00485600	-0.31697600	-0.25450800
C	5.00111700	-2.62128500	-2.75361700
H	3.22280600	-3.59534800	-3.52995600
H	6.55665100	-1.50651500	-1.78609600
C	0.59740700	1.63244500	-1.56663600
C	0.45237100	2.83475800	-0.85571800
C	1.28281100	1.66304200	-2.78409500
C	0.98010300	4.02507400	-1.34598400
H	-0.05869100	2.84530500	0.10248000
C	1.82568100	2.85557200	-3.28831300
H	1.42774000	0.74838300	-3.35418800
C	1.67778300	4.04212600	-2.56224100
H	0.88204900	4.95455600	-0.79374500
H	2.35889900	2.83640400	-4.23191000
C	-2.26495000	0.78875900	-1.47603800
C	-1.86869800	0.00519300	-2.53156000
H	-2.01607200	1.84753500	-1.55819800
H	-1.35480000	0.43689300	-3.39076200
I	-1.01890600	-2.75234100	-0.37898700
O	2.17757600	5.25869600	-2.94163600
C	2.90166000	5.33100400	-4.15775600
H	3.20943400	6.37250400	-4.26678700
H	3.79560800	4.69209400	-4.13867700
H	2.28218200	5.04712000	-5.01961300
Sn	-3.72521000	0.30649600	0.08537100
C	-5.05590100	2.04833300	0.04743700
H	-4.50282800	2.91880600	0.42320500
H	-5.30261800	2.27000500	-0.99842900
C	-4.87919800	-1.45446100	-0.46350800
H	-5.59195900	-1.65559300	0.34630200
C	-2.74943800	0.26219500	2.03707400
H	-3.53077700	0.37544100	2.79939600

H	-2.30895600	-0.73091900	2.17223100
C	-6.34533100	1.85126900	0.85996600
H	-6.89361200	0.97374300	0.48715500
H	-6.10132500	1.62755600	1.90925800
C	-7.28205600	3.06772300	0.82368500
H	-6.74199900	3.94636700	1.20208200
H	-7.53375000	3.29255000	-0.22173100
C	-8.56663800	2.86057000	1.63258900
H	-8.34071900	2.66327600	2.68708600
H	-9.21735600	3.74033800	1.59010900
H	-9.13710700	2.00484500	1.25298500
H	-2.18401700	-1.02944000	-2.63307900
C	-1.68805600	1.36094500	2.19966700
H	-0.86768000	1.18022300	1.48996400
H	-2.10795100	2.34132400	1.92842300
C	-1.10383200	1.46435000	3.61561100
H	-0.63346400	0.51015100	3.88555100
H	-1.92252600	1.61642400	4.33213200
C	-0.08079900	2.59772300	3.74503400
H	0.34599400	2.64448000	4.75292100
H	0.74557200	2.46526100	3.03903600
H	-0.54293100	3.56931600	3.53352700
H	-4.18823600	-2.30173700	-0.49988700
C	-5.62347400	-1.30072300	-1.79860700
H	-6.30186600	-0.43549600	-1.76151500
H	-4.90749100	-1.08663200	-2.60506800
C	-6.43337800	-2.54852800	-2.17927100
H	-7.15350700	-2.76596000	-1.37855300
H	-5.75620500	-3.41179300	-2.22341700
C	-7.17178200	-2.39859200	-3.51324900
H	-6.46854500	-2.21028900	-4.33292400
H	-7.74093500	-3.30017600	-3.76321900
H	-7.87470000	-1.55764800	-3.48287300
O	5.94092500	-3.20748000	-3.54406500
O	4.94370100	4.57247100	2.05502000
O	2.10794600	-3.70575500	5.31273500

C	5.06145400	4.90017600	3.43215800
H	5.59822500	5.84923000	3.47112800
H	4.07770800	5.02131000	3.90439300
H	5.63190300	4.14024100	3.98239200
C	5.51399500	-4.16501800	-4.50400400
H	4.82997100	-3.72272500	-5.23999700
H	6.41781500	-4.50425300	-5.01222700
H	5.02266900	-5.02343200	-4.02809500
C	0.96841000	-3.82082700	6.15383900
H	1.27385300	-4.45258400	6.98929500
H	0.64863600	-2.84339000	6.53869800
H	0.12680800	-4.29320800	5.63102400

(L) Transition state for the transmetalation

imaginary mode 39.33 i cm^{-1}

Total energy: -4312.61976682 Hartree

Free energy: -4311.816807 Hartree

Pd	-0.06056900	-0.84660700	-1.40624900
C	-0.66699100	1.41819600	1.43978800
C	-0.09159400	2.69058800	1.45355800
C	-0.49205400	0.59341800	2.56508800
C	0.62643700	3.14988300	2.56273300
H	-0.19986100	3.34185300	0.59267900
C	0.22333700	1.03279100	3.67134400
H	-0.94101300	-0.39580300	2.58516100
C	0.78122000	2.32100500	3.68017600
H	1.05327600	4.14552700	2.54215700
H	0.35156400	0.40619900	4.54795600
C	-3.25251500	0.07574100	0.62798100
C	-4.02262600	-0.84239900	-0.10537200
C	-3.74654800	0.53614600	1.85062800
C	-5.24483900	-1.28737200	0.37533300
H	-3.65158800	-1.23641500	-1.04488500
C	-4.97548700	0.09395000	2.34870100
H	-3.17114800	1.24115200	2.44251900
C	-5.73015800	-0.82382000	1.60767700

H	-5.83487500	-2.01131100	-0.17635300
H	-5.32601600	0.46760700	3.30343200
C	-2.15887900	2.31105500	-1.05780900
C	-1.88207900	2.46604400	-2.42447600
C	-2.89265400	3.30478100	-0.40427900
C	-2.32071000	3.58921100	-3.11479700
H	-1.31570400	1.70356900	-2.94973800
C	-3.33447500	4.44195500	-1.08166900
H	-3.13230500	3.19757900	0.64983100
C	-3.04666600	4.58652800	-2.44666700
H	-2.11326100	3.71963800	-4.17170900
H	-3.89959000	5.19500800	-0.54558600
C	-1.24160100	-2.44288900	-1.03200200
C	-1.47481400	-2.90750000	0.27433300
C	-1.94961200	-3.05906300	-2.07108600
C	-2.39283100	-3.92218700	0.53354400
H	-0.95484200	-2.46164200	1.11617000
C	-2.89211800	-4.06832200	-1.82485500
H	-1.77918700	-2.75002700	-3.09797100
C	-3.11891600	-4.50113200	-0.51423900
H	-2.58086100	-4.26651700	1.54612800
H	-3.42705600	-4.50558600	-2.66054000
C	1.70475500	-1.98458500	-3.56709000
C	1.11708800	-2.19829400	-2.38039800
Sn	2.94782800	-0.54609500	0.03175800
C	4.42731200	-1.54732800	-1.21341800
H	3.96522700	-2.49108500	-1.51752100
H	5.26684000	-1.78861300	-0.54650700
C	1.85079200	-1.97205200	1.26397400
H	1.31703500	-2.63758800	0.58397100
H	1.10308900	-1.40732800	1.82549500
C	3.71678200	1.09040400	1.26426700
H	4.62732200	1.46169200	0.77843400
H	2.97605200	1.89412400	1.20654400
H	1.22448600	-3.19435800	-1.94369500
H	2.27512900	-2.76506700	-4.07572000

H	1.64980900	-1.02875800	-4.08342900
O	1.44863900	2.66691900	4.81864400
O	-3.42817500	5.64883200	-3.20932300
O	-6.93599500	-1.32838800	1.99422700
C	-7.46980800	-0.91526200	3.24243100
H	-8.41984600	-1.44049100	3.35330700
H	-6.80862000	-1.18633700	4.07634500
H	-7.65192100	0.16756200	3.26847100
C	-4.17297600	6.68933800	-2.59438200
H	-4.36817800	7.42346000	-3.37763200
H	-5.12892200	6.32370300	-2.19656100
H	-3.60783000	7.16877900	-1.78399000
C	1.85583100	4.01950500	4.97957400
H	1.00060500	4.70387200	4.91033200
H	2.29553600	4.08312500	5.97567500
H	2.61055600	4.31093200	4.23907100
C	3.97870300	0.72796800	2.73231100
H	3.04233300	0.39893500	3.20146200
H	4.67891600	-0.11568000	2.81352500
C	4.54229700	1.91131100	3.53232200
H	3.89147000	2.77902700	3.37002700
H	5.52418600	2.18631600	3.12432800
C	4.65220200	1.62333100	5.03204000
H	5.08931700	2.47019300	5.57253100
H	3.66167400	1.42855900	5.45547600
H	5.28369900	0.74760300	5.22192200
C	4.91542700	-0.77539100	-2.44218200
H	4.05769000	-0.52830600	-3.07773000
H	5.36207700	0.18291700	-2.14131700
C	5.93471900	-1.56954400	-3.27104900
H	5.47798000	-2.52109100	-3.57527700
H	6.79720600	-1.83023900	-2.64199000
C	6.40867900	-0.80512200	-4.51121600
H	7.12918100	-1.38850800	-5.09418200
H	5.56477300	-0.56252700	-5.16700300
H	6.89073300	0.13899800	-4.23187300

C	2.75539400	-2.77118400	2.21473200
H	3.30406800	-2.10139500	2.88968900
H	3.51479400	-3.32644800	1.64560000
C	1.94615100	-3.76760600	3.06133400
H	1.19275000	-3.21182000	3.63629800
H	1.38786000	-4.43438300	2.39139100
C	2.82005000	-4.59172500	4.01167500
H	3.36547400	-3.94397100	4.70794700
H	2.22004600	-5.28960600	4.60479200
H	3.56116000	-5.17782700	3.45613000
As	-1.57291900	0.70363700	-0.13312900
I	1.73633100	1.38193900	-1.88533100
O	-4.01675400	-5.47297000	-0.15238100
C	-4.79314600	-6.07016600	-1.17441400
H	-5.44388100	-6.79410600	-0.67983800
H	-5.41357100	-5.33135400	-1.70132700
H	-4.16847300	-6.59427900	-1.91125700

(M) Complex between vinyl−PdAr−L and Bu_3SnI

Total energy: -4312.62297391 Hartree

Free energy: -4311.822872 Hartree

Pd	0.36407900	1.10794100	-1.27779700
As	1.80436500	-0.63627800	-0.18743400
C	0.74392600	-1.60577800	1.13315400
C	0.45312100	-2.96654300	1.03704400
C	0.16617900	-0.87009100	2.18224400
C	-0.39036500	-3.59506000	1.95985200
H	0.87815200	-3.55546900	0.23082700
C	-0.66847500	-1.47936600	3.10898500
H	0.37272800	0.19192700	2.27754100
C	-0.95391800	-2.85009500	3.00174600
H	-0.59491300	-4.65373000	1.85416800
H	-1.10746000	-0.92023600	3.92894000
C	3.35519200	-0.11588500	0.86564600
C	4.22136600	0.86464600	0.35267000
C	3.64901800	-0.68714600	2.10538600

C	5.34555000	1.25837900	1.06193100
H	3.99708500	1.34963300	-0.59128200
C	4.77888300	-0.29848600	2.83204200
H	2.99038400	-1.43943000	2.52862400
C	5.63262600	0.67969800	2.30819100
H	6.00697100	2.03024500	0.68333100
H	4.97554400	-0.75870900	3.79304400
C	2.54032600	-2.05813400	-1.28993700
C	2.17137000	-2.14652300	-2.64146000
C	3.44763500	-2.99088400	-0.77946800
C	2.68496000	-3.14932900	-3.45408600
H	1.48124100	-1.42078300	-3.06056900
C	3.96954500	-4.00669000	-1.58225400
H	3.76687700	-2.92441300	0.25684200
C	3.58436800	-4.08917700	-2.92800800
H	2.40937300	-3.22559200	-4.50068900
H	4.67198900	-4.71323300	-1.15651900
C	1.54924000	2.61208400	-0.67269900
C	1.65534800	2.94027700	0.69008800
C	2.36312400	3.30752400	-1.57352700
C	2.55920700	3.90045700	1.13779800
H	1.04378300	2.42606700	1.42630300
C	3.29096100	4.26469500	-1.13576400
H	2.29022800	3.10410900	-2.63769500
C	3.39382700	4.56034500	0.22759100
H	2.64992700	4.14063200	2.19282300
H	3.91275800	4.76879400	-1.86718800
C	-1.66004500	2.45934400	-3.06740400
C	-0.84493100	2.57510900	-2.00647300
Sn	-3.37524300	-0.01778500	-0.14883500
C	-4.12039000	-1.78107900	0.89741800
H	-5.02855900	-2.11384000	0.38088300
H	-3.36965900	-2.56780800	0.76646300
C	-4.77527400	0.91737400	-1.52449400
H	-4.18438800	1.64488100	-2.09089100
H	-5.10183800	0.14799100	-2.23316400

C	-2.29935700	1.40620700	1.09388800
H	-2.34602900	1.06177200	2.13269600
H	-1.25598500	1.34691200	0.76656800
H	-0.82995500	3.54488400	-1.50352300
H	-2.28091500	3.29212500	-3.40748700
H	-1.74240900	1.54514100	-3.65144000
C	-2.81661200	2.84385400	0.94239000
H	-2.87276800	3.10575700	-0.12106300
H	-3.83747800	2.92849400	1.34210000
C	-4.38813800	-1.55260100	2.39252600
H	-3.44976500	-1.28962400	2.89480100
H	-5.06949500	-0.70305100	2.54635800
C	-5.98292800	1.58839500	-0.85186700
H	-5.64359000	2.35242400	-0.13949200
H	-6.55423300	0.85427300	-0.26488000
C	-6.92744500	2.25066800	-1.86671500
H	-6.35920300	2.98510400	-2.45257500
H	-7.27439100	1.49202600	-2.58103900
C	-1.91528200	3.86795500	1.64621600
H	-0.90728300	3.79920900	1.22133900
H	-1.82574900	3.60456600	2.70967800
C	-4.98358000	-2.79108900	3.07772100
H	-4.36761100	-3.66203000	2.82333900
H	-5.98037800	-2.99032000	2.66165900
C	-5.06216000	-2.64714800	4.60007900
H	-5.51649400	-3.52901100	5.06485700
H	-4.05881000	-2.51911900	5.01949300
H	-5.66283300	-1.77582800	4.88599200
C	-8.13003700	2.93121300	-1.20547900
H	-7.80619100	3.71408200	-0.50993700
H	-8.78675100	3.39600900	-1.94803000
H	-8.72799200	2.21014000	-0.63593400
C	-2.43225800	5.30274200	1.50609000
H	-1.77003900	6.01709900	2.00575700
H	-2.49675200	5.59093000	0.45045200
H	-3.43297300	5.41108600	1.94135700

O	-1.78900700	-3.35468800	3.95651100
O	6.75640600	1.14121400	2.92691600
O	4.02914200	-5.03296400	-3.80380300
C	-2.03329000	-4.75433200	3.96688200
H	-2.70545400	-4.93438200	4.80677600
H	-2.51940300	-5.08968300	3.04196000
H	-1.10478800	-5.32180200	4.11049800
C	7.08381600	0.61843300	4.20473100
H	7.99739900	1.12838000	4.51472500
H	6.29250700	0.81774700	4.93966500
H	7.27085300	-0.46323300	4.16603700
C	4.95228300	-6.00571000	-3.33752400
H	5.16981500	-6.64840500	-4.19199700
H	5.88487700	-5.54456300	-2.98638900
H	4.52682000	-6.61394700	-2.52819800
I	-1.54563400	-1.20096600	-2.01069800
O	4.26747000	5.46872500	0.77021900
C	5.14371200	6.14990700	-0.10813900
H	5.80356700	5.45573000	-0.64786600
H	4.59762300	6.75837900	-0.84263400
H	5.75244100	6.80676100	0.51652300

(N) vinyl−PdAr−L

Total energy: -3824.11566540 Hartree

Free energy: -3823.655952 Hartree

Pd	0.55984800	-1.33851000	-2.18202400
As	-0.68337500	-0.18026100	-0.34967300
C	-2.59516900	0.09745000	-0.57697100
C	-3.49825800	0.07912800	0.48860300
C	-3.08616700	0.33828900	-1.87121200
C	-4.86280200	0.29511000	0.28307500
H	-3.14268100	-0.11306500	1.49651000
C	-4.43887100	0.56112400	-2.09094900
H	-2.40117700	0.35177200	-2.71593100
C	-5.33762900	0.53975600	-1.01276800
H	-5.53768100	0.26894000	1.13025500

H	-4.82905000	0.74706200	-3.08612700
C	-0.06259500	1.59617200	0.14838000
C	1.28469400	1.76955000	0.51630200
C	-0.90230500	2.71103300	0.12880700
C	1.76791200	3.02529900	0.85206900
H	1.96122000	0.92313100	0.54412000
C	-0.42390800	3.98300800	0.45959800
H	-1.94659200	2.60121800	-0.14686900
C	0.91842900	4.14284700	0.82271900
H	2.80552400	3.16754400	1.13574100
H	-1.10229100	4.82734700	0.43160500
C	-0.57391200	-1.12304500	1.34500000
C	-0.49208100	-2.52519300	1.33122800
C	-0.55652700	-0.46256600	2.57520800
C	-0.40482400	-3.24459800	2.51460600
H	-0.47882300	-3.05422200	0.38127500
C	-0.46715700	-1.17261700	3.77552600
H	-0.59733000	0.62210800	2.60746900
C	-0.39200600	-2.57124100	3.74707700
H	-0.33427500	-4.32733200	2.51638300
H	-0.44985000	-0.62987600	4.71302100
C	2.35122700	-0.94636700	-1.39187600
C	3.15293100	0.06217100	-1.93048600
C	2.74482200	-1.54813900	-0.18514700
C	4.29545400	0.51651100	-1.25667000
H	2.88654600	0.52844000	-2.87406500
C	3.88250200	-1.10690900	0.48829300
H	2.15066000	-2.34137300	0.25597200
C	4.65837400	-0.06369700	-0.03699800
H	4.88076000	1.31725300	-1.69387500
H	4.18596800	-1.55528500	1.42944000
C	1.20657600	-3.53631400	-4.01058600
C	1.53095500	-2.28407700	-3.65256800
H	2.27414200	-1.74428900	-4.24578700
H	1.61106800	-4.00754300	-4.90930900
H	0.51955900	-4.15271600	-3.43134800

O	-6.64252400	0.76353500	-1.33106000
O	1.49509500	5.33034200	1.16453500
O	-0.29728700	-3.36547700	4.84911300
C	-7.60621900	0.74007900	-0.28777300
H	-8.56885400	0.93441300	-0.76302100
H	-7.64026800	-0.23778500	0.21022700
H	-7.41076000	1.51783100	0.46231400
C	0.69117100	6.49986200	1.14018800
H	1.34519500	7.32215900	1.43485000
H	0.29282400	6.69771200	0.13617200
H	-0.14498700	6.43304200	1.84916000
C	-0.25059900	-2.74546400	6.12610600
H	-0.16600600	-3.55612500	6.85137100
H	0.61897400	-2.08219500	6.22257300
H	-1.16384300	-2.17145400	6.33184900
O	5.74374200	0.30620000	0.71444900
C	6.54577900	1.37254500	0.23945500
H	5.97091600	2.30467900	0.14368500
H	7.33468900	1.51407400	0.98071100
H	7.00382700	1.13954900	-0.73176700

(O) Bu_3SnI

Total energy: -488.462274643 Hartree

Free energy: -488.151937 Hartree

Sn	-0.42025900	0.00003400	-0.00061800
C	0.19718200	-1.89411900	-0.88407200
H	0.02067800	-2.68198800	-0.14338100
H	-0.46763300	-2.10097400	-1.72932700
C	0.20128400	0.18389900	2.08014300
H	0.03004400	1.22096200	2.38952600
H	-0.46511500	-0.44003700	2.68495800
C	0.19707000	1.71175300	-1.20010900
H	0.02485500	1.46179400	-2.25290500
H	-0.47057700	2.54605900	-0.96051700
C	1.66527200	2.10760200	-0.96684300
H	1.82622200	2.35165200	0.09278700

H	2.32992400	1.25958400	-1.18555300
C	1.66713700	-1.89199700	-1.33787700
H	1.83273800	-1.09476100	-2.07631700
H	2.32890400	-1.66119100	-0.49082900
C	1.66996300	-0.21606700	2.30318700
H	2.33318000	0.39584000	1.67510900
H	1.82953400	-1.25644900	1.98635500
C	2.10940000	-0.07316900	3.76810900
H	1.95653700	0.96647500	4.08712800
H	1.45234100	-0.68616600	4.39922700
C	2.10050000	3.30741200	-1.82153900
H	1.44203100	4.15862800	-1.60324100
H	1.94602300	3.06561900	-2.88157100
C	2.10195800	-3.23133000	-1.95161300
H	1.44627500	-3.46428100	-2.80109600
H	1.94312600	-4.03015700	-1.21497300
C	3.56421600	-3.22880800	-2.40836700
H	3.85088800	-4.19231000	-2.84180500
H	3.73916900	-2.45657800	-3.16637900
H	4.23933900	-3.02634600	-1.56882500
C	3.57028800	-0.47608500	3.99232000
H	4.24687500	0.14346900	3.39231500
H	3.86032100	-0.36590200	5.04214400
H	3.73935900	-1.52092600	3.70729000
C	3.56100000	3.70575900	-1.58688100
H	3.84789400	4.56170600	-2.20610500
H	3.73160600	3.97964200	-0.53931100
H	4.23892300	2.87831700	-1.82645100
I	-3.23494600	-0.00080100	0.00271500

(P) Transition state for the reductive elimination

imaginary mode 269.56 i cm^{-1}

Total energy: -3824.10954752 Hartree

Free energy: -3823.647260 Hartree

Pd	-0.68720600	0.32441000	-2.40938200
As	0.79163300	0.12270300	-0.45604700

C	2.12357200	-1.29669200	-0.48664700
C	3.26742000	-1.28757100	0.31473400
C	1.90899200	-2.39189500	-1.34008600
C	4.18419900	-2.34132000	0.27892700
H	3.45987300	-0.44768000	0.97573100
C	2.80758700	-3.44937400	-1.38284300
H	1.02897500	-2.41003800	-1.97886100
C	3.95337900	-3.43038400	-0.57210900
H	5.06434800	-2.30074000	0.90953700
H	2.65273300	-4.29934800	-2.03932300
C	-0.30264400	-0.38308200	1.07597300
C	-1.39688300	0.43635200	1.39937200
C	-0.12261500	-1.57168100	1.78361500
C	-2.29433100	0.06835100	2.38915200
H	-1.57992100	1.34717600	0.83956600
C	-1.02626600	-1.96164300	2.77941900
H	0.71689500	-2.22080300	1.55406600
C	-2.12428100	-1.14545700	3.07147300
H	-3.16192100	0.67875000	2.61538600
H	-0.86795800	-2.89835900	3.30065000
C	1.79525200	1.63226900	0.24744500
C	2.35485200	2.55333200	-0.65259600
C	1.98716800	1.83273700	1.61677600
C	3.09500400	3.63517900	-0.19628800
H	2.19961800	2.42552700	-1.72109900
C	2.72690200	2.91883500	2.09222700
H	1.54722400	1.14224500	2.33049300
C	3.28703800	3.82432800	1.18170300
H	3.52974700	4.35510100	-0.88189600
H	2.85291000	3.04859000	3.16050100
C	-2.64217300	0.35104300	-1.81565300
C	-3.18096500	-0.84517500	-1.32769200
C	-3.22157500	1.56244300	-1.39532600
C	-4.19581400	-0.84381400	-0.36307800
H	-2.78276100	-1.79791000	-1.66369500
C	-4.23218500	1.57365700	-0.44044800

H	-2.86493600	2.50382800	-1.80230700
C	-4.70261500	0.37043900	0.10743200
H	-4.54982200	-1.78873000	0.03218500
H	-4.66125600	2.50593000	-0.08567400
C	-2.29710300	1.35512200	-4.66992000
C	-2.07240700	0.28677600	-3.88687300
H	-2.35629000	-0.70594500	-4.24288300
H	-2.69141300	1.25254100	-5.68119200
H	-2.11273000	2.37219900	-4.33088300
O	-3.09875700	-1.44618500	3.98332100
O	4.02363100	4.91704600	1.52770200
O	4.77522700	-4.51077900	-0.68983000
C	5.95945100	-4.54607700	0.09291800
H	5.73580100	-4.53568100	1.16801200
H	6.45980900	-5.48217900	-0.15975900
H	6.62603000	-3.70579500	-0.14203700
C	-2.99791600	-2.67092700	4.69378000
H	-3.86888100	-2.71251800	5.34991700
H	-3.01346400	-3.53540800	4.01670400
H	-2.08557200	-2.71198800	5.30346100
C	4.23888900	5.17609800	2.90715400
H	4.83830400	6.08664900	2.95272600
H	3.29358600	5.33917400	3.44138500
H	4.78800900	4.35840100	3.39272800
O	-5.63869600	0.49605600	1.10028300
C	-6.01556200	-0.67540200	1.80912400
H	-6.72717400	-0.34971500	2.57045100
H	-6.50693000	-1.40875300	1.15504500
H	-5.15271600	-1.14448200	2.30039900

(Q) The final product complex

Total energy: -3824.18681583 Hartree

Free energy: -3823.720296 Hartree

Pd	-0.41830600	-0.19003500	-2.60383400
As	0.82462900	-0.00468600	-0.55933500
C	1.94472300	-1.51151200	-0.03169900

C	3.08943800	-1.37582000	0.75667000
C	1.57043900	-2.79686200	-0.45668000
C	3.84930300	-2.48910200	1.12851900
H	3.40735000	-0.39104500	1.08633300
C	2.31121000	-3.91250200	-0.09192000
H	0.69450800	-2.91473800	-1.08998900
C	3.45742100	-3.76527600	0.70533600
H	4.73508500	-2.34807400	1.73646900
H	2.03298500	-4.90979600	-0.41698300
C	-0.34723700	0.17433500	0.99219600
C	-1.53001300	0.91750900	0.84799300
C	-0.07570100	-0.41968900	2.22665300
C	-2.40820400	1.07155400	1.91141000
H	-1.78434700	1.34907800	-0.11581800
C	-0.96066500	-0.28954000	3.30240700
H	0.82730600	-1.00759900	2.36071900
C	-2.13400900	0.45563000	3.14070600
H	-3.33206300	1.62876200	1.80251500
H	-0.72848800	-0.77605100	4.24245200
C	2.04767000	1.49277300	-0.30454100
C	2.82281300	1.91540500	-1.39716500
C	2.19643900	2.15597900	0.91539100
C	3.72543800	2.96187300	-1.26958800
H	2.71004700	1.42188600	-2.35952000
C	3.09791000	3.21515000	1.05912500
H	1.59941900	1.85549500	1.77135600
C	3.86912000	3.61959200	-0.03747200
H	4.32723100	3.29772600	-2.10775500
H	3.18454000	3.71166200	2.01832000
C	-3.31445100	-0.57739600	-2.07650800
C	-3.65637500	-1.40249100	-0.99541900
C	-3.87141100	0.71771800	-2.10563800
C	-4.48215000	-0.96381300	0.03954300
H	-3.23904300	-2.40508700	-0.94493200
C	-4.69554700	1.16808500	-1.08665200
H	-3.63858200	1.38548900	-2.92879000

C	-4.99510900	0.33646900	0.00501000
H	-4.68917400	-1.62485700	0.87216500
H	-5.11233500	2.17006100	-1.10006600
C	-1.89641300	-0.39922400	-4.21517200
C	-2.37181200	-1.07934900	-3.09610400
H	-2.20223800	-2.15545800	-3.05168000
H	-1.44352400	-0.96039500	-5.02856100
H	-2.24792100	0.59734800	-4.47200900
O	-3.08934700	0.62255500	4.10689100
O	4.77694700	4.63675000	-0.01604600
O	4.11839000	-4.91992800	1.00478800
C	5.29699100	-4.83602100	1.79115100
H	5.09307500	-4.41691400	2.78566800
H	5.65968900	-5.85925100	1.90158500
H	6.07031200	-4.23029700	1.30028000
C	-2.87466100	0.02134100	5.37469100
H	-3.74321900	0.27961700	5.98283100
H	-2.79885000	-1.07164500	5.29887100
H	-1.96829300	0.40871600	5.85842800
C	4.95500000	5.35435100	1.19559500
H	5.71035600	6.11403300	0.98818700
H	4.02705600	5.84636600	1.51606700
H	5.31182800	4.70315800	2.00483700
O	-5.76411900	0.90107500	0.98259000
C	-6.02699100	0.13904200	2.15477900
H	-6.65616800	0.76996600	2.78501900
H	-6.56851300	-0.78726800	1.92122600
H	-5.10268200	-0.09752700	2.69572600

(R) PdL

Total energy: -3399.93864822 Hartree

Free energy: -3399.627061 Hartree

Pd	0.00094700	-0.00258800	3.27466000
As	0.00071200	-0.00067400	0.94710100
C	-0.53944500	1.65968100	0.07502700
C	0.01343900	2.09840900	-1.13000000

C	-1.53980000	2.43866700	0.67882300
C	-0.41838500	3.28242400	-1.73597700
H	0.79716000	1.52044700	-1.61048200
C	-1.98283700	3.61304000	0.08715100
H	-1.96360800	2.12084500	1.62820900
C	-1.42382600	4.04324500	-1.12699300
H	0.03537800	3.59703300	-2.66828600
H	-2.75391400	4.22355000	0.54572700
C	-1.16750200	-1.29717400	0.07322800
C	-1.34659600	-2.55183200	0.67806600
C	-1.82035500	-1.03745600	-1.13367600
C	-2.14334500	-3.52129800	0.08573100
H	-0.86223100	-2.76003400	1.62886800
C	-2.63091500	-2.00202700	-1.74040400
H	-1.70812800	-0.07054900	-1.61494300
C	-2.79189500	-3.25199900	-1.13021600
H	-2.29016900	-4.49337600	0.54516100
H	-3.12742000	-1.76622200	-2.67418600
C	1.70788300	-0.36234200	0.07303500
C	2.88340100	0.11124300	0.67798300
C	1.81022900	-1.05730000	-1.13393100
C	4.12161200	-0.09252300	0.08570500
H	2.82084700	0.63476100	1.62876700
C	3.05117100	-1.27561600	-1.74054100
H	0.91717800	-1.44422300	-1.61545300
C	4.21357000	-0.78875400	-1.13023600
H	5.03642400	0.26744500	0.54517500
H	3.09585500	-1.82339400	-2.67436100
O	-3.55563800	-4.26644000	-1.62696000
O	5.47417600	-0.94144700	-1.62686000
O	-1.92260900	5.21116400	-1.62326300
C	-1.38583000	5.70946400	-2.83910300
H	-1.54782300	5.01111000	-3.67115600
H	-1.91706300	6.64021600	-3.04453100
H	-0.31133200	5.91890400	-2.75277400
C	-4.25179300	-4.05053100	-2.84492900

H	-4.79412700	-4.97482100	-3.05053100
H	-4.96847700	-3.22270700	-2.76161400
H	-3.56326100	-3.84457200	-3.67544200
C	5.63626100	-1.65269400	-2.84446600
H	6.70792100	-1.65907200	-3.04991800
H	5.27887100	-2.68764200	-2.76069400
H	5.11315700	-1.16038700	-3.67527100

(S) p-methoxystyrene (2)

Total energy: -424.191461370 Hartree

Free energy: -424.059966 Hartree

C	-1.44959400	-0.24023200	-0.00021400
C	-0.50827500	-1.27902700	-0.00006200
C	-0.95383800	1.08081000	-0.00033000
C	0.86704500	-1.03684600	0.00009900
H	-0.85683300	-2.30904800	-0.00002400
C	0.40623500	1.34017000	-0.00017700
H	-1.64517100	1.91778300	-0.00060700
C	1.33175300	0.28243200	0.00006800
H	1.55464600	-1.87406600	0.00023400
H	0.78732200	2.35620200	-0.00029600
C	-3.91642600	0.28646300	0.00056100
C	-2.88270500	-0.56558200	-0.00029100
H	-3.10289300	-1.63338200	-0.00110500
H	-4.93862600	-0.07733400	0.00038500
H	-3.78992300	1.36525100	0.00152400
O	2.64558100	0.64883900	0.00006200
C	3.62721800	-0.37606500	0.00015500
H	4.59363300	0.13069600	0.00017500
H	3.55231000	-1.00972300	0.89407000
H	3.55240900	-1.00982300	-0.89370200

(2) Optimized geometries in Figure S20, obtained from B3LYP calculations without dispersion correction.

***L* = As(PhOMe)$_3$ [1i]**

(A) PdL_2

Total energy: -6671.87761680 Hartree

Free energy: -6671.234361 Hartree

Pd	0.09857600	0.00190400	0.01039200
As	2.50537300	0.00158300	0.00383800
C	3.38364700	-0.69906600	1.60724600
C	4.60687600	-1.38732800	1.58349300
C	2.75409800	-0.50813100	2.84111400
C	5.18432800	-1.85793600	2.75710300
H	5.11055700	-1.56863000	0.63886600
C	3.32342900	-0.97036900	4.03011800
H	1.79370400	0.00029300	2.87691100
C	4.54758400	-1.64919200	3.98968600
H	6.12792600	-2.39429300	2.74632000
H	2.80484700	-0.80500700	4.96719600
C	3.37628000	1.74333000	-0.19805500
C	2.73641900	2.71445700	-0.97441700
C	4.60392100	2.07090300	0.39873200
C	3.29982100	3.97714700	-1.17367500
H	1.77260200	2.48810900	-1.42380000
C	5.17560200	3.32450000	0.21440100
H	5.11583300	1.34510100	1.02325900
C	4.52848800	4.28552100	-0.57680300
H	2.77325100	4.70431800	-1.78059600
H	6.12261600	3.58637000	0.67565800
C	3.36922300	-1.04190600	-1.40972300
C	2.73314300	-2.20610200	-1.85172200
C	4.58787700	-0.68185100	-2.00609300
C	3.29170000	-3.00919700	-2.84894700
H	1.77601900	-2.48781500	-1.41962900
C	5.15454500	-1.46738700	-3.00321500
H	5.09659200	0.22655700	-1.69806500
C	4.51144000	-2.63929900	-3.42899400
H	2.76827800	-3.90340300	-3.16647000
H	6.09457600	-1.19344700	-3.47168700
As	-2.30330200	0.00083800	0.00698400
C	-3.18370800	0.92959800	1.48968500

C	-4.38649700	0.50599400	2.05910600
C	-2.56535500	2.07738900	2.01482100
C	-4.97448400	1.20289900	3.12025800
H	-4.87869800	-0.38706200	1.68584100
C	-3.13907500	2.78398500	3.06301400
H	-1.61588800	2.40869500	1.60180500
C	-4.35068000	2.35004100	3.62379500
H	-5.90541700	0.84164600	3.54161800
H	-2.66533100	3.66980800	3.47396600
C	-3.17158000	0.82253900	-1.54437200
C	-4.37123900	1.53358400	-1.46992900
C	-2.54703500	0.69810300	-2.79738000
C	-4.95025800	2.10507400	-2.60820200
H	-4.86797400	1.66083500	-0.51276100
C	-3.11182300	1.25342000	-3.93742400
H	-1.59981100	0.16979300	-2.87157200
C	-4.32041600	1.96223500	-3.84977200
H	-5.87901300	2.65540500	-2.51209200
H	-2.63332300	1.16226100	-4.90733300
C	-3.17736800	-1.75089600	0.06491300
C	-4.37513200	-2.03651100	-0.59400000
C	-2.56009400	-2.77722400	0.80052300
C	-4.95928400	-3.30589800	-0.52430500
H	-4.86619000	-1.26847100	-1.18399400
C	-3.13008100	-4.04019500	0.88520500
H	-1.61443500	-2.58182200	1.29986800
C	-4.33666700	-4.31318000	0.22158200
H	-5.88631600	-3.49353400	-1.05354900
H	-2.65714600	-4.83720500	1.45009900
O	5.17018500	5.48375600	-0.69603900
O	5.14767600	-3.34029600	-4.41165800
O	5.19426700	-2.14925100	5.08217200
O	-4.81331000	-5.58440100	0.35921000
O	-4.79155700	2.47577300	-5.02299100
O	-4.83074700	3.10632400	4.65320300
C	-6.02082900	-5.92433600	-0.30250900

H	-5.93235600	-5.81286500	-1.39092500
H	-6.21119800	-6.97194300	-0.06386400
H	-6.86315800	-5.31569200	0.05140800
C	4.54122300	-4.53144300	-4.88704100
H	5.20961600	-4.92438700	-5.65486200
H	4.43106300	-5.27713100	-4.08911700
H	3.55690100	-4.33601100	-5.33169500
C	-6.00155400	3.21511000	-4.99489200
H	-5.91954000	4.10366800	-4.35562300
H	-6.18714300	3.52943600	-6.02320700
H	-6.84391200	2.60239100	-4.64815300
C	4.56005600	6.49732300	-1.47901300
H	5.23368200	7.35488500	-1.44006700
H	4.43589700	6.18371000	-2.52356900
H	3.58200700	6.78859200	-1.07482300
C	4.59442800	-1.97496200	6.35590800
H	5.27042700	-2.44202700	7.07394700
H	4.47861600	-0.91295300	6.60809300
H	3.61374000	-2.46465700	6.41288600
C	-6.04378200	2.70792500	5.27072600
H	-5.96205400	1.70934200	5.71913600
H	-6.23642300	3.43925300	6.05731600
H	-6.88153100	2.71320300	4.56124600

(B) Ar−X (p-iodoanisole)

Total energy: -357.584630669Hartree

Free energy: -357.497083 Hartree

C	-0.18260700	0.07515900	-0.00013700
C	0.41886700	1.33582000	-0.00008900
C	0.58935500	-1.08037600	-0.00027900
C	1.80579500	1.43077300	-0.00008500
H	-0.18262000	2.23777500	-0.00004100
C	1.98540400	-0.98484200	-0.00034000
H	0.12302900	-2.05917600	-0.00034800
C	2.59864300	0.27317400	-0.00018800
H	2.29779500	2.39784800	0.00002600

H	2.57249100	-1.89540000	-0.00047100
I	-2.33197600	-0.07730200	0.00007000
O	3.94552900	0.48009500	-0.00008700
C	4.80061900	-0.65296900	0.00045500
H	5.81881500	-0.26146700	0.00086600
H	4.65182900	-1.27177600	0.89465200
H	4.65272000	-1.27202100	-0.89373400

(C)The transition state for the oxidative addition by Pd**L**$_2$

imaginary mode 90.1 i cm^{-1}

Total energy: -7029.45030694 Hartree

Free energy: -7028.698173 Hartree

Pd	-0.07719100	-0.94559500	-0.58126600
As	2.05062800	0.30893800	0.03396700
C	2.25213100	1.01654200	1.85639700
C	3.48984400	1.20371300	2.47855800
C	1.09310500	1.36282800	2.57136100
C	3.58401600	1.71713000	3.77634900
H	4.40466600	0.93912700	1.95790700
C	1.16929500	1.88110200	3.85735100
H	0.11823000	1.22930600	2.11335400
C	2.41837900	2.05955400	4.47122700
H	4.56170400	1.84179000	4.22737100
H	0.27439500	2.15347600	4.40754400
C	2.23981300	1.95466700	-1.02382700
C	1.64496100	2.00805800	-2.29599300
C	2.92996200	3.08098400	-0.56863800
C	1.74357900	3.14736700	-3.08678600
H	1.09123500	1.14894500	-2.66589600
C	3.03454500	4.23605300	-1.34913500
H	3.39003200	3.07488900	0.41476700
C	2.44088400	4.27059400	-2.61738400
H	1.28631900	3.19230400	-4.07014100
H	3.57555000	5.09165400	-0.96148400
C	3.83372600	-0.48150200	-0.22058800
C	4.23447500	-1.55173300	0.60069000

C	4.69572800	-0.08228300	-1.24435100
C	5.45572400	-2.18497100	0.41277400
H	3.58251000	-1.89548600	1.39897500
C	5.92422500	-0.71862000	-1.45584300
H	4.41760000	0.73890400	-1.89725300
C	6.31045000	-1.77353400	-0.62265000
H	5.77056200	-3.00530800	1.05007300
As	-2.26257700	0.13995700	0.06803800
C	-3.74838900	0.22174000	-1.21014800
C	-4.71263500	1.23339200	-1.19516800
C	-3.85406500	-0.78300900	-2.18632100
C	-5.76659700	1.24804600	-2.11416300
H	-4.64904700	2.03385200	-0.46443300
C	-4.89742000	-0.78576500	-3.10275600
H	-3.09769900	-1.56004800	-2.24411200
C	-5.86386200	0.23121800	-3.07140600
H	-6.49408900	2.05042100	-2.07408600
H	-4.98024300	-1.55821700	-3.86052900
C	-3.10774100	-0.76769500	1.58654000
C	-2.27976700	-1.37951000	2.53364800
C	-4.49749700	-0.84408900	1.77236400
C	-2.80565200	-2.03619500	3.64942400
H	-1.20177300	-1.35692000	2.39535000
C	-5.03697700	-1.49933900	2.87311000
H	-5.16748000	-0.39348600	1.04664200
C	-4.19372300	-2.09612000	3.82269000
H	-2.13076900	-2.49605900	4.36182000
H	-6.11035600	-1.56460100	3.02078000
C	-2.24381800	1.99956100	0.70107700
C	-1.48384800	2.93154600	-0.01399600
C	-2.93424500	2.44006000	1.84132500
C	-1.41278100	4.27019900	0.37721700
H	-0.92122500	2.61571200	-0.88831400
C	-2.86807600	3.76855700	2.24777700
H	-3.52527400	1.73988500	2.42341800
C	-2.10861800	4.69362300	1.51643900

H	-0.80756200	4.95808900	-0.20115600
H	-3.39667300	4.11510500	3.13028000
C	0.42585300	-2.93456500	-1.14032000
C	-0.66765100	-3.63047300	-0.60017600
C	1.73569100	-3.40567500	-0.91514400
C	-0.45156400	-4.70423500	0.28020800
H	-1.68127300	-3.36600100	-0.87537100
C	1.94073500	-4.47350000	-0.05720400
H	2.57980200	-2.91778900	-1.38651700
C	0.85071500	-5.12384300	0.55462300
H	-1.30993600	-5.21110300	0.70494600
H	2.94427100	-4.82655000	0.15811700
O	-2.10817800	5.97113900	1.99591400
O	-4.81998400	-2.71119200	4.86729300
O	-6.84643200	0.14448400	-4.01368100
O	1.17716100	-6.16834000	1.37403700
O	2.39025600	2.56619300	5.73818400
O	2.47949200	5.34158100	-3.46267600
C	-7.84384400	1.15254000	-4.03952700
H	-7.41340300	2.14455300	-4.22805900
H	-8.51515200	0.89164400	-4.85923600
H	-8.41475500	1.18304300	-3.10236100
C	-4.01841400	-3.32763300	5.86222200
H	-3.36115300	-2.60323500	6.36021200
H	-4.71279200	-3.74395700	6.59376400
H	-3.40584800	-4.13766600	5.44550100
C	-1.34415500	6.94637800	1.30499700
H	-1.69288700	7.07864100	0.27258100
H	-1.48200000	7.88041300	1.85217000
H	-0.27701200	6.68991400	1.29145000
C	3.62345100	2.76159000	6.41069700
H	3.37121500	3.16506300	7.39269700
H	4.17044000	1.81841300	6.53830400
H	4.26583900	3.47758100	5.88161600
C	3.18629600	6.49932900	-3.04947800
H	3.09843000	7.21507700	-3.86841600

H	2.75345400	6.93762900	-2.14056300
H	4.24787700	6.28494300	-2.87048000
C	0.12256700	-6.88254200	1.99488600
H	-0.53722200	-7.35634100	1.25616500
H	0.59615900	-7.65701500	2.60070300
H	-0.47977700	-6.23370900	2.64470900
I	0.03095400	-1.97531200	-3.30309900
H	6.56320400	-0.38017400	-2.26314800
O	7.48384600	-2.46173100	-0.73031300
C	8.37590700	-2.10646000	-1.77459800
H	7.91601500	-2.23744800	-2.76251200
H	8.72310300	-1.06958100	-1.67675300
H	9.22971600	-2.77986300	-1.68420900

(D) Ar−Pd$\mathbf{L}_2$−I

Total energy: -7029.48545279 Hartree

Free energy: -7028.729828 Hartree

Pd	0.42468900	-1.33976000	0.05164600
As	-2.02208400	-0.52140200	-0.20777000
C	-2.61422900	0.82682300	1.08227300
C	-3.46420500	1.88652000	0.75795000
C	-2.15511800	0.72009600	2.40705300
C	-3.85399000	2.82545100	1.71860400
H	-3.82732400	1.99915700	-0.25870000
C	-2.53590900	1.64262000	3.37335900
H	-1.48940200	-0.09233500	2.68415500
C	-3.38995500	2.70377500	3.03472200
H	-4.51609200	3.63444000	1.43208800
H	-2.18240700	1.56503900	4.39628800
C	-3.47926200	-1.82054000	-0.08413800
C	-3.46465300	-2.93791500	-0.93660600
C	-4.54494600	-1.67418700	0.80293200
C	-4.49316300	-3.86708100	-0.91063100
H	-2.63453100	-3.09176100	-1.61898800
C	-5.58385600	-2.61116100	0.85040400
H	-4.58139300	-0.82537800	1.47756700

C	-5.56120400	-3.71155500	-0.01190200
H	-4.48551600	-4.73396100	-1.56308600
H	-6.39304500	-2.46877300	1.55695900
C	-2.47478200	0.27527900	-1.93963000
C	-1.46304500	0.79451600	-2.76259400
C	-3.79230500	0.31577500	-2.40936000
C	-1.75724700	1.34791500	-4.00198700
H	-0.43170300	0.76499300	-2.43048500
C	-4.10605900	0.86946000	-3.65310900
H	-4.59371400	-0.10394500	-1.80951600
C	-3.08362900	1.39033800	-4.45638800
H	-0.97633600	1.75239500	-4.63741300
As	1.66054400	0.81860100	0.01314700
C	1.89772400	1.34606400	1.87851500
C	2.29168600	2.63968800	2.23684500
C	1.65522500	0.41418300	2.90153000
C	2.46329400	3.00183900	3.57499000
H	2.45835600	3.38997300	1.47006100
C	1.81969900	0.76034300	4.23647000
H	1.31998000	-0.58779600	2.64729200
C	2.23018000	2.05687600	4.58306800
H	2.76909100	4.01311600	3.81583000
H	1.63261200	0.04413500	5.03001600
C	3.46434600	0.83567300	-0.73668200
C	3.67652700	0.25256000	-1.98909100
C	4.55175700	1.43875500	-0.08782800
C	4.93312700	0.27383300	-2.59826300
H	2.86128800	-0.25160000	-2.49830800
C	5.80897700	1.46125100	-0.67781000
H	4.42509000	1.88498900	0.89250800
C	6.00905500	0.88008000	-1.93904700
H	5.06106500	-0.19851000	-3.56467000
H	6.65664500	1.91936700	-0.17840400
C	0.95862300	2.49331800	-0.73975100
C	-0.13018100	3.12907400	-0.13430500
C	1.49387500	3.05894600	-1.90819200

C	-0.68170400	4.29488600	-0.66982200
H	-0.56212600	2.72530200	0.77516100
C	0.95188600	4.21574900	-2.45489700
H	2.34699100	2.59846500	-2.39526000
C	-0.14218500	4.84229000	-1.84020100
H	-1.52558500	4.75470200	-0.16960900
H	1.36465800	4.65910700	-3.35541800
C	2.25199400	-2.24621500	-0.08107800
C	3.23747800	-2.30845100	0.90330500
C	2.50562400	-2.88146100	-1.30840800
C	4.45800500	-2.96206400	0.67674700
H	3.07744900	-1.85869200	1.87806400
C	3.71309800	-3.53262300	-1.54849100
H	1.74832800	-2.88918400	-2.08859100
C	4.70114600	-3.57273400	-0.55578900
H	5.19625900	-2.98675800	1.47052100
H	3.90472300	-4.03013500	-2.49482300
O	-0.59829000	5.97200800	-2.45113900
O	7.27766700	0.95250400	-2.43026600
O	2.36398400	2.29911200	5.91571700
O	5.85738900	-4.23325200	-0.88895100
O	-3.70404000	3.55801500	4.04957500
O	-6.51998800	-4.68042900	-0.06018500
C	2.77701100	3.59260200	6.33030200
H	2.05985400	4.36436500	6.02285400
H	2.82216100	3.55862400	7.41972400
H	3.76915600	3.84624400	5.93578900
C	7.55031700	0.33971600	-3.68205500
H	6.96778900	0.79701400	-4.49218200
H	8.61279500	0.50090000	-3.87047400
H	7.34634300	-0.73795000	-3.65670900
C	-1.71636200	6.63773400	-1.88598800
H	-1.50516400	6.99353800	-0.86920400
H	-1.91437100	7.49496900	-2.53125600
H	-2.60272100	5.99090600	-1.86256400
C	-4.57906200	4.64001000	3.77389400

H	-4.69892200	5.17818500	4.71533200
H	-4.15896400	5.32023300	3.02143200
H	-5.56124300	4.29021400	3.43098100
C	-7.59457000	-4.60746000	0.86231500
H	-8.21895200	-5.48103700	0.66814200
H	-7.23964400	-4.64072700	1.90028900
H	-8.19331100	-3.69834300	0.71811100
C	6.86141200	-4.34709300	0.10166000
H	6.49987000	-4.88349100	0.98928400
H	7.67491900	-4.91647500	-0.35261100
H	7.24209700	-3.36475300	0.41369900
I	-0.38707700	-3.70791500	1.09886800
H	-5.13782000	0.87824100	-3.98459100
O	-3.27213400	1.94852700	-5.68536800
C	-4.58964400	1.99197300	-6.21096100
H	-5.25884100	2.59093500	-5.57975700
H	-4.50705400	2.46214400	-7.19201800
H	-5.01267100	0.98607800	-6.32731800

(E) L

Total energy: -3271.93908835 Hartree

Free energy: -3271.625358 Hartree

As	0.00015000	0.00032300	1.47566400
C	-0.44315100	-1.68246700	0.56325300
C	-1.19257000	-1.77145900	-0.62115600
C	-0.01352200	-2.87494500	1.15515500
C	-1.48619800	-3.00256300	-1.19587900
H	-1.55411200	-0.86689600	-1.10020500
C	-0.29328400	-4.12184600	0.58969300
H	0.55336000	-2.84128000	2.08261200
C	-1.03585400	-4.18763400	-0.59526600
H	-2.06526500	-3.07410400	-2.11125800
H	0.06172300	-5.02099500	1.07958900
C	1.67907700	0.45777800	0.56304500
C	2.49607700	1.42753600	1.15384800
C	2.13194000	-0.14848400	-0.62005300

C	3.71597300	1.80840400	0.58855700
H	2.18266000	1.90298300	2.08033900
C	3.34512400	0.21244100	-1.19456000
H	1.53011400	-0.91507100	-1.09815200
C	4.14534400	1.19640500	-0.59506000
H	4.31646500	2.56653900	1.07757800
H	3.69750200	-0.25467900	-2.10888000
C	-1.23575300	1.22543700	0.56330000
C	-2.48444600	1.44707400	1.15373000
C	-0.93719800	1.92142400	-0.61942800
C	-3.42461600	2.31266300	0.58838900
H	-2.73949600	0.93741900	2.07994100
C	-1.85675300	2.79115800	-1.19399500
H	0.02787200	1.78444200	-1.09724200
C	-3.10937900	2.99107900	-0.59492600
H	-4.38167900	2.45281300	1.07714300
H	-1.62842800	3.33035400	-2.10804700
O	5.31693900	1.47960800	-1.23536100
O	-3.94086500	3.86365000	-1.23530300
O	-1.37570000	-5.34384800	-1.23596700
C	-0.94742400	-6.57368600	-0.67393800
H	-1.31933600	-7.35506400	-1.33864400
H	0.14725800	-6.63655100	-0.62114700
H	-1.36282000	-6.72760800	0.33047100
C	-5.22116900	4.10522200	-0.67471900
H	-5.71176200	4.81858200	-1.33890400
H	-5.82197100	3.18784800	-0.62439000
H	-5.14873000	4.54027800	0.33054800
C	6.16723200	2.46642600	-0.67412200
H	7.03048800	2.53407800	-1.33813600
H	5.67417900	3.44591100	-0.62335400
H	6.50732800	2.18528400	0.33105300

(F) Ar−PdI−L

Total energy: -3757.51708224 Hartree

Free energy: -3757.101510 Hartree

Pd	1.60564800	-0.10368500	-0.10202300
As	-0.91365200	0.20336500	-0.00590100
C	-1.99260100	-0.85160900	-1.23570800
C	-3.31113900	-1.21790900	-0.95459000
C	-1.42420600	-1.26750400	-2.45125300
C	-4.06264800	-1.96971800	-1.86178100
H	-3.76635100	-0.92829700	-0.01221800
C	-2.15940600	-2.01110100	-3.36390900
H	-0.39001100	-1.02305400	-2.67628900
C	-3.48648000	-2.36687700	-3.07511500
H	-5.08090700	-2.24209600	-1.61047500
H	-1.72550300	-2.34235700	-4.30158100
C	-1.46896600	2.03549900	-0.39679800
C	-0.71949400	3.09238600	0.15075000
C	-2.55496800	2.34967200	-1.21661200
C	-1.05039000	4.41513000	-0.10651100
H	0.13671000	2.87852400	0.78656900
C	-2.89837300	3.67753200	-1.49025500
H	-3.14652800	1.55492000	-1.66021900
C	-2.14530900	4.71749900	-0.93260900
H	-0.47467900	5.23389700	0.31261800
H	-3.74491700	3.88382300	-2.13453400
C	-1.75903000	-0.13055800	1.71910100
C	-1.30694600	-1.21515300	2.49210500
C	-2.79126400	0.66547900	2.22108400
C	-1.88017300	-1.49485200	3.72468700
H	-0.49662900	-1.84099600	2.12780900
C	-3.37479400	0.39634200	3.46293300
H	-3.14878100	1.51656300	1.64938100
C	-2.91959200	-0.69042800	4.21926000
H	-1.53703600	-2.32873000	4.32835800
H	-4.17063700	1.03635100	3.82537100
C	3.57003500	0.02571200	-0.17431600
C	4.20429000	0.19404200	-1.41726300
C	4.28365200	0.26661600	1.00454900
C	5.49170000	0.71800700	-1.47423100

H	3.69255600	-0.07147100	-2.33770000
C	5.57926700	0.79477000	0.95191900
H	3.83705000	0.05318300	1.97138800
C	6.18290100	1.02600200	-0.29101800
H	5.99196400	0.88092600	-2.42378700
H	6.10573500	0.99931200	1.87701200
O	-2.38679100	6.04300500	-1.12998300
O	-4.12219700	-3.09997300	-4.03040200
O	-3.41153400	-1.04513700	5.43902200
C	-5.45510000	-3.52111600	-3.78330300
H	-5.75666600	-4.09466700	-4.66092200
H	-5.51856600	-4.16121900	-2.89428400
H	-6.13367500	-2.66715800	-3.66028800
C	-3.46903500	6.41403000	-1.97090100
H	-3.47304500	7.50469800	-1.99196400
H	-3.33671100	6.03350300	-2.99160000
H	-4.42899100	6.05733800	-1.57617700
C	-4.45633300	-0.26439900	5.99851700
H	-4.68915100	-0.71963500	6.96222700
H	-4.14430200	0.77584900	6.15684100
H	-5.35428500	-0.27730900	5.36741600
I	1.97313000	-2.72386000	0.00489200
O	7.44239200	1.52481100	-0.45899600
C	8.20976700	1.81721000	0.69738600
H	9.16750700	2.19523800	0.33612600
H	7.73077700	2.58519000	1.31878900
H	8.38273200	0.92085600	1.30682900

(G) Transition state for the isomerization

(TS connecting between Ar−PdI−L and Ar−PdL−I)

imaginary mode 62.6 i cm^{-1}

Total energy: -3757.51174141 Hartree

Free energy: -3757.097434Hartree

Pd	1.45487200	-0.83301100	0.05040700
As	-0.97890000	0.08855700	0.00896600
C	-2.30226600	-1.03192500	-0.88182400

C	-3.63849300	-1.08726100	-0.47821100
C	-1.89248200	-1.82781500	-1.96531300
C	-4.56002900	-1.90429200	-1.13930300
H	-3.97567500	-0.49687000	0.36832000
C	-2.79756000	-2.63975000	-2.63395100
H	-0.85197300	-1.82260600	-2.27901300
C	-4.14034000	-2.68313500	-2.22511300
H	-5.58831100	-1.92814700	-0.79830700
H	-2.48824400	-3.26145700	-3.46762200
C	-1.16147100	1.79921400	-0.91018000
C	-0.13698000	2.75158600	-0.76873200
C	-2.26041400	2.11695000	-1.71138600
C	-0.21636300	3.98450000	-1.40045000
H	0.73740300	2.52276900	-0.16459700
C	-2.35177700	3.35283700	-2.35884600
H	-3.05911400	1.39441400	-1.84807900
C	-1.32711700	4.29414900	-2.20226000
H	0.57169400	4.72325800	-1.29746600
H	-3.21566300	3.56452200	-2.97781400
C	-1.80103300	0.44196800	1.74096300
C	-1.53761200	-0.44306600	2.80116100
C	-2.63157900	1.53949800	1.97872200
C	-2.09775200	-0.24060400	4.05442000
H	-0.88103500	-1.29523500	2.64497500
C	-3.19851200	1.75958900	3.23768700
H	-2.83939400	2.24611000	1.18097400
C	-2.93365400	0.86495800	4.28182200
H	-1.89784600	-0.91816900	4.87804300
H	-3.83380200	2.62419100	3.38978300
C	3.29971300	-0.16522800	0.14300500
C	3.95824800	0.19942500	-1.03093600
C	3.82287600	0.19198000	1.39331200
C	5.08504500	1.03022000	-0.96733200
H	3.60214600	-0.14474800	-1.99640600
C	4.94287100	1.01677400	1.45470900
H	3.35861600	-0.15738600	2.30991500

C	5.57603800	1.44383100	0.27692100
H	5.57202700	1.32606000	-1.88925200
H	5.35601100	1.32819200	2.40896600
I	2.58494000	-3.19579000	0.01692500
O	6.67028900	2.24324100	0.45255500
C	7.38178700	2.66731800	-0.69801700
H	8.20906300	3.27848600	-0.33345600
H	7.78415500	1.81653500	-1.26314100
H	6.75343900	3.27325900	-1.36426300
O	-3.42841600	0.98010600	5.54494200
O	-1.30966900	5.52493800	-2.78409800
O	-4.94794400	-3.51344400	-2.94005500
C	-6.31072000	-3.62563500	-2.55791600
H	-6.75882700	-4.34019900	-3.24970400
H	-6.41314600	-4.00269300	-1.53253700
H	-6.83511900	-2.66508500	-2.64183400
C	-2.39528200	5.89113100	-3.62285400
H	-2.17279100	6.89754200	-3.98009500
H	-2.48807500	5.21506800	-4.48219400
H	-3.34482700	5.90543700	-3.07269000
C	-4.26530600	2.08710700	5.84468300
H	-4.53615000	1.98299300	6.89624900
H	-3.74200500	3.04064500	5.69923200
H	-5.17787200	2.08142600	5.23495200

(H) Ar−PdL−X

Total energy: -3757.52742306 Hartree

Free energy: -3757.109301 Hartree

Pd	0.12109800	-1.97363000	-0.18812500
As	-0.33070900	0.33809300	-0.00021100
C	-2.18834400	0.69916000	-0.45215200
C	-2.87129800	1.76083600	0.14856500
C	-2.85548700	-0.08692100	-1.40517800
C	-4.19433200	2.04844800	-0.19150200
H	-2.38024800	2.37322500	0.89854200
C	-4.16876400	0.19391700	-1.75579500

H	-2.35685300	-0.93979300	-1.85497300
C	-4.84846100	1.26323300	-1.15094000
H	-4.69988200	2.87315100	0.29649500
H	-4.69655100	-0.41353200	-2.48328600
C	0.64673100	1.64243600	-1.06325200
C	2.01674300	1.87396000	-0.83987700
C	0.00370300	2.35488000	-2.07877400
C	2.71040000	2.80031700	-1.60425000
H	2.54597100	1.32665000	-0.06734200
C	0.69564700	3.28178300	-2.86279900
H	-1.05186600	2.19482100	-2.27111700
C	2.05609000	3.50988800	-2.62527300
H	3.76573000	2.98828500	-1.43643500
H	0.16569900	3.81396600	-3.64363300
C	-0.15833300	0.97009700	1.82653300
C	-0.50204100	0.10006400	2.87646800
C	0.26364100	2.26527200	2.13476300
C	-0.42583400	0.51973400	4.19610900
H	-0.82579700	-0.91382700	2.65590800
C	0.34710700	2.69886100	3.46098400
H	0.54186700	2.95192700	1.34166400
C	0.00089600	1.82426000	4.49866600
H	-0.68656500	-0.14385400	5.01396300
H	0.68225700	3.70811100	3.66823500
C	2.04096200	-1.45355100	-0.06619900
C	2.80548600	-1.51968400	-1.23518200
C	2.69036300	-1.27659700	1.16570500
C	4.20425500	-1.47260400	-1.18115800
H	2.32333500	-1.62070200	-2.20381500
C	4.08181000	-1.22247700	1.22568500
H	2.11914600	-1.19142100	2.08539600
C	4.84666300	-1.32386300	0.05404400
H	4.77076400	-1.54655900	-2.10232800
H	4.59783100	-1.10325700	2.17348700
I	-1.73260600	-3.89751900	-0.37226400
O	6.20109700	-1.25518800	0.22277200

C	7.02598400	-1.38084100	-0.92374000
H	8.05442100	-1.31869900	-0.56423600
H	6.87756000	-2.34527900	-1.42653100
H	6.84768200	-0.57175600	-1.64443600
O	0.04624000	2.13655200	5.82062700
O	2.82747500	4.38853200	-3.31967500
O	-6.13185900	1.45219800	-1.55729900
C	-6.88810400	2.49343600	-0.95620400
H	-7.87577400	2.45100800	-1.41711300
H	-6.98782900	2.34622400	0.12641700
H	-6.44311800	3.47844500	-1.14672300
C	2.22944200	5.12459400	-4.37783600
H	3.02082400	5.75008400	-4.79279900
H	1.84338300	4.46175800	-5.16218900
H	1.41584300	5.76504300	-4.01460400
C	0.48210800	3.43554900	6.19661500
H	0.44386500	3.46065100	7.28632200
H	1.51070600	3.62710500	5.86632200
H	-0.17720600	4.21479700	5.79395500

(I) vinyl$SnBu_3$

Total energy: -554.945721001 Hartree

Free energy: -554.595839 Hartree

C	4.06393500	0.26585000	-1.23351700
C	2.84459900	0.36369100	-1.77524600
Sn	0.99766600	0.14197100	-0.66733100
H	4.97504400	0.38454000	-1.82087000
H	4.21955200	0.06236000	-0.17497600
H	2.78579400	0.57055000	-2.84589300
C	1.52033300	-0.31947200	1.41541000
H	2.40943900	-0.96225100	1.39501600
H	1.83163200	0.61475700	1.89901500
C	-0.15871900	-1.49509000	-1.56918300
H	0.30786300	-2.43766100	-1.25676100
H	-0.01415100	-1.43344600	-2.65528900
C	-0.12337300	2.02926800	-0.78872200

H	0.61226700	2.84183700	-0.74442100
H	-0.57902800	2.08654000	-1.78535400
C	-1.19571000	2.23230300	0.29406700
H	-1.93412000	1.41937300	0.25250000
H	-0.73734500	2.16913100	1.29109800
C	-1.66054200	-1.51350100	-1.24181900
H	-2.12270400	-0.56416500	-1.54730600
H	-1.80976300	-1.58245700	-0.15511800
C	0.41027700	-0.99437700	2.23820900
H	0.09529700	-1.92661500	1.74864600
H	-0.48267200	-0.35420300	2.26486000
C	-2.41625300	-2.66901400	-1.91712000
H	-2.27383900	-2.60271300	-3.00443900
H	-1.96289000	-3.62141200	-1.61017800
C	-1.93376100	3.57514300	0.17523600
H	-1.20040200	4.39180700	0.22070400
H	-2.39924300	3.64130600	-0.81764600
C	0.83084300	-1.31328900	3.68153400
H	1.72044700	-1.95757400	3.66105600
H	1.14161000	-0.38378100	4.17782400
C	-3.91417500	-2.68481100	-1.59455300
H	-4.40002400	-1.75808800	-1.92133200
H	-4.42294800	-3.51839600	-2.08996800
H	-4.08671700	-2.78415100	-0.51661400
C	-2.99932000	3.77955700	1.25733600
H	-3.50589700	4.74387400	1.14501500
H	-3.76435500	2.99569000	1.21379600
H	-2.55683700	3.75192100	2.25987100
C	-0.27462700	-1.98851200	4.50012900
H	-0.58168500	-2.93737200	4.04516200
H	0.05596900	-2.20241900	5.52192500
H	-1.16465100	-1.35198600	4.56568700

(J) Cation−π complex between Ar−PdL−X and vinylSnBu3

Total energy: -4312.49790913Hartree

Free energy: -4311.703396 Hartree

Pd	-0.15406200	-0.01887000	-0.91594600
As	2.06822600	-0.35673700	0.11953700
C	2.22176200	-1.68915100	1.53391100
C	3.40991100	-2.41289200	1.71860700
C	1.16083000	-1.90402500	2.41547300
C	3.52956400	-3.32467900	2.75860000
H	4.24582200	-2.27523400	1.04029200
C	1.27051200	-2.81082900	3.47217000
H	0.22235600	-1.37940300	2.27307800
C	2.45985800	-3.52948200	3.64457500
H	4.44014300	-3.89655800	2.90460800
H	0.42384100	-2.96009900	4.13126600
C	2.99358000	1.15463500	0.94670000
C	3.45670000	2.23589100	0.17538000
C	3.19013700	1.19495300	2.32994200
C	4.10421500	3.30892300	0.77056100
H	3.30757500	2.24552600	-0.89868200
C	3.82901400	2.27657400	2.94348900
H	2.85081500	0.37374100	2.95188100
C	4.29353900	3.33975500	2.16135100
H	4.46412200	4.14427400	0.17912600
H	3.96309600	2.27027900	4.01864700
C	3.33380600	-0.96777700	-1.22896500
C	2.88092800	-1.81351700	-2.24750400
C	4.69353500	-0.61771700	-1.19831400
C	3.75494600	-2.30523300	-3.21899000
H	1.83533200	-2.10632100	-2.28302500
C	5.57187400	-1.09905600	-2.16094400
H	5.07090400	0.04135100	-0.42340100
C	5.10895300	-1.94778800	-3.17859200
H	3.37035800	-2.96124000	-3.99075400
H	6.62383800	-0.83287600	-2.14665300
C	0.47753000	1.86159500	-1.37816400
C	0.23865900	2.97839500	-0.55969500
C	1.10464800	2.07555800	-2.60958400

C	0.60527000	4.25987700	-0.96336600
H	-0.23495800	2.85542200	0.41067500
C	1.48633300	3.36087600	-3.02767600
H	1.31764300	1.23761100	-3.26930400
C	1.23248500	4.46030500	-2.20154200
H	0.41972200	5.12265700	-0.33063500
H	1.97216300	3.48171800	-3.98950900
C	-2.30646800	0.80724500	-1.33252500
C	-1.86103800	0.16700300	-2.46422300
H	-2.12457000	1.88148500	-1.30456800
H	-1.38336500	0.72088400	-3.27184300
I	-0.86102300	-2.72527500	-0.63450900
O	1.55600900	5.75580600	-2.50307600
C	2.17675900	6.01459100	-3.74990900
H	2.33711100	7.09336700	-3.79088700
H	3.14539500	5.50420600	-3.83724100
H	1.53998100	5.71330600	-4.59235100
Sn	-3.80984500	0.11022200	0.11020200
C	-5.15390600	1.85144100	0.20524000
H	-4.55715800	2.72412200	0.50099600
H	-5.51077600	2.05918100	-0.81136600
C	-4.90453200	-1.61625100	-0.66568700
H	-5.57134200	-1.96287600	0.13428600
C	-2.97944100	-0.20134400	2.11155200
H	-3.82921500	-0.36828200	2.78613400
H	-2.40722900	-1.13454100	2.08579400
C	-6.34828200	1.68505600	1.15840000
H	-6.94565600	0.81017200	0.86351000
H	-5.99071800	1.47249500	2.17636100
C	-7.27000700	2.91410900	1.20874400
H	-6.68029600	3.79122800	1.50840300
H	-7.63673800	3.12777400	0.19554500
C	-8.45852400	2.74336600	2.16078300
H	-8.12105900	2.56144500	3.18780000
H	-9.09443300	3.63484500	2.17374700
H	-9.08453200	1.89345300	1.86514000

H	-2.11099600	-0.86785300	-2.67718900
C	-2.11159400	0.95522600	2.63110900
H	-1.23923200	1.08260900	1.97374200
H	-2.66839200	1.90229100	2.58139500
C	-1.62011600	0.75602800	4.07396500
H	-1.06441600	-0.18945200	4.13789600
H	-2.48967700	0.64172800	4.73552700
C	-0.73677400	1.90317600	4.57642400
H	-0.41447600	1.73835100	5.61019900
H	0.16373300	2.00949600	3.96015100
H	-1.27298400	2.85882700	4.54499800
H	-4.17341500	-2.41377300	-0.83139800
C	-5.71062300	-1.34108200	-1.94463700
H	-6.42706000	-0.52452300	-1.77499000
H	-5.04065400	-0.99051900	-2.74253000
C	-6.47680900	-2.57296900	-2.45236600
H	-7.15224100	-2.92599000	-1.66107700
H	-5.76353400	-3.38894600	-2.62896700
C	-7.27846700	-2.30310400	-3.73011700
H	-6.62353900	-1.98120900	-4.54811900
H	-7.81213400	-3.19855300	-4.06578900
H	-8.02187200	-1.51268700	-3.57334800
O	6.04714700	-2.36507300	-4.07184900
O	4.93532400	4.43812600	2.64684500
O	2.67660000	-4.44310400	4.63039000
C	5.14460300	4.53217100	4.04801000
H	5.66099300	5.47903900	4.21204200
H	4.19560500	4.53818400	4.59898700
H	5.77036700	3.71079200	4.41980400
C	5.64230200	-3.23590700	-5.11894000
H	4.89255700	-2.76616700	-5.76796400
H	6.54140500	-3.44368900	-5.70071800
H	5.23904100	-4.17806600	-4.72737100
C	1.61451000	-4.73066700	5.52835800
H	1.99580600	-5.49189300	6.21052800
H	1.32087200	-3.84433900	6.10526700

H	0.73619200	-5.12369400	5.00141700

(K) Transition state for the transmetalation

imaginary mode 40.9 i cm^{-1}

Total energy: -4312.46567440 Hartree

Free energy: -4311.671108 Hartree

Pd	0.09455300	0.77728800	-1.30732200
C	0.91212500	-1.63838300	1.50371800
C	0.72036500	-3.02048900	1.47193800
C	0.38112100	-0.91815300	2.58912200
C	0.01899300	-3.68157000	2.48613200
H	1.11224000	-3.60277100	0.64466900
C	-0.30950400	-1.56021100	3.60846200
H	0.51644700	0.15907100	2.64427900
C	-0.50302900	-2.95026500	3.55845600
H	-0.11548200	-4.75488400	2.42260200
H	-0.71383300	-1.00927500	4.45160500
C	3.30027500	0.14022800	0.96662900
C	4.06628100	1.11234100	0.29982500
C	3.70793800	-0.26717400	2.23913000
C	5.20184500	1.65090400	0.88763400
H	3.76413200	1.46554000	-0.68044200
C	4.84707400	0.27183900	2.84624000
H	3.13693200	-1.01284500	2.78262300
C	5.60141200	1.23463100	2.16706900
H	5.79129300	2.40720500	0.38001200
H	5.13031900	-0.06665000	3.83605200
C	2.66448800	-2.03844400	-0.98709600
C	2.36579000	-2.20514100	-2.34879800
C	3.65196700	-2.85002500	-0.41939000
C	3.02566600	-3.15954400	-3.11382600
H	1.61057500	-1.58084400	-2.81499400
C	4.31899900	-3.81802400	-1.17241200
H	3.92356200	-2.72652300	0.62483700
C	4.00476600	-3.97604400	-2.52920800
H	2.80063900	-3.29037800	-4.16724800

H	5.07876700	-4.42909700	-0.69944800
C	1.15962800	2.48147500	-1.02280900
C	1.21781000	3.13234600	0.22175000
C	1.89593800	3.04111900	-2.07508600
C	1.98111900	4.28403100	0.40821300
H	0.66895100	2.73881600	1.07238500
C	2.68190100	4.19005400	-1.90019400
H	1.86212000	2.58785200	-3.06139700
C	2.72230100	4.81976200	-0.65234000
H	2.02359500	4.77982200	1.37369200
H	3.23840700	4.58242200	-2.74436400
C	-1.50292200	1.69357700	-3.69408900
C	-1.07171200	1.99529500	-2.45999700
Sn	-2.98792600	0.49106100	-0.14955000
C	-4.58956400	0.89798500	-1.58392200
H	-4.10240600	1.27593000	-2.48654000
H	-5.17626300	1.72510800	-1.16267100
C	-2.34216200	2.29156900	0.93551200
H	-1.66799300	2.85902100	0.29311000
H	-1.76015600	1.94892200	1.79846300
C	-3.52366300	-1.06489400	1.30731800
H	-4.09484100	-1.82141500	0.75736500
H	-2.59184500	-1.54317900	1.62380100
H	-1.25997600	3.00946500	-2.10217700
H	-2.02360400	2.42919000	-4.31118300
H	-1.35775900	0.71554600	-4.14669100
O	-1.21381100	-3.48479500	4.59312000
O	4.59368500	-4.88220100	-3.35866500
O	6.72752600	1.82635800	2.65794600
C	7.17029400	1.45792400	3.95413500
H	8.06730800	2.04880700	4.14579400
H	6.41773000	1.68644800	4.71981300
H	7.42337500	0.39107200	4.00870300
C	5.60028300	-5.72980500	-2.82732700
H	5.92741600	-6.36279600	-3.65351600
H	6.45692600	-5.15556000	-2.45191200

H	5.21174400	-6.36359800	-2.01980400
C	-1.44681700	-4.88617300	4.59550200
H	-0.50674400	-5.45110800	4.63241100
H	-2.02565700	-5.09297700	5.49669900
H	-2.02165200	-5.20151100	3.71588600
C	-4.31014300	-0.56167500	2.52732100
H	-3.73220100	0.20883400	3.05670100
H	-5.24397900	-0.07489100	2.20973300
C	-4.65622000	-1.68383800	3.52164500
H	-3.72759600	-2.16289900	3.85809900
H	-5.23011400	-2.45985400	2.99719200
C	-5.45035200	-1.18881600	4.73515900
H	-5.68122700	-2.00842300	5.42373000
H	-4.88768400	-0.43380800	5.29639100
H	-6.40008400	-0.73355400	4.43102600
C	-5.49164400	-0.30137100	-1.90017500
H	-4.88477400	-1.12717900	-2.29410400
H	-5.96261900	-0.67890200	-0.98142300
C	-6.59378100	0.03400500	-2.91842600
H	-6.12626900	0.40384900	-3.84056400
H	-7.20338800	0.86246200	-2.53227900
C	-7.49625300	-1.16122200	-3.24229100
H	-8.26891900	-0.89360700	-3.97063700
H	-6.91714200	-1.99178400	-3.66166400
H	-8.00168400	-1.53236000	-2.34307600
C	-3.53448100	3.15145500	1.38746800
H	-4.23086400	2.56186800	2.00063100
H	-4.10804600	3.48780800	0.51276500
C	-3.09701700	4.38722000	2.19337200
H	-2.53036400	4.05706300	3.07436000
H	-2.40013400	4.97949700	1.58641900
C	-4.27312500	5.26414000	2.63574700
H	-4.97030800	4.70436300	3.26995400
H	-3.92948300	6.13302700	3.20649400
H	-4.83715800	5.63593600	1.77270900
As	1.76027100	-0.64633200	0.04616800

I	-1.49985100	-1.56783000	-1.80739600
O	3.44497500	5.95068600	-0.36788100
C	4.19851100	6.53552500	-1.41324200
H	4.68660500	7.41235200	-0.98326300
H	4.96665400	5.85025500	-1.79718600
H	3.56053000	6.85344000	-2.24903100

(L) Complex between vinyl−PdAr−L and Bu_3SnI

Total energy: -4312.47181564 Hartree

Free energy: -4311.684294 Hartree

Pd	-0.30656900	1.06415700	0.41278100
As	-2.21222000	-0.59899000	-0.01366700
C	-1.69666300	-2.31589300	-0.80303400
C	-2.02726200	-3.55002700	-0.24180900
C	-0.92879500	-2.30449300	-1.98087000
C	-1.61189100	-4.75084400	-0.82785700
H	-2.61438200	-3.59142500	0.66998000
C	-0.51993100	-3.48658400	-2.58223500
H	-0.64410200	-1.35745900	-2.43224000
C	-0.85663900	-4.72188500	-2.00519200
H	-1.88292600	-5.68997400	-0.35991400
H	0.06805400	-3.48326800	-3.49449200
C	-3.76358400	-0.14158700	-1.11964300
C	-4.41739400	1.08811900	-0.92031800
C	-4.25954200	-1.00497300	-2.09973800
C	-5.52824900	1.43384500	-1.67696300
H	-4.05215000	1.78680000	-0.17580400
C	-5.37512500	-0.66586700	-2.87270000
H	-3.77754400	-1.96038900	-2.27783000
C	-6.01539400	0.55968100	-2.66083800
H	-6.03010700	2.38474900	-1.53134700
H	-5.72850600	-1.36083500	-3.62551400
C	-3.08835000	-1.14162000	1.64713700
C	-2.39044900	-1.01529200	2.86035300
C	-4.39249900	-1.64341800	1.68082700
C	-2.97394600	-1.38999300	4.06399600

H	-1.38329400	-0.60781600	2.86161200
C	-4.99419000	-2.02323400	2.88356100
H	-4.96147500	-1.73395300	0.76043800
C	-4.28173100	-1.89857600	4.08311000
H	-2.44097100	-1.29156800	5.00415300
H	-6.00870200	-2.40419100	2.87267700
C	-1.46530400	2.68174000	0.07659500
C	-1.58440800	3.23816300	-1.20924100
C	-2.19890800	3.27797900	1.10899600
C	-2.42375600	4.32319500	-1.45712200
H	-1.02259800	2.81790700	-2.03940900
C	-3.05130700	4.36829400	0.87510800
H	-2.11515200	2.89949100	2.12385000
C	-3.16636100	4.89415600	-0.41560500
H	-2.51946100	4.74406700	-2.45388400
H	-3.60246700	4.79570600	1.70572300
C	1.72360400	2.69401400	1.95391800
C	1.07959300	2.49851700	0.79284200
Sn	4.01411600	-0.08401200	0.06382500
C	4.99727700	-1.93316800	-0.57775800
H	5.21164600	-2.52222200	0.32125400
H	4.25729500	-2.50058900	-1.15338700
C	4.97295300	0.84823500	1.79065700
H	4.34423000	1.69962300	2.06628900
H	4.90786900	0.12440400	2.61092200
C	3.45567000	1.19809800	-1.61557000
H	3.67932300	0.63622300	-2.53044300
H	2.36869600	1.31121800	-1.55718700
H	1.28835500	3.20765500	-0.01328300
H	2.43428700	3.51362100	2.08871900
H	1.55953300	2.06880200	2.83004400
C	4.14056400	2.57329600	-1.63349600
H	3.91880600	3.10701700	-0.70062400
H	5.23355000	2.45903200	-1.67314300
C	6.27574400	-1.72191500	-1.40622700
H	6.05560000	-1.10895300	-2.29179200

H	7.01770000	-1.15663300	-0.82462600
C	6.43082800	1.28036000	1.56202700
H	6.48886600	1.99746300	0.73153800
H	7.04323200	0.41779200	1.26329800
C	7.05938000	1.92125200	2.81057000
H	6.45306400	2.78583000	3.11093500
H	7.00599700	1.20764600	3.64358300
C	3.69237400	3.44059400	-2.82095800
H	2.60287500	3.56792300	-2.77547100
H	3.89999200	2.90503100	-3.75740000
C	6.91449200	-3.04209200	-1.86786700
H	6.17829700	-3.60846800	-2.45367400
H	7.14005800	-3.65719100	-0.98650400
C	8.18775300	-2.83949900	-2.69566200
H	8.61672700	-3.79687800	-3.00875200
H	7.98442600	-2.25517100	-3.60039200
H	8.95349000	-2.30435100	-2.12237200
C	8.51232800	2.35794600	2.59689500
H	8.59043400	3.09698800	1.79128900
H	8.93010000	2.80943900	3.50253400
H	9.14776000	1.50654000	2.32692000
C	4.37024400	4.81432900	-2.85116700
H	4.02904500	5.40832300	-3.70516400
H	4.14976400	5.38414000	-1.94149500
H	5.45980700	4.71895800	-2.92670800
O	-0.40341100	-5.82581300	-2.66548500
O	-7.10861200	0.99417800	-3.35168300
O	-4.76811800	-2.23470500	5.31130400
C	-0.69173700	-7.10207600	-2.11661200
H	-0.23339500	-7.82966000	-2.78824100
H	-0.26333200	-7.21717500	-1.11274300
H	-1.77250700	-7.28803300	-2.06788600
C	-7.63273600	0.16084800	-4.37243700
H	-8.48372000	0.69841500	-4.79378400
H	-6.89514000	-0.02372200	-5.16414300
H	-7.97709200	-0.80246900	-3.97388400

C	-6.09214000	-2.73766100	5.39736800
H	-6.27207600	-2.93227000	6.45574800
H	-6.82724900	-2.00781400	5.03474000
H	-6.20827400	-3.67277900	4.83436200
I	1.54315800	-1.15305100	1.06490200
O	-3.96609000	5.95601100	-0.76103600
C	-4.71218700	6.58268100	0.26431200
H	-5.42614700	5.89135400	0.73323100
H	-4.06325700	7.00107700	1.04581000
H	-5.26467400	7.39459700	-0.21298700

(M) vinyl−PdAr−L

Total energy: -3824.03586941 Hartree

Free energy: -3823.579884 Hartree

Pd	0.86877300	-2.07567900	-1.02311800
As	-0.62300300	-0.21610900	-0.15695600
C	-2.49241200	-0.44644600	-0.67787300
C	-3.56287700	-0.24556300	0.19647900
C	-2.77295300	-0.86042600	-1.99269600
C	-4.88426700	-0.44501600	-0.21545400
H	-3.37564100	0.06482200	1.21979200
C	-4.07911400	-1.05774400	-2.41806300
H	-1.95838700	-1.03218800	-2.69239700
C	-5.14668200	-0.85163500	-1.52918900
H	-5.68992700	-0.28357400	0.49108100
H	-4.30131100	-1.37845600	-3.43062100
C	-0.25866000	1.61707300	-0.71437700
C	1.07811600	2.03478900	-0.84292700
C	-1.27574400	2.53244900	-0.99621400
C	1.38067700	3.33247100	-1.23198800
H	1.88680100	1.33719500	-0.64777600
C	-0.98399400	3.84087500	-1.39308400
H	-2.31567800	2.23050000	-0.91743800
C	0.35123300	4.24564900	-1.51004000
H	2.40914300	3.66264500	-1.33553100
H	-1.79715800	4.52394700	-1.60882700

C	-0.74274600	-0.06007800	1.78397300
C	-0.62107800	-1.22607500	2.55959400
C	-0.92904500	1.15868300	2.44028800
C	-0.69644000	-1.17479100	3.94460400
H	-0.45386400	-2.18331400	2.07190800
C	-1.00207700	1.22771300	3.83473300
H	-1.00990900	2.07675100	1.86634000
C	-0.88779000	0.05603300	4.59300200
H	-0.60004800	-2.07048200	4.54960000
H	-1.14141300	2.19075000	4.31164300
C	2.69084300	-1.38198300	-0.56357200
C	3.58896500	-0.97526800	-1.55384800
C	3.05850200	-1.20928600	0.78208100
C	4.81013900	-0.36766500	-1.22461300
H	3.34968500	-1.11918900	-2.60332900
C	4.27399100	-0.61704800	1.11899300
H	2.39464900	-1.52785100	1.57978500
C	5.15643100	-0.18838600	0.11773100
H	5.47473100	-0.05437600	-2.02212500
H	4.56062200	-0.47996600	2.15744800
C	1.41185300	-4.90592100	-1.44594900
C	1.80202500	-3.66693200	-1.78048000
H	2.55656600	-3.54127200	-2.56057900
H	1.77665800	-5.79058200	-1.97252900
H	0.70887300	-5.10186400	-0.63717900
O	-6.38983200	-1.07630800	-2.03801300
O	0.75255900	5.49164100	-1.88848300
O	-0.94222100	0.00436900	5.95278600
C	-7.51029400	-0.90333200	-1.18354900
H	-8.38783800	-1.13970900	-1.78696800
H	-7.47073900	-1.58224600	-0.32230200
H	-7.58858400	0.13024900	-0.82267900
C	-0.24198600	6.45568000	-2.19751400
H	0.29503700	7.36380500	-2.47534300
H	-0.86881500	6.13533200	-3.03952000
H	-0.88414600	6.66711500	-1.33277500

C	-1.10768800	1.21920400	6.66854100
H	-1.11435400	0.94712300	7.72495800
H	-0.28066800	1.91538100	6.48007700
H	-2.05590000	1.71148100	6.41705100
O	6.32208300	0.38601300	0.55541200
C	7.25717600	0.81275400	-0.41766600
H	6.84071100	1.59124700	-1.07150100
H	8.10341900	1.22637900	0.13420700
H	7.60770200	-0.02119600	-1.04061300

(N) Bu_3SnI

Total energy: -488.427131111 Hartree

Free energy: -488.118854 Hartree

Sn	0.35401000	0.00096000	0.00022000
C	-0.19604700	-0.73102600	1.98775000
H	0.06994100	-1.79335400	2.02354000
H	0.45942500	-0.22148400	2.70221500
C	-0.19131600	-1.35420200	-1.62930400
H	0.07241000	-0.85165800	-2.56658300
H	0.46815900	-2.22482400	-1.54644900
C	-0.18880200	2.09025300	-0.35984500
H	0.07763900	2.65112400	0.54294800
H	0.46955300	2.45203700	-1.15698900
C	-1.66365300	2.32089200	-0.72968800
H	-1.92112800	1.74577000	-1.63003800
H	-2.32064100	1.94525300	0.06728200
C	-1.67250100	-0.52542400	2.36583000
H	-1.92847300	0.54226900	2.31879000
H	-2.32651600	-1.02550200	1.63777600
C	-1.66572000	-1.79145600	-1.64110100
H	-2.32390800	-0.91416800	-1.71199900
H	-1.92040800	-2.28475800	-0.69268400
C	-1.99303400	-2.74867000	-2.79886100
H	-1.74343700	-2.25852700	-3.74934000
H	-1.33992700	-3.62872400	-2.72983200
C	-1.98911000	3.80241500	-0.98048200

H	-1.33701200	4.18084000	-1.77884300
H	-1.73667500	4.38090500	-0.08182900
C	-2.00567100	-1.05159000	3.77151500
H	-1.35682200	-0.55162700	4.50284700
H	-1.75465200	-2.11947800	3.82222800
C	-3.47385200	-0.84745500	4.15906900
H	-3.67826200	-1.23214900	5.16338800
H	-3.74311500	0.21495300	4.14948600
H	-4.14422900	-1.36435400	3.46279900
C	-3.45902500	-3.19363600	-2.81688000
H	-4.13355700	-2.33566400	-2.91824000
H	-3.65915400	-3.87311100	-3.65156200
H	-3.72674500	-3.71670600	-1.89165700
C	-3.45545400	4.04267900	-1.35406100
H	-3.65408200	5.10546400	-1.52572900
H	-3.72596800	3.50259500	-2.26863900
H	-4.12897700	3.70338300	-0.55868400
I	3.18889000	-0.00289100	0.00398400

(O) Transition state for the reductive elimination

imaginary mode 263.0 i cm^{-1}

Total energy: -3824.03010905 Hartree

Free energy: -3823.573200 Hartree

Pd	1.13308100	-1.42426300	-1.36773200
As	-0.68873000	-0.18387900	-0.20762900
C	-2.43890100	-0.23013900	-1.07750200
C	-3.64156400	-0.33191200	-0.37484300
C	-2.48870900	-0.17382100	-2.48154400
C	-4.87081900	-0.37165600	-1.04077500
H	-3.63273400	-0.39095000	0.70923400
C	-3.70064200	-0.20673500	-3.15683700
H	-1.56537900	-0.11067400	-3.05219700
C	-4.90324500	-0.30643200	-2.43872300
H	-5.78420800	-0.45617900	-0.46371500
H	-3.74527000	-0.16605700	-4.24033100
C	-0.39636200	1.73137600	0.02885200

C	0.91840500	2.19060500	0.21964000
C	-1.43441300	2.66595600	0.01062400
C	1.17999700	3.54186700	0.40077900
H	1.74391000	1.48434100	0.21056200
C	-1.18485500	4.03043500	0.18673200
H	-2.45690400	2.33893900	-0.15300000
C	0.12875600	4.47222200	0.38617300
H	2.19216900	3.90498100	0.54664200
H	-2.01267600	4.72936900	0.16151900
C	-1.11210200	-0.77753700	1.60368500
C	-1.02647900	-2.15007800	1.89396400
C	-1.48405200	0.09608300	2.62785000
C	-1.31748000	-2.63251700	3.16231400
H	-0.71709300	-2.84580100	1.11803400
C	-1.77401000	-0.37339600	3.91281400
H	-1.54242200	1.16317900	2.43635000
C	-1.69383400	-1.74467500	4.18300800
H	-1.25138000	-3.69069500	3.39370600
H	-2.05310100	0.33336000	4.68545700
C	3.12809400	-1.15852300	-0.98709800
C	3.83220700	-0.12513300	-1.61712100
C	3.67703700	-1.71139100	0.18661000
C	5.02110600	0.38579200	-1.07752900
H	3.45818500	0.30108200	-2.54360300
C	4.85503800	-1.21267100	0.72983200
H	3.18037900	-2.54096500	0.68050200
C	5.53555900	-0.15705600	0.10302500
H	5.52902100	1.19438000	-1.59119100
H	5.27488200	-1.63182600	1.63935600
C	2.52104400	-3.85690700	-2.28974400
C	2.40645700	-2.53107600	-2.46719700
H	2.70591200	-2.08889500	-3.41913200
H	2.84223300	-4.51294300	-3.09911900
H	2.31430600	-4.33870300	-1.33735400
O	0.48912100	5.77432100	0.56692900
O	-1.95242900	-2.31288500	5.39422800

O	-6.03909000	-0.33772500	-3.19076000
C	-7.28607000	-0.45835500	-2.52376100
H	-7.47157500	0.39163300	-1.85448900
H	-8.04603800	-0.47056300	-3.30640400
H	-7.34774400	-1.38950200	-1.94620600
C	-0.52741100	6.76414100	0.54623300
H	-0.02212700	7.71814600	0.70410500
H	-1.05005800	6.78813600	-0.41858500
H	-1.26145400	6.60838700	1.34737100
C	-2.31456000	-1.46482800	6.47312300
H	-2.46521500	-2.11929800	7.33290500
H	-1.52131500	-0.74243900	6.70394600
H	-3.24551700	-0.92123400	6.26651900
O	6.68743000	0.25685700	0.71855000
C	7.42258700	1.30572600	0.11555700
H	8.29148600	1.47460000	0.75438400
H	7.76474700	1.03682100	-0.89288800
H	6.83636400	2.23272800	0.05461400

(P) p-methoxystyrene (2)

Total energy: -424.178044808 Hartree

Free energy: -424.046626 Hartree

C	-1.44930600	-0.23902600	-0.00022700
C	-0.50812900	-1.27762700	-0.00011300
C	-0.95348900	1.08183000	-0.00034900
C	0.86723200	-1.03537400	0.00001500
H	-0.85773000	-2.30727000	-0.00007900
C	0.40658100	1.34138400	-0.00024300
H	-1.64542000	1.91848400	-0.00066000
C	1.33215000	0.28345500	-0.00004600
H	1.55542800	-1.87234000	0.00016300
H	0.78624400	2.35807600	-0.00040200
C	-3.91811200	0.28386400	0.00062300
C	-2.88224100	-0.56541500	-0.00023800
H	-3.09961900	-1.63364700	-0.00099100
H	-4.93899800	-0.08349500	0.00048300

H	-3.79573600	1.36310200	0.00153600
O	2.64677300	0.64769400	0.00017100
C	3.62649800	-0.37809400	0.00021600
H	4.59334100	0.12756500	0.00057700
H	3.55033800	-1.01117100	0.89377700
H	3.55086900	-1.01084200	-0.89359200

(Q) PdL

Total energy: -3399.88481954 Hartree

Free energy: -3399.574284 Hartree

Pd	0.00041900	-0.00192000	3.25277700
As	0.00014500	-0.00094900	0.91661200
C	-0.08861400	1.75263400	0.05127300
C	0.58566200	2.05286800	-1.13437700
C	-0.85974800	2.76047100	0.65441000
C	0.49639000	3.32011000	-1.72014800
H	1.20084500	1.29840400	-1.61520900
C	-0.96408300	4.02064600	0.08258200
H	-1.37196400	2.55281700	1.59046800
C	-0.28426900	4.30960400	-1.11160100
H	1.03810900	3.52006900	-2.63726500
H	-1.55649700	4.80400300	0.54438400
C	-1.47423600	-0.95358600	0.05045900
C	-1.96627200	-2.12226100	0.65562500
C	-2.06727700	-0.52139300	-1.13786600
C	-3.00629900	-2.84119400	0.08339000
H	-1.53351700	-2.46074600	1.59361500
C	-3.12081300	-1.23080800	-1.72413700
H	-1.71759700	0.38624300	-1.62035000
C	-3.59237400	-2.39849000	-1.11335700
H	-3.39226100	-3.74348500	0.54681700
H	-3.56162700	-0.86290100	-2.64331100
C	1.56302500	-0.80016300	0.05045700
C	2.82214500	-0.63243200	0.65108100
C	1.48532800	-1.53745100	-1.13314500
C	3.96571100	-1.17143800	0.07868800

H	2.89904200	-0.08263100	1.58569400
C	2.62750000	-2.09308000	-1.71943300
H	0.52389700	-1.69623500	-1.61199300
C	3.87545100	-1.90775000	-1.11355100
H	4.94087100	-1.04702200	0.53851900
H	2.52935100	-2.66469600	-2.63495100
O	-0.44294700	5.57650400	-1.59030400
O	5.05211100	-2.40251000	-1.59317700
O	-4.61148700	-3.16753700	-1.59221000
C	0.23582700	5.93471000	-2.78361000
H	-0.02383000	6.97668300	-2.97686700
H	1.32432900	5.84885500	-2.67201200
H	-0.08629400	5.31958200	-3.63385100
C	-5.25719900	-2.76010400	-2.78807300
H	-6.03132800	-3.50434900	-2.98120700
H	-5.72464700	-1.77293600	-2.68010300
H	-4.56138400	-2.73559800	-3.63677200
C	5.02247600	-3.17141700	-2.78521800
H	6.05500300	-3.46541300	-2.97997600
H	4.40621500	-4.07245500	-2.67108300
H	4.64781300	-2.58708600	-3.63565200

(3) Optimized geometries in Figure S22, obtained from dispersion corrected B3LYP (B3LYP-GD3) calculations

***L* = P(PhOMe)$_3$**

(A) PdL_2

Total energy: -2887.87196958 Hartree

Free energy: -2887.222729 Hartree

Pd	0.00000100	-0.00004200	0.00000600
P	2.29925100	0.00040400	0.00074700
C	3.08392500	1.61459300	0.41710800
C	4.29053900	1.73653500	1.11418200
C	2.43565200	2.79151900	-0.00401600
C	4.85164500	2.98872500	1.38376000
H	4.80581300	0.84668800	1.46288200
C	2.98549900	4.03987800	0.24791800

H	1.48420300	2.71529500	-0.52457000
C	4.19911200	4.14727900	0.94580200
H	5.78417200	3.04441100	1.93279500
H	2.49079200	4.95130700	-0.07175600
C	3.08596800	-0.44534900	-1.60460600
C	2.44399000	-1.40564200	-2.40990500
C	4.28824100	0.10466400	-2.06134000
C	2.99573700	-1.81120700	-3.61622800
H	1.49597800	-1.82459600	-2.08166900
C	4.85101700	-0.28731200	-3.28005700
H	4.79880100	0.85674200	-1.46751500
C	4.20481000	-1.25283200	-4.06103500
H	2.50585900	-2.54927300	-4.24305200
H	5.78000700	0.16615200	-3.60487400
C	3.08684500	-1.16667200	1.18910400
C	2.43969000	-1.39413100	2.41877200
C	4.29530100	-1.82744800	0.94471500
C	2.99229600	-2.23647600	3.37235200
H	1.48709000	-0.90805200	2.61433000
C	4.85920600	-2.68695400	1.89271800
H	4.80970800	-1.68117800	-0.00024700
C	4.20762300	-2.89079600	3.11491600
H	2.49848000	-2.41822900	4.32142800
H	5.79310000	-3.18720900	1.66526900
P	-2.29925000	-0.00040500	-0.00075500
C	-3.08682700	1.16671100	-1.18908300
C	-4.29526000	1.82752200	-0.94467900
C	-2.43967400	1.39416100	-2.41875600
C	-4.85914600	2.68705300	-1.89267100
H	-4.80966600	1.68125900	0.00028500
C	-2.99226200	2.23652900	-3.37232500
H	-1.48709100	0.90805300	-2.61432600
C	-4.20756700	2.89088500	-3.11487300
H	-5.79302200	3.18733600	-1.66521000
H	-2.49844800	2.41827400	-4.32140300
C	-3.08396700	-1.61456600	-0.41714300

C	-4.29053100	-1.73647300	-1.11430700
C	-2.43577300	-2.79151000	0.00405400
C	-4.85166500	-2.98864700	-1.38390500
H	-4.80574600	-0.84661200	-1.46305900
C	-2.98565000	-4.03985200	-0.24789800
H	-1.48436100	-2.71531600	0.52468000
C	-4.19921300	-4.14721800	-0.94587500
H	-5.78415300	-3.04430500	-1.93301000
H	-2.49100400	-4.95129400	0.07183300
C	-3.08594200	0.44530500	1.60462200
C	-4.28829000	-0.10461600	2.06127300
C	-2.44388000	1.40545300	2.41002400
C	-4.85105800	0.28731200	3.28000800
H	-4.79891200	-0.85658900	1.46736800
C	-2.99561700	1.81097000	3.61636900
H	-1.49581300	1.82433100	2.08185000
C	-4.20476400	1.25269100	4.06109100
H	-5.78010700	-0.16607700	3.60476000
H	-2.50567500	2.54892500	4.24327300
O	4.65027000	5.41838300	1.15082400
O	4.65808900	-1.71090200	-5.26354800
O	4.66138800	-3.70431800	4.11169800
O	-4.66131500	3.70442800	-4.11164500
O	-4.65802600	1.71070100	5.26363300
O	-4.65040500	-5.41830900	-1.15090700
C	5.87607300	-4.40771600	3.90452300
H	6.04548900	-4.99178100	4.81068400
H	5.81043500	-5.08746600	3.04444300
H	6.72182500	-3.72322400	3.75403300
C	5.86323100	5.59393200	1.86571500
H	6.03082300	6.67109000	1.91676800
H	5.79620600	5.19077800	2.88506900
H	6.71079000	5.12175100	1.35077500
C	5.86619200	-1.17152400	-5.77607900
H	6.03627100	-1.66703100	-6.73342600
H	5.79051500	-0.08812600	-5.93927200

H	6.71629400	-1.37310700	-5.11037100
C	-5.87597600	4.40786300	-3.90445300
H	-5.81030900	5.08760500	-3.04436800
H	-6.04538200	4.99194000	-4.81060800
H	-6.72174800	3.72339700	-3.75396100
C	-5.86331400	-5.59382500	-1.86589200
H	-5.79619200	-5.19069300	-2.88524900
H	-6.03094300	-6.67097700	-1.91694000
H	-6.71089800	-5.12160200	-1.35103100
C	-5.86621500	1.17142700	5.77607000
H	-5.79067700	0.08800600	5.93917500
H	-6.03627200	1.66687400	6.73345200
H	-6.71626600	1.37317000	5.11034500

(B) the first complex between Ar−X and Pd**L**$_2$

Total energy: -3245.50613153 Hartree

Free energy: -3244.737552 Hartree

Pd	-0.03029700	-0.92717600	-0.35921900
P	1.85323700	0.33007200	0.29916300
C	1.90764700	0.73790400	2.09544200
C	3.07570200	1.12948000	2.76299200
C	0.71865000	0.65359200	2.84310500
C	3.06591800	1.45247000	4.12203000
H	4.01655000	1.17036700	2.22190800
C	0.69056400	0.97529700	4.19323400
H	-0.19234600	0.31686400	2.36162500
C	1.86558700	1.38175700	4.84272900
H	3.99079900	1.74818100	4.60297800
H	-0.22829000	0.90654700	4.76662400
C	1.92583500	1.96556300	-0.54916300
C	1.33818400	2.06149400	-1.82465600
C	2.47240400	3.12351600	0.01229400
C	1.29430800	3.26819700	-2.50654100
H	0.88161000	1.17947200	-2.26567200
C	2.41919100	4.35028700	-0.65408500
H	2.92234800	3.08855800	0.99917700

C	1.81771000	4.42659200	-1.91588300
H	0.81891900	3.35041300	-3.47792400
H	2.82668700	5.23226200	-0.17472800
C	3.52355400	-0.38064200	0.00793000
C	3.95628900	-1.45655800	0.80796500
C	4.31845200	-0.00792200	-1.07916200
C	5.13643400	-2.12821600	0.52948800
H	3.35950000	-1.76479900	1.66181800
C	5.50703200	-0.68087400	-1.37698000
H	4.01078500	0.81622700	-1.71530300
C	5.91800200	-1.75048800	-0.57436700
H	5.47630100	-2.95539400	1.14435100
P	-2.01569200	0.32055000	-0.25513500
C	-3.32931100	-0.19343700	-1.43999600
C	-4.69659900	-0.19652300	-1.14564600
C	-2.92524300	-0.62464500	-2.71841800
C	-5.64270100	-0.61517500	-2.08569500
H	-5.04059500	0.12421700	-0.16729500
C	-3.85331900	-1.02746200	-3.66833100
H	-1.86561500	-0.64913800	-2.96055700
C	-5.22214700	-1.02937200	-3.35575000
H	-6.69267200	-0.61156400	-1.81783800
H	-3.54682100	-1.35948000	-4.65491800
C	-2.82456000	0.19519000	1.39547900
C	-2.55493600	-0.93618700	2.17710000
C	-3.68214700	1.17704600	1.92479500
C	-3.12129200	-1.10595100	3.44176700
H	-1.87863800	-1.69613700	1.80068900
C	-4.25005800	1.02513600	3.18340800
H	-3.89182000	2.07494600	1.35118100
C	-3.97491900	-0.11843900	3.95108300
H	-2.87901200	-1.99696100	4.00846800
H	-4.90652100	1.78101400	3.60230600
C	-1.90380700	2.14047900	-0.51623100
C	-2.37421800	2.77766000	-1.66742200
C	-1.18134200	2.90872700	0.41862200

C	-2.11947700	4.13307200	-1.90530000
H	-2.93948500	2.21662000	-2.40503000
C	-0.94122500	4.25560500	0.20537200
H	-0.78876700	2.44268900	1.31701000
C	-1.39189400	4.87436900	-0.97037000
H	-2.48325700	4.58664700	-2.81947200
H	-0.36913700	4.84340600	0.91454100
C	0.63351300	-3.03774500	-0.72127600
C	-0.76172800	-3.03006200	-1.02283900
C	1.07383900	-3.65221900	0.49129700
C	-1.68510800	-3.61452500	-0.10194800
H	-1.10490800	-2.83790900	-2.03292700
C	0.15780400	-4.14669700	1.39014600
H	2.13546300	-3.69946700	0.70448800
C	-1.23492400	-4.12168100	1.09971400
H	-2.73569100	-3.60682800	-0.36493300
H	0.47625800	-4.56850800	2.33808700
O	-1.06000300	6.19370300	-1.10736000
O	-4.57819200	-0.16898100	5.17150600
O	-6.05262200	-1.45508300	-4.34953400
O	-2.03736000	-4.61816800	2.09675200
O	1.73855900	1.67243100	6.16880300
O	1.67670700	5.57524400	-2.64127500
C	-7.44818900	-1.48941700	-4.09240000
H	-7.84352600	-0.49097900	-3.86242300
H	-7.91466000	-1.85733200	-5.00766700
H	-7.69194600	-2.16918300	-3.26505000
C	-4.31088100	-1.28749300	6.00554000
H	-3.24336400	-1.36371700	6.25034500
H	-4.87949100	-1.12286600	6.92209200
H	-4.63827500	-2.22714100	5.54122000
C	-1.34506900	6.82297300	-2.34908900
H	-2.42378500	6.85899800	-2.54933000
H	-0.96732900	7.84331900	-2.26200800
H	-0.82948700	6.31509800	-3.17282400
C	2.89557300	2.08007300	6.88291600

H	2.56941300	2.26014700	7.90859300
H	3.66908500	1.30056500	6.88225200
H	3.32115300	3.00556400	6.47256200
C	2.04013600	6.80171000	-2.02162800
H	1.81036700	7.58374600	-2.74761200
H	1.45364100	6.96713200	-1.11008300
H	3.11206600	6.83759100	-1.78784700
C	-3.43846900	-4.60132200	1.87551800
H	-3.72077800	-5.21895200	1.01199900
H	-3.89376700	-5.01768900	2.77636900
H	-3.80893100	-3.57870600	1.72186700
I	2.07043500	-3.05691900	-2.40641900
H	6.09450500	-0.36292900	-2.23009300
O	7.05602400	-2.47912200	-0.76737100
C	7.85600500	-2.18272800	-1.90055700
H	7.29542400	-2.30884800	-2.83649500
H	8.25713700	-1.16076800	-1.86029600
H	8.68480200	-2.89251900	-1.87998700

(C) The transition state for the oxidative addition by Pd**L**$_2$

imaginary mode 106.75 i cm^{-1}

Total energy: -3245.49522038 Hartree

Free energy: -3244.727255 Hartree

Pd	0.14188100	-0.90393600	-0.58247800
P	1.70394300	0.72576700	0.24838600
C	1.83277800	0.87755700	2.07907200
C	2.84929700	1.58378000	2.73839900
C	0.84567900	0.26090200	2.86850800
C	2.87425800	1.69917000	4.12991200
H	3.65126900	2.03795000	2.16399700
C	0.84972900	0.37270000	4.25248600
H	0.06791700	-0.32123000	2.38971400
C	1.86398200	1.09788400	4.89431900
H	3.67972900	2.24988000	4.60107400
H	0.08121200	-0.10198400	4.85387000
C	1.22717000	2.41784400	-0.32431300

C	0.48056200	2.52169800	-1.51335300
C	1.51833300	3.59547200	0.37221000
C	0.04078600	3.75212100	-1.97980700
H	0.22159500	1.62196600	-2.06326200
C	1.06975100	4.83895200	-0.07748600
H	2.07512100	3.55734100	1.30181800
C	0.31658300	4.91856100	-1.25481900
H	-0.55435600	3.82954100	-2.88330900
H	1.29265000	5.72454200	0.50537300
C	3.45337200	0.57520000	-0.29261900
C	4.40570900	-0.13682400	0.46185700
C	3.80809500	0.97597100	-1.58749200
C	5.66450400	-0.41803000	-0.05329500
H	4.15666300	-0.48557600	1.45876000
C	5.06721100	0.69325500	-2.12018500
H	3.09010400	1.50769100	-2.20389800
C	6.00431200	-0.00947600	-1.35167900
H	6.40164200	-0.96405200	0.52658100
P	-2.06263000	-0.28423200	0.06220200
C	-3.41956700	-0.95094700	-0.98700000
C	-4.73950300	-1.06331200	-0.53292300
C	-3.13079700	-1.34230700	-2.30670400
C	-5.75207900	-1.55280900	-1.35923200
H	-4.98888400	-0.77470700	0.48380400
C	-4.13057800	-1.82352100	-3.14268500
H	-2.11254300	-1.27187600	-2.67893900
C	-5.44807300	-1.93370100	-2.67418600
H	-6.76078300	-1.63343500	-0.97186100
H	-3.91428000	-2.12783100	-4.16149200
C	-2.48347400	-0.88401300	1.75283700
C	-1.88655200	-2.07381200	2.19262500
C	-3.33523600	-0.20217300	2.63994000
C	-2.12231100	-2.57904400	3.47244900
H	-1.20403200	-2.60481200	1.53289900
C	-3.57559400	-0.69043800	3.91795000
H	-3.79767400	0.73108900	2.33413400

C	-2.96913500	-1.88190400	4.34497800
H	-1.63352600	-3.49639400	3.77778500
H	-4.22391600	-0.16439600	4.61118700
C	-2.43823000	1.51442400	0.13726500
C	-3.20984700	2.15435700	-0.83677000
C	-1.80595200	2.31000100	1.11315900
C	-3.34198800	3.54642100	-0.86109900
H	-3.71009000	1.56893900	-1.60177200
C	-1.94714100	3.68784700	1.11225800
H	-1.18658500	1.84689600	1.87501800
C	-2.70098300	4.31890100	0.11161500
H	-3.93118600	4.00744300	-1.64454100
H	-1.44721600	4.30385800	1.85125600
C	1.35307100	-2.42403500	-1.32082500
C	0.39878800	-3.42260800	-1.04843700
C	2.71241400	-2.63352400	-1.01541700
C	0.77429800	-4.54677000	-0.28246700
H	-0.59887800	-3.37384900	-1.47030400
C	3.06982500	-3.74751300	-0.27943500
H	3.45625700	-1.90635500	-1.31158500
C	2.10121200	-4.69830200	0.11284200
H	0.02865200	-5.30253400	-0.06505500
H	4.10059700	-3.90681500	0.02146800
O	-2.73628100	5.68391400	0.17117700
O	-3.26011000	-2.26828400	5.61890600
O	-6.35388400	-2.42295600	-3.56739200
O	2.58584200	-5.75123600	0.84157200
O	1.78657700	1.14894000	6.25396100
O	-0.20551300	6.07264100	-1.76606600
C	-7.70372300	-2.56342900	-3.15154500
H	-8.14444000	-1.59801200	-2.86895600
H	-8.24351800	-2.96568200	-4.01034900
H	-7.79851300	-3.25985600	-2.30777100
C	-2.64759200	-3.44713500	6.12091200
H	-1.55279100	-3.36283600	6.12795700
H	-3.00557200	-3.55988200	7.14544900

H	-2.93461100	-4.33310500	5.53917900
C	-3.35364000	6.37864300	-0.90440400
H	-4.42303400	6.14312300	-0.98037600
H	-3.24020200	7.44061000	-0.67942700
H	-2.85317100	6.15425700	-1.85373000
C	2.78992000	1.86289800	6.96049300
H	2.53272900	1.77806000	8.01753600
H	3.78660800	1.43214900	6.79634100
H	2.80823000	2.92394800	6.67814900
C	-0.07647100	7.25921400	-0.99448600
H	-0.58773500	8.04110700	-1.55903900
H	-0.55663500	7.14277800	-0.01548600
H	0.97489200	7.54575000	-0.86203600
C	1.66854800	-6.74682000	1.25704500
H	1.20905300	-7.26126600	0.40171200
H	2.24422900	-7.46809100	1.84014900
H	0.87101200	-6.32758100	1.88689800
I	0.89775100	-1.22453100	-3.46068300
H	5.29828500	1.01859100	-3.12728600
O	7.26034400	-0.34211600	-1.76752600
C	7.63867400	-0.00343700	-3.09331300
H	6.98190900	-0.47639500	-3.83533900
H	7.63326400	1.08322000	-3.25275100
H	8.65533800	-0.37857400	-3.22218300

(D) Ar–Pd**L**$_2$–I

Total energy: -3245.53985719 Hartree

Free energy: -3244.765224 Hartree

Pd	-0.60303500	1.12738300	-0.16560500
C	2.41754200	-0.25483700	1.17960900
C	3.26937000	-1.36299200	1.13125400
C	1.91433000	0.14176700	2.43436300
C	3.58118400	-2.09278500	2.28273700
H	3.66716600	-1.70252600	0.18159800
C	2.23040100	-0.56209700	3.58681000
H	1.24998600	0.99872200	2.49806000

C	3.04525300	-1.70066800	3.51455200
H	4.22314000	-2.96170800	2.19989400
H	1.82107400	-0.27731900	4.54937500
C	2.95565700	2.12265400	-0.35870500
C	2.73294100	3.09577100	-1.35082800
C	4.05376300	2.27280800	0.48947700
C	3.59444600	4.16954900	-1.49818300
H	1.86564400	3.01788400	-1.99925800
C	4.92419200	3.36069500	0.36088700
H	4.24398200	1.54175700	1.26854700
C	4.69669300	4.31225600	-0.63851100
H	3.42635900	4.92878400	-2.25449400
H	5.76264200	3.45026200	1.04109400
C	2.34835400	-0.24534400	-1.77394000
C	1.39046000	-0.68154700	-2.70458200
C	3.69832500	-0.50734700	-2.04342800
C	1.76172500	-1.40424700	-3.82945400
H	0.34169900	-0.46539300	-2.53324300
C	4.08726400	-1.24818500	-3.16091600
H	4.46499300	-0.11882800	-1.37910500
C	3.11034800	-1.71503100	-4.05203900
H	1.02338400	-1.76459300	-4.53661300
C	-1.16451600	-1.46748200	1.87787500
C	-0.84709400	-2.73134500	2.38880300
C	-1.30325000	-0.39958200	2.78740900
C	-0.60569700	-2.92303500	3.75102100
H	-0.75504900	-3.58040700	1.71999100
C	-1.10801300	-0.58604300	4.14584800
H	-1.51590300	0.59896100	2.41981700
C	-0.71767800	-1.84215800	4.63439000
H	-0.32140500	-3.90638000	4.10549400
H	-1.18947400	0.24095300	4.84340800
C	-3.14694500	-1.39515200	-0.26323900
C	-3.65145500	-0.97801200	-1.50185300
C	-4.05087000	-1.86264900	0.70299000
C	-5.01494100	-0.99381600	-1.77414200

H	-2.98024200	-0.56678800	-2.24811300
C	-5.41750900	-1.87148400	0.44845400
H	-3.68956900	-2.18810100	1.67311100
C	-5.91023900	-1.40610900	-0.77895600
H	-5.36620200	-0.61679600	-2.72549900
H	-6.12754200	-2.20075700	1.20003000
C	-0.52445900	-2.50529000	-0.78068900
C	0.75920100	-2.90134200	-0.38511200
C	-1.05530900	-3.07716100	-1.95209100
C	1.52078100	-3.78774600	-1.14406500
H	1.18840800	-2.50601800	0.52517800
C	-0.30648100	-3.95905400	-2.71912300
H	-2.05910600	-2.82718500	-2.27597300
C	1.00289100	-4.29236100	-2.34194600
H	2.51809400	-4.04495800	-0.80807800
H	-0.70426200	-4.38497300	-3.63440700
C	-2.55954500	1.70689100	-0.36624800
C	-3.56170200	1.60303200	0.59904500
C	-2.92746200	2.16924200	-1.64051500
C	-4.90362000	1.86211100	0.29863000
H	-3.32713000	1.27575600	1.60624700
C	-4.26084700	2.42957300	-1.95836700
H	-2.17188700	2.31958400	-2.40798400
C	-5.26018500	2.24691500	-0.99588300
H	-5.65023500	1.72761700	1.07222400
H	-4.54792500	2.76455100	-2.95091600
O	1.68214200	-5.09961300	-3.20189500
O	-7.26665200	-1.36268600	-0.90346500
O	-0.44974000	-1.89942900	5.96617300
O	-6.55592700	2.44394100	-1.42084100
O	3.24197100	-2.36331900	4.69377400
O	5.47777500	5.40710400	-0.86207900
C	0.20770000	-3.05808600	6.46817300
H	1.15433400	-3.22620900	5.94021600
H	0.40831200	-2.85437100	7.52120300
H	-0.42632100	-3.95121000	6.39306800

C	-7.80815000	-0.82847200	-2.10912200
H	-7.54466400	-1.44890500	-2.97573400
H	-8.89155300	-0.83947600	-1.97923500
H	-7.46778500	0.20009800	-2.27928100
C	3.07361200	-5.28238900	-2.98433000
H	3.27052600	-5.86350200	-2.07334600
H	3.44333600	-5.83760700	-3.84787200
H	3.59496700	-4.31923600	-2.91780900
C	4.07425500	-3.51414200	4.68627000
H	4.10069900	-3.87443500	5.71591800
H	3.66971200	-4.30258400	4.03757000
H	5.09514400	-3.27299000	4.36288500
C	6.57204900	5.64086200	0.01019400
H	7.03544200	6.56909000	-0.32827400
H	6.24222300	5.76012900	1.05070400
H	7.31226000	4.83055900	-0.03916900
C	-7.58543000	2.33349000	-0.45023600
H	-7.44892000	3.05143900	0.36943300
H	-8.51869200	2.55908200	-0.97071600
H	-7.64245500	1.31898900	-0.03202000
I	-0.23198000	3.67222600	0.71827500
H	5.14004300	-1.43864100	-3.33243400
O	3.36776200	-2.47255500	-5.15596300
C	4.71905700	-2.77281000	-5.46959900
H	5.19952600	-3.36235700	-4.67677800
H	4.69135800	-3.36374500	-6.38633100
H	5.30778300	-1.86273800	-5.64330500
P	-1.37198000	-1.11981200	0.08524800
P	1.81448600	0.68784300	-0.28202100

(E) L

Total energy: -1379.92157124 Hartree

Free energy: -1379.606128 Hartree

P	-0.00074100	-0.00078700	-1.75142600
C	0.54287200	1.56330400	-0.92990700
C	-0.03645500	2.09306100	0.22898800

C	1.61293700	2.26985400	-1.51222700
C	0.42767800	3.28140700	0.80128400
H	-0.86738200	1.57669900	0.69952000
C	2.09352000	3.44403200	-0.95018600
H	2.07511600	1.89119400	-2.42064300
C	1.50095200	3.96044100	0.21264500
H	-0.05185400	3.66082300	1.69597200
H	2.91969200	3.98939900	-1.39478200
C	1.08200400	-1.25293600	-0.92885400
C	1.16110800	-2.53261800	-1.51149100
C	1.82891900	-1.01545800	0.23089500
C	1.93853900	-3.53499800	-0.94902100
H	0.60340400	-2.74397400	-2.42061600
C	2.62676300	-2.01068000	0.80368200
H	1.79537300	-0.03777100	0.70151500
C	2.68061100	-3.27936900	0.21457800
H	1.99965000	-4.52290100	-1.39395100
H	3.19384900	-1.78463700	1.69905500
C	-1.62685500	-0.31231900	-0.92968200
C	-2.77600500	0.24823500	-1.51992200
C	-1.79332000	-1.06687200	0.23750500
C	-4.03304300	0.07642900	-0.95777400
H	-2.68106300	0.82807500	-2.43477500
C	-3.05414700	-1.25971700	0.81027100
H	-0.92853400	-1.51800200	0.71406200
C	-4.18130900	-0.68273800	0.21336800
H	-4.92028700	0.50917400	-1.40852900
H	-3.14093600	-1.85509000	1.71159000
O	2.03854700	5.12360700	0.68181400
O	-5.45743300	-0.80072800	0.68196800
O	3.42031900	-4.32558800	0.68398300
C	4.20254500	-4.12470400	1.85076100
H	4.70741600	-5.07284400	2.04331000
H	4.95535000	-3.33850900	1.70483500
H	3.58019900	-3.86554000	2.71787400
C	-5.67310900	-1.56613700	1.85724300

H	-6.74704300	-1.53126100	2.04799100
H	-5.36444900	-2.61159400	1.72361900
H	-5.14020200	-1.14482400	2.72029900
C	1.47415200	5.70150400	1.84847800
H	2.04451900	6.61167100	2.04139000
H	0.41744000	5.96242900	1.70221900
H	1.55926400	5.03263700	2.71550900

(F) L−PdAr−I

Total energy: -1865.55610707 Hartree

Free energy: -1865.131581 Hartree

Pd	0.07454800	1.72877800	-0.31985400
C	-1.90534500	-0.90454700	-1.34859200
C	-2.98627600	-1.78180300	-1.19752900
C	-1.58817500	-0.44418700	-2.64112800
C	-3.73461200	-2.20141700	-2.29743900
H	-3.25929900	-2.14197900	-0.21053800
C	-2.32065600	-0.85936100	-3.74372900
H	-0.76420900	0.25159100	-2.77783600
C	-3.40051300	-1.74190300	-3.57997100
H	-4.56793300	-2.87645300	-2.14485300
H	-2.08677700	-0.50692300	-4.74266000
C	0.32388400	-1.75083300	0.31227400
C	1.13350600	-1.71798100	1.45564600
C	0.60686500	-2.69814100	-0.68440800
C	2.22082000	-2.57315700	1.59584700
H	0.94107100	-0.98669100	2.23415900
C	1.69278200	-3.55625200	-0.55640000
H	-0.00859900	-2.74854300	-1.57710700
C	2.52802400	-3.47378700	0.56690500
H	2.84556600	-2.49210300	2.47578900
H	1.93457100	-4.27761900	-1.32997100
C	-1.94483000	-0.42329700	1.53164600
C	-2.57585800	0.75492300	1.95101500
C	-2.19497900	-1.60888400	2.24865300
C	-3.44396400	0.76493500	3.04302800

H	-2.38540600	1.68890600	1.42821600
C	-3.05411900	-1.61198800	3.33790600
H	-1.70093600	-2.53050100	1.95671400
C	-3.68766500	-0.42508100	3.74249500
H	-3.90930400	1.69651100	3.34063300
H	-3.25038500	-2.51885500	3.90026100
C	1.91126500	0.99491900	-0.13391700
C	2.43825600	0.18500100	-1.13545500
C	2.63847200	1.22402500	1.03842800
C	3.66576200	-0.46060900	-0.94854200
H	1.88824900	0.00506700	-2.05324600
C	3.86053500	0.57841300	1.22785500
H	2.25849500	1.88977100	1.80574000
C	4.36429000	-0.28838400	0.24987400
H	4.03480200	-1.11635600	-1.72742000
H	4.43357800	0.72596600	2.13803100
O	-4.50661100	-0.53572000	4.82074300
O	3.62031400	-4.28775900	0.56218300
O	-4.05723600	-2.08346200	-4.71900200
O	5.53110900	-0.94030800	0.56608300
C	-5.17131000	-2.96185600	-4.62457700
H	-5.96973600	-2.53576900	-4.00352100
H	-5.53855900	-3.09060100	-5.64355500
H	-4.88161300	-3.93973500	-4.21854200
C	4.52982700	-4.19196900	1.65636200
H	4.05391000	-4.48891500	2.59974200
H	5.34002200	-4.88711900	1.43118700
H	4.93227600	-3.17626400	1.75210500
C	-5.16776600	0.63209900	5.29307100
H	-5.83430200	1.05472600	4.53036300
H	-5.76000600	0.31423600	6.15211700
H	-4.45130500	1.40006100	5.61134900
C	6.10052300	-1.78736700	-0.42278000
H	6.33914300	-1.23381100	-1.34036000
H	7.02427900	-2.17681100	0.00942000
H	5.43485500	-2.62562700	-0.66864700

I	0.72864900	4.23195500	-0.76567400
P	-0.85820900	-0.38297700	0.06047600

(G) Transition state for the isomerization

(TS connecting between L−PdAr−I and Ar−PdL−I)

imaginary mode 25.99 i cm^{-1}

Total energy: -1865.55271661 Hartree

Free energy: -1865.126228 Hartree

Pd	0.32335700	-1.60492600	-0.56982800
P	0.42609200	0.55735000	0.15662900
C	1.27844100	1.58061900	-1.09636800
C	1.97287300	2.74259000	-0.73719100
C	1.20235800	1.23172200	-2.45773300
C	2.57281300	3.55010600	-1.70300600
H	2.05684400	3.02427800	0.30798300
C	1.79211100	2.02918700	-3.42723600
H	0.69060700	0.31977000	-2.75294300
C	2.48160000	3.19532400	-3.05727400
H	3.10664300	4.43991000	-1.39237300
H	1.74727900	1.76567700	-4.47848400
C	-1.12764900	1.43781100	0.52670100
C	-1.91200200	0.97675100	1.59315600
C	-1.68095800	2.37871600	-0.35685500
C	-3.22817600	1.39358700	1.75438700
H	-1.50813700	0.24364800	2.28399100
C	-2.99546600	2.80314800	-0.20501900
H	-1.09179700	2.75769800	-1.18584800
C	-3.79059900	2.27958700	0.82470500
H	-3.81552700	0.98421900	2.56598000
H	-3.44233800	3.50988400	-0.89634600
C	1.43196100	0.67123000	1.67850900
C	2.45505100	-0.26096600	1.90347500
C	1.24000900	1.70211000	2.61804600
C	3.27406600	-0.17399900	3.02839800
H	2.61701600	-1.07427300	1.20071500
C	2.04933000	1.79623700	3.74105800

H	0.44599600	2.42769900	2.47224500
C	3.07355500	0.85902800	3.95498600
H	4.05084700	-0.91486000	3.17202700
H	1.90846700	2.58369600	4.47397800
C	-1.65337700	-1.48369200	-0.41719100
C	-2.42517800	-0.77423800	-1.33650500
C	-2.28126000	-2.14289400	0.64833500
C	-3.81293400	-0.68507800	-1.18522000
H	-1.95653900	-0.23949000	-2.15675700
C	-3.66398300	-2.05367400	0.80579400
H	-1.69986500	-2.71151100	1.36839400
C	-4.43061100	-1.29707500	-0.09011800
H	-4.38143800	-0.10220900	-1.89948500
H	-4.16535000	-2.54263700	1.63538000
O	3.80540000	1.03815900	5.08484400
O	-5.09520000	2.66811600	0.83078800
O	3.02669000	3.90366000	-4.07953900
O	-5.76609700	-1.18590500	0.20662600
C	3.76075600	5.08297700	-3.77541800
H	4.62778600	4.86532000	-3.13867900
H	4.10690200	5.47537500	-4.73244700
H	3.13089900	5.83512900	-3.28289200
C	-5.96168600	2.08697700	1.80300200
H	-5.66811900	2.36925000	2.82211400
H	-6.95448200	2.48815800	1.59409100
H	-5.98088000	0.99354200	1.71671500
C	4.85062900	0.11520600	5.36963000
H	5.61873100	0.12153100	4.58587200
H	5.29325600	0.44548400	6.31023800
H	4.46547300	-0.90535900	5.48881200
C	-6.58172700	-0.44555000	-0.69107700
H	-6.57555100	-0.88301100	-1.69803500
H	-7.59483100	-0.49316600	-0.28744100
H	-6.26506700	0.60446800	-0.75261300
I	1.90304400	-3.63940800	-1.20956800

(H) Ar−PdL−X

Total energy: -1865.55581910 Hartree

Free energy: -1865.129907 Hartree

Pd	0.14327300	-0.56588500	-1.78905100
C	1.38404700	1.59620200	0.47611400
C	1.95151600	1.96934400	1.70132800
C	1.58189800	2.42419600	-0.64241000
C	2.69478500	3.14257200	1.82231700
H	1.82493000	1.33880000	2.57594300
C	2.31555300	3.59632600	-0.53205500
H	1.18089800	2.13344000	-1.60797800
C	2.87765600	3.96468900	0.70031000
H	3.12650600	3.39941700	2.78189700
H	2.48449700	4.23657800	-1.39104800
C	-1.19680800	0.52623800	1.24000800
C	-2.08154500	-0.50192800	1.59384200
C	-1.63775600	1.85577000	1.34192200
C	-3.38461500	-0.22924900	1.99164600
H	-1.76671600	-1.53703900	1.51549900
C	-2.93918900	2.14065800	1.73774000
H	-0.96932700	2.67101000	1.08385400
C	-3.83332400	1.09862300	2.02369600
H	-4.04892000	-1.05242200	2.22016400
H	-3.29848900	3.16265300	1.79659300
C	1.14848100	-1.17574400	1.40826300
C	2.08312100	-2.05853400	0.85035200
C	0.89427800	-1.24974000	2.79263100
C	2.75471200	-2.98976000	1.64157300
H	2.30081400	-2.01965800	-0.21219800
C	1.55790800	-2.17309700	3.58669900
H	0.16707000	-0.58641100	3.24933300
C	2.49488900	-3.05122200	3.01741800
H	3.46946900	-3.65568000	1.17390600
H	1.36793700	-2.23951000	4.65280400
C	-1.84209900	-0.61830600	-1.54655200
C	-2.60522700	0.55048100	-1.63011000

C	-2.50432500	-1.83810000	-1.33028200
C	-3.99568900	0.52197000	-1.49026200
H	-2.12022200	1.51384500	-1.76044400
C	-3.89064900	-1.87826100	-1.18525800
H	-1.94058500	-2.76448300	-1.25016300
C	-4.63803900	-0.69407700	-1.23442300
H	-4.54973100	1.45165000	-1.53787200
H	-4.41115300	-2.81360800	-1.00305300
O	3.08612100	-3.91764800	3.88000200
O	-5.11409100	1.46519900	2.30086400
O	3.58154700	5.12658900	0.70152800
O	-5.98108300	-0.81909500	-0.98091700
C	4.20529700	5.54243700	1.90926900
H	4.94135100	4.80644100	2.25744200
H	4.71513800	6.47828500	1.67659300
H	3.46934800	5.72018100	2.70433600
C	-6.07250200	0.43279900	2.51991200
H	-5.83616100	-0.15022800	3.41929100
H	-7.02802100	0.93922300	2.66418200
H	-6.13978800	-0.24103500	1.65668300
C	4.04597300	-4.83493700	3.36752400
H	4.90252800	-4.31437300	2.92093600
H	4.38597600	-5.42097000	4.22238400
H	3.60316500	-5.50632000	2.62094100
C	-6.78580300	0.34615000	-1.09643200
H	-6.73829200	0.77120400	-2.10757500
H	-7.80922000	0.02856300	-0.88842500
H	-6.49150100	1.11665500	-0.37093400
I	2.59130700	-0.68293100	-2.89951600
P	0.34689700	0.09510200	0.36580800

(I) Cation−π complex between Ar−PdL−X and vinylSnBu3

Total energy: -2420.59056550 Hartree

Free energy: -2419.788602 Hartree

Pd	0.05469200	-0.26235500	-0.84732600
C	1.97328800	-1.28756900	1.92719700

C	3.03588200	-2.00981200	2.49578400
C	0.80665300	-1.11182500	2.67678500
C	2.92846100	-2.53298500	3.77653300
H	3.94745200	-2.17746700	1.93183500
C	0.68926500	-1.62060600	3.96963600
H	-0.03457500	-0.58834200	2.24101100
C	1.75565100	-2.33981900	4.52475100
H	3.73689500	-3.10259700	4.22263000
H	-0.23588600	-1.47128400	4.51251600
C	2.99573000	1.06738100	0.65626100
C	3.74682100	1.72767400	-0.33498400
C	2.83176500	1.69831300	1.89342400
C	4.30267900	2.97323900	-0.09543600
H	3.87407200	1.27468200	-1.31101400
C	3.38149600	2.95779700	2.14517600
H	2.26660500	1.21229100	2.68154700
C	4.11579500	3.60480600	1.14467900
H	4.86712800	3.49352400	-0.86158000
H	3.22777100	3.41452500	3.11520900
C	3.28439700	-1.48650900	-0.69127000
C	2.80402500	-2.42270200	-1.61633900
C	4.67755400	-1.37389700	-0.51370700
C	3.67616300	-3.23126600	-2.34606600
H	1.73478000	-2.54068500	-1.75913000
C	5.55336300	-2.17231600	-1.23443600
H	5.07952900	-0.64873600	0.18644300
C	5.05895200	-3.10934500	-2.15654900
H	3.26592700	-3.94647500	-3.04843700
H	6.62749400	-2.09139700	-1.10486500
C	0.80860700	1.46754000	-1.59409100
C	0.65523200	2.70671400	-0.95083000
C	1.49356300	1.43605000	-2.81071000
C	1.18054400	3.87040300	-1.50237900
H	0.14328100	2.76893600	0.00445300
C	2.03475500	2.60152300	-3.37655300
H	1.63981100	0.49324200	-3.33291100

C	1.88226500	3.82394300	-2.71577700
H	1.07749600	4.82819900	-1.00181100
H	2.56898000	2.53383800	-4.31745200
C	-2.04650000	0.59473000	-1.57032200
C	-1.58949000	-0.27221000	-2.52866100
H	-1.79179000	1.64383100	-1.72635900
H	-1.02539900	0.08686500	-3.38974500
I	-0.86626300	-2.80761700	-0.08219400
O	2.37949900	5.02060700	-3.15831900
C	3.11829200	5.02714000	-4.36697400
H	3.42717200	6.06140100	-4.52944800
H	4.01230500	4.39112400	-4.30202800
H	2.51022700	4.69563700	-5.22007700
Sn	-3.59875300	0.24903500	-0.06426600
C	-4.93027100	1.96302200	-0.37575900
H	-4.37520800	2.88047600	-0.14065600
H	-5.17537700	2.01923300	-1.44379000
C	-4.70830400	-1.57839900	-0.46789600
H	-5.50945200	-1.65339400	0.27856800
C	-2.75289300	0.44912000	1.93727100
H	-3.58556200	0.58495600	2.63904100
H	-2.26532500	-0.49636500	2.19601300
C	-6.22039000	1.89988600	0.45658200
H	-6.77371800	0.97844400	0.22304600
H	-5.97673100	1.83902000	1.52776900
C	-7.15035800	3.10146300	0.23310700
H	-6.60457800	4.02473400	0.47103100
H	-7.40195200	3.16373000	-0.83439900
C	-8.43514200	3.02982900	1.06473500
H	-8.20903400	2.99634000	2.13698400
H	-9.08047300	3.89658100	0.88712900
H	-9.01145600	2.12939200	0.82208400
H	-1.89074300	-1.31564000	-2.55457800
C	-1.77222200	1.62677900	2.04416600
H	-0.90820300	1.44017000	1.39087000
H	-2.24018100	2.54721700	1.66427400

C	-1.26393800	1.89821400	3.46728100
H	-0.74291200	1.00872600	3.84373500
H	-2.12326300	2.05521700	4.13319700
C	-0.32725400	3.10969500	3.53228300
H	0.05698800	3.27092800	4.54544500
H	0.53059700	2.97900500	2.86389100
H	-0.84712200	4.02416300	3.22325700
H	-4.02962500	-2.41911900	-0.29828000
C	-5.29898500	-1.63543500	-1.88489100
H	-5.96463300	-0.77678900	-2.05755400
H	-4.49567800	-1.54793200	-2.63011900
C	-6.08006200	-2.92959600	-2.15491500
H	-6.88730900	-3.02193500	-1.41537800
H	-5.41435700	-3.78696300	-1.98925200
C	-6.66435700	-2.99143600	-3.56982900
H	-5.87208800	-2.93128900	-4.32517000
H	-7.21546100	-3.92260200	-3.73868600
H	-7.35400900	-2.15805200	-3.74891700
O	5.99921600	-3.84116800	-2.81087100
O	4.68595800	4.83400500	1.27166200
O	1.75403900	-2.89045300	5.76863700
C	4.49172500	5.54337600	2.48683000
H	5.00294700	6.49919000	2.36280800
H	3.42678000	5.72508700	2.68254400
H	4.92717500	5.00975500	3.34204200
C	5.56396200	-4.81916000	-3.74709900
H	5.00444900	-4.36484700	-4.57502100
H	6.47002500	-5.28424500	-4.13802100
H	4.94027000	-5.58552900	-3.26951300
C	0.57772500	-2.76924200	6.55698900
H	0.78872300	-3.28757700	7.49353200
H	0.34051500	-1.71877100	6.77128900
H	-0.28531600	-3.23970800	6.06862200
P	2.10062800	-0.49089200	0.28500900

(J) Transition state for the transmetalation

imaginary mode 38.06 i cm^{-1}

Total energy: -2420.55990952 Hartree

Free energy: -2419.754448 Hartree

Pd	-0.23987300	-0.52751600	-1.38166800
C	-0.70217600	1.28189100	1.57016700
C	-0.11613100	2.53806000	1.75669900
C	-0.44276300	0.28245600	2.52929400
C	0.68111000	2.81139500	2.87286400
H	-0.27569800	3.32219100	1.02509300
C	0.34924700	0.53825600	3.63960100
H	-0.88750800	-0.70122100	2.41476200
C	0.91220600	1.81121500	3.82374500
H	1.11138900	3.79933800	2.98477200
H	0.53804000	-0.22569800	4.38669300
C	-3.21492700	0.13313300	0.68702000
C	-4.03964200	-0.54931400	-0.22763800
C	-3.66058000	0.27059300	2.00497400
C	-5.25288700	-1.08713700	0.16817200
H	-3.71069200	-0.68866500	-1.25095200
C	-4.88118700	-0.27127400	2.41936000
H	-3.05503900	0.79855100	2.73440400
C	-5.68096300	-0.95841500	1.49895600
H	-5.87913900	-1.63336700	-0.52878500
H	-5.18989300	-0.15101300	3.45093100
C	-2.19349400	2.43432700	-0.65656300
C	-1.98057700	2.70790800	-2.01840500
C	-2.89474600	3.37382900	0.11032100
C	-2.44111300	3.88806000	-2.58807800
H	-1.44715500	1.99093500	-2.63389700
C	-3.35556800	4.56675300	-0.44524900
H	-3.09019500	3.17362100	1.16012200
C	-3.12708200	4.82794200	-1.80474800
H	-2.28096800	4.10737300	-3.63841600
H	-3.89142800	5.27218300	0.17836500
C	-1.41531200	-2.15881900	-1.17709300
C	-1.60746000	-2.78010100	0.06895000

C	-2.14514500	-2.65643900	-2.26328800
C	-2.50993100	-3.82844800	0.23022000
H	-1.06233300	-2.43648700	0.94192600
C	-3.07235500	-3.69799500	-2.11467200
H	-2.00414200	-2.22632000	-3.25036900
C	-3.26053500	-4.28576800	-0.85952300
H	-2.66390800	-4.29589600	1.19827400
H	-3.62566600	-4.03938300	-2.98249000
C	1.40939900	-1.40074800	-3.75626600
C	0.88063600	-1.75930200	-2.57616800
Sn	2.87052500	-0.55472200	-0.11930200
C	4.27670500	-1.35781400	-1.57569600
H	3.79223800	-2.24310400	-1.99778000
H	5.14493300	-1.69984900	-0.99514300
C	1.82783400	-2.15267000	0.93826600
H	1.17634900	-2.65102500	0.21972400
H	1.19010600	-1.68187300	1.69019700
C	3.74654500	0.83967500	1.32272900
H	4.64992100	1.25767800	0.86195000
H	3.03516700	1.66452200	1.43094800
H	0.98922600	-2.80731800	-2.28512400
H	1.93208200	-2.11598700	-4.39548500
H	1.35163300	-0.38368200	-4.13804200
O	1.66128100	1.96792500	4.95266500
O	-3.53313300	5.95317100	-2.45449700
O	-6.88077900	-1.53487200	1.79025400
C	-7.35242500	-1.46881700	3.12707200
H	-8.30479500	-2.00133700	3.13803800
H	-6.65893300	-1.95519300	3.82592100
H	-7.51618800	-0.43175800	3.44966200
C	-4.24050700	6.94132100	-1.71976900
H	-4.46287700	7.74104600	-2.42786500
H	-5.18134600	6.54791400	-1.31277300
H	-3.63551600	7.34579400	-0.89747900
C	2.09584400	3.27672800	5.29836000
H	1.24584900	3.96187700	5.41066100

H	2.61490300	3.17736300	6.25243900
H	2.79191600	3.68610600	4.55596600
C	4.05412900	0.23216500	2.69787000
H	3.12466300	-0.13679600	3.15079400
H	4.71963900	-0.63816400	2.60728100
C	4.70182800	1.24575300	3.65282200
H	4.10082200	2.16259300	3.64485600
H	5.69021600	1.52540700	3.26415600
C	4.82201600	0.72487300	5.08742000
H	5.32332200	1.44996700	5.73804000
H	3.82841100	0.52836900	5.50334500
H	5.39787900	-0.20724400	5.12446800
C	4.71339100	-0.40690100	-2.69311200
H	3.82886800	-0.06009300	-3.23914900
H	5.18483600	0.49135700	-2.26971500
C	5.68273400	-1.06581500	-3.68454100
H	5.20162800	-1.95689300	-4.11019200
H	6.57147100	-1.42433600	-3.14678100
C	6.10527600	-0.11916900	-4.81252400
H	6.79029500	-0.60708700	-5.51398100
H	5.23367300	0.22602300	-5.38020800
H	6.61085100	0.76802200	-4.41368800
C	2.79054300	-3.15590100	1.59213200
H	3.45535500	-2.65282500	2.30725400
H	3.44189200	-3.61232800	0.83312700
C	2.03220300	-4.27317300	2.32766400
H	1.38800500	-3.81887900	3.09291200
H	1.35873400	-4.77263400	1.61911300
C	2.96443800	-5.30035000	2.97730300
H	3.62737900	-4.82441900	3.70935900
H	2.40039100	-6.08232800	3.49617300
H	3.59699400	-5.78781600	2.22653900
P	-1.63999400	0.83571000	0.05297700
I	1.62358700	1.68370000	-1.63234400
O	-4.13895900	-5.30534200	-0.59324600
C	-4.94529200	-5.77782500	-1.65622800

H	-5.57756000	-6.56198300	-1.23480500
H	-5.58457400	-4.98418000	-2.06835300
H	-4.34281100	-6.20285200	-2.47130700

(K) Complex between vinyl−PdAr−L and Bu_3SnI

Total energy: -2420.56373281 Hartree

Free energy: -2419.761316 Hartree

Pd	0.53561600	0.85840300	-1.21745400
C	0.79754700	-1.63611200	1.19360400
C	0.45053100	-2.98921400	1.17517800
C	0.20152100	-0.81170100	2.16809300
C	-0.45720000	-3.52074300	2.09719200
H	0.87749600	-3.64720400	0.42615600
C	-0.69203600	-1.32604500	3.09566500
H	0.44171000	0.24639200	2.19861600
C	-1.03319500	-2.68813400	3.06227800
H	-0.70466100	-4.57419600	2.04668300
H	-1.14208100	-0.69558100	3.85553800
C	3.33299800	-0.26526000	0.83029000
C	4.28663500	0.48198700	0.11130600
C	3.55191200	-0.48680700	2.19158700
C	5.40862000	0.99611300	0.73727100
H	4.12524100	0.69326900	-0.94015100
C	4.68053700	0.03006400	2.83764200
H	2.83836400	-1.06226900	2.77228600
C	5.61072300	0.78012600	2.11047100
H	6.13274200	1.59324000	0.19387300
H	4.81566700	-0.15727700	3.89619700
C	2.50412300	-2.20529600	-1.10677100
C	2.15884400	-2.29252400	-2.46678800
C	3.37684800	-3.16542200	-0.57750000
C	2.65548300	-3.31604600	-3.26354100
H	1.50140900	-1.54737000	-2.90333400
C	3.88023300	-4.20118200	-1.36429000
H	3.67806900	-3.10084700	0.46444400
C	3.51573100	-4.28018500	-2.71676500

H	2.39696700	-3.38917200	-4.31463900
H	4.55359900	-4.92582500	-0.92250400
C	1.77500800	2.34731000	-0.68305900
C	1.88004500	2.74378300	0.66137700
C	2.61814100	2.96861200	-1.61016600
C	2.81443600	3.69235800	1.06860500
H	1.24353100	2.29291500	1.41728600
C	3.57506700	3.91460200	-1.21340600
H	2.54523300	2.71414700	-2.66339000
C	3.67947100	4.27434100	0.13395200
H	2.90385600	3.98447900	2.11057700
H	4.21898600	4.35944900	-1.96394100
C	-1.35793200	2.21590600	-3.15083000
C	-0.58539700	2.34476800	-2.05956700
Sn	-3.35949100	0.08578900	-0.19789600
C	-4.31279600	-1.52423900	0.92859900
H	-5.29320100	-1.71259100	0.47478400
H	-3.70885600	-2.42386900	0.76866000
C	-4.61199800	1.02366900	-1.70681700
H	-3.93701700	1.65364500	-2.29507800
H	-4.97473300	0.23186500	-2.37192900
C	-2.22725100	1.49778700	1.00792900
H	-2.32560800	1.21140600	2.06073000
H	-1.18208100	1.35200100	0.71594300
H	-0.54710000	3.33790200	-1.60540100
H	-1.92292700	3.05800800	-3.55916300
H	-1.46004600	1.27832900	-3.69367500
C	-2.63575400	2.95887600	0.77171600
H	-2.65076200	3.16907100	-0.30455400
H	-3.65566100	3.13823500	1.14165100
C	-4.44744200	-1.23724800	2.43116900
H	-3.45299800	-1.08819600	2.86696100
H	-5.00241400	-0.30335300	2.60243800
C	-5.78324400	1.84338900	-1.14332500
H	-5.40802600	2.62828500	-0.47278500
H	-6.44096300	1.20731000	-0.53275700

C	-6.62269700	2.50351200	-2.24797400
H	-5.96793300	3.13985800	-2.85778000
H	-7.00518500	1.72444900	-2.92098800
C	-1.67391300	3.94830600	1.44474900
H	-0.66405300	3.77709800	1.05387800
H	-1.63193100	3.73862000	2.52302300
C	-5.14816400	-2.37365500	3.18932800
H	-4.64711700	-3.31916100	2.94655500
H	-6.17907000	-2.47266100	2.82336500
C	-5.14210800	-2.16477900	4.70647500
H	-5.66150700	-2.97681600	5.22701700
H	-4.11328200	-2.12227600	5.07891200
H	-5.63872300	-1.22624500	4.97897500
C	-7.78700400	3.33256600	-1.69689500
H	-7.42453400	4.13608600	-1.04534900
H	-8.36842500	3.79321400	-2.50217500
H	-8.46970300	2.71081500	-1.10593700
C	-2.07158200	5.40891100	1.21270400
H	-1.36750200	6.09618200	1.69274600
H	-2.08602600	5.64193800	0.14169000
H	-3.07126700	5.61906300	1.61160800
O	-1.93306700	-3.09335500	4.00461700
O	6.73721700	1.34122400	2.63366500
O	3.94660200	-5.24171300	-3.57859900
C	-2.28686600	-4.46865000	4.05248000
H	-3.01333600	-4.56231300	4.86056700
H	-2.74911600	-4.80092000	3.11426800
H	-1.41515200	-5.10005600	4.26734400
C	6.96984000	1.20736000	4.02693100
H	7.89571700	1.74722200	4.23207600
H	6.15600700	1.64874500	4.61740600
H	7.09412700	0.15594300	4.31965900
C	4.83141800	-6.24025200	-3.09168800
H	5.04329700	-6.89367900	-3.93934400
H	5.77153700	-5.80588800	-2.72701400
H	4.37334500	-6.83056000	-2.28704700

I	-1.52380000	-1.36478700	-1.84654900
O	4.58030900	5.17860300	0.63821500
C	5.50762200	5.75796700	-0.25992500
H	6.13718900	4.99774900	-0.74401200
H	5.00939300	6.35046100	-1.04022800
H	6.14073400	6.41733600	0.33737600
P	1.84782700	-0.83330800	-0.08454700

(L) vinyl−PdAr−L

Total energy: -1932.05773671 Hartree

Free energy: -1931.595553 Hartree

Pd	0.32653500	-0.52421800	-2.37755900
C	-2.52933100	0.30136100	-0.40806500
C	-3.46173500	-0.04966400	0.57454000
C	-2.99156200	0.96485800	-1.56116700
C	-4.81808500	0.24620700	0.42532900
H	-3.13229900	-0.56791700	1.46983700
C	-4.33526100	1.27340700	-1.71882600
H	-2.28669000	1.24727800	-2.34008700
C	-5.25996700	0.91311800	-0.72560800
H	-5.51302000	-0.04647200	1.20325000
H	-4.69925500	1.78375300	-2.60431200
C	-0.06377000	1.39880600	0.64980700
C	1.29117000	1.38877800	1.04201700
C	-0.82933300	2.53490100	0.92967000
C	1.84738500	2.47819000	1.69340100
H	1.91412600	0.52489700	0.84004700
C	-0.27505500	3.64190900	1.57997100
H	-1.87544300	2.56927800	0.64270700
C	1.07040400	3.61627800	1.96379600
H	2.88949500	2.47560800	1.99524900
H	-0.89918700	4.50488000	1.77877300
C	-0.61511600	-1.42154900	0.93476300
C	-0.59828600	-2.74031800	0.44279400
C	-0.53816600	-1.22694300	2.31816200
C	-0.51894200	-3.82322600	1.30544700

H	-0.63196500	-2.91184700	-0.63035000
C	-0.45226300	-2.30795800	3.19885000
H	-0.53120200	-0.21881300	2.72111200
C	-0.44365400	-3.61418300	2.69236900
H	-0.49856000	-4.84260000	0.93447800
H	-0.38679500	-2.12001300	4.26376100
C	2.18280000	-0.48996600	-1.64653100
C	2.99904900	0.62324100	-1.85648100
C	2.62436500	-1.49395000	-0.76947600
C	4.20713700	0.77666300	-1.16166700
H	2.69394800	1.40348900	-2.54693900
C	3.82683400	-1.35233000	-0.07888100
H	2.01991200	-2.37697900	-0.59146600
C	4.61978500	-0.21037100	-0.26118000
H	4.80346900	1.66547100	-1.33304700
H	4.16961800	-2.11608500	0.61263900
C	0.71554500	-1.94358200	-4.91899600
C	1.14607300	-0.91934800	-4.16518200
H	1.88950300	-0.23788800	-4.58846600
H	1.03476400	-2.08077900	-5.95483200
H	0.02031000	-2.69511800	-4.54489500
O	-6.55378300	1.25182200	-0.97697300
O	1.71703700	4.63319100	2.60131200
O	-0.35884500	-4.74019000	3.45207700
C	-7.54314000	0.90277700	-0.01886500
H	-8.49162100	1.26031100	-0.42227400
H	-7.59934400	-0.18382500	0.12727300
H	-7.35768200	1.38608700	0.94942200
C	0.98898100	5.81727400	2.88910900
H	1.69055500	6.49033300	3.38459300
H	0.61462400	6.29572100	1.97436200
H	0.14284500	5.62061200	3.56112700
C	-0.25040600	-4.59840200	4.86143300
H	-0.18520800	-5.61129000	5.26150500
H	0.65143100	-4.03955300	5.14357700
H	-1.13032200	-4.09831900	5.28729700

O	5.77179300	-0.16180200	0.48123600
C	6.59749800	0.98089000	0.34760600
H	6.07024100	1.90187900	0.63457600
H	7.44169700	0.82767800	1.02275700
H	6.97485200	1.09611200	-0.67796900
P	-0.73271600	-0.04381700	-0.26773500

(M) Transition state for the reductive elimination

imaginary mode 273.29 i cm^{-1}

Total energy: -1932.05184893 Hartree

Free energy: -1931.586927 Hartree

Pd	0.43455300	0.32626000	2.31931400
P	-0.87587500	0.07471800	0.36544900
C	-2.21899500	-1.17807100	0.41330700
C	-3.31561800	-1.17001000	-0.45611500
C	-2.12189700	-2.22048800	1.35428000
C	-4.29272000	-2.16580800	-0.40141000
H	-3.42200400	-0.37259900	-1.18514000
C	-3.08030300	-3.22277600	1.41394500
H	-1.28165900	-2.23966800	2.04442900
C	-4.17509500	-3.20130100	0.53591600
H	-5.13226200	-2.12294000	-1.08493400
H	-3.01283200	-4.02888700	2.13706500
C	0.22606300	-0.50883500	-0.98561800
C	1.28418000	0.33056000	-1.38434300
C	0.16592700	-1.80014600	-1.51447000
C	2.25197200	-0.11261800	-2.26999700
H	1.37398200	1.32614800	-0.96346300
C	1.14272000	-2.26397700	-2.40367100
H	-0.63960700	-2.46849900	-1.22667700
C	2.19740600	-1.42252400	-2.77005500
H	3.08810800	0.51879900	-2.55007600
H	1.07168200	-3.27532900	-2.78599200
C	-1.66473100	1.57461000	-0.33508000
C	-2.11955000	2.56805500	0.55116400
C	-1.84236900	1.77817200	-1.70889000

C	-2.74721900	3.71251000	0.08075300
H	-1.96634900	2.44082900	1.61994500
C	-2.46619100	2.92820900	-2.19780000
H	-1.47757500	1.03695600	-2.41386800
C	-2.92568200	3.90040600	-1.29919500
H	-3.09828800	4.48510600	0.75682900
H	-2.58111700	3.05564900	-3.26755100
C	2.41797500	0.38906800	1.82640400
C	3.02295900	-0.81088500	1.43472700
C	2.98148200	1.59669600	1.37454500
C	4.09650000	-0.82327100	0.53604200
H	2.63463900	-1.75852200	1.79568000
C	4.05011400	1.59443100	0.48527400
H	2.56921700	2.54464600	1.70700100
C	4.59525000	0.38234400	0.03538500
H	4.50553300	-1.77423300	0.21541300
H	4.47041700	2.52187500	0.10797200
C	1.89582300	1.50954700	4.60868800
C	1.75128700	0.40007900	3.86434900
H	2.05230700	-0.56408000	4.28029400
H	2.24102600	1.46816500	5.64208900
H	1.69351700	2.50289000	4.21360900
O	3.23291800	-1.78089800	-3.58952000
O	-3.54483800	5.05856000	-1.65953200
O	-5.06419200	-4.22295000	0.67846000
C	-6.20236100	-4.25166000	-0.17062500
H	-5.91757500	-4.33228300	-1.22806300
H	-6.76967900	-5.13836500	0.11628200
H	-6.83101900	-3.36167800	-0.03579300
C	3.24916000	-3.10094900	-4.11126700
H	4.15204800	-3.17459300	-4.71970000
H	3.28918400	-3.85267900	-3.31172300
H	2.37246700	-3.29797200	-4.74238100
C	-3.73777900	5.31959700	-3.04214900
H	-4.23910800	6.28699600	-3.09883400
H	-2.78280000	5.37572000	-3.58100500

H	-4.37124600	4.55698500	-3.51432500
O	5.59391800	0.48955700	-0.89684900
C	6.05529800	-0.70357800	-1.51313800
H	6.80381100	-0.39364800	-2.24523600
H	6.52789300	-1.38140800	-0.78881400
H	5.24191300	-1.23058200	-2.02941500

(N) The final product complex

Total energy: -1932.12922407 Hartree

Free energy: -1931.660519 Hartree

Pd	-0.22143200	0.09517900	-2.50659800
C	2.01454700	-1.39198900	-0.19075200
C	3.14549700	-1.33086800	0.63102800
C	1.70434500	-2.61921100	-0.80615100
C	3.94839500	-2.45421600	0.84812000
H	3.41597000	-0.39459300	1.10975100
C	2.48660700	-3.74489800	-0.59271000
H	0.84274500	-2.67671200	-1.46639700
C	3.61682500	-3.66984600	0.23678400
H	4.82079600	-2.36718000	1.48481700
H	2.25549800	-4.69369900	-1.06594800
C	-0.26949200	-0.02812100	0.93975500
C	-1.43758500	0.75564100	0.88154400
C	-0.06309500	-0.82773100	2.06858700
C	-2.35618800	0.74796600	1.92006900
H	-1.64308200	1.35109600	-0.00310400
C	-0.99296400	-0.86294200	3.11357100
H	0.82593800	-1.44616800	2.14042200
C	-2.14598800	-0.07519500	3.03593500
H	-3.26585100	1.33611600	1.87074100
H	-0.80839800	-1.50745100	3.96490900
C	1.95447800	1.48964000	-0.09754900
C	2.69478800	2.07416300	-1.14241000
C	2.07452100	2.03550000	1.18495500
C	3.53424700	3.15327500	-0.90829500
H	2.60245000	1.67591300	-2.15007900

C	2.90998200	3.12819000	1.43466700
H	1.50589000	1.61090000	2.00684400
C	3.64681700	3.68959800	0.38459700
H	4.10634000	3.61056000	-1.70892300
H	2.97274300	3.52863000	2.43952400
C	-3.14519300	-0.34191500	-2.20106800
C	-3.54591300	-1.29782400	-1.25669600
C	-3.69676500	0.95108000	-2.08972000
C	-4.42209400	-0.98933800	-0.21616800
H	-3.13560500	-2.30276300	-1.31672600
C	-4.57038600	1.27316900	-1.06362400
H	-3.41984200	1.71800700	-2.80585900
C	-4.92700800	0.30988400	-0.10544000
H	-4.67459800	-1.75142500	0.51086700
H	-4.98261100	2.27246000	-0.96695400
C	-1.61462000	0.10213000	-4.21798400
C	-2.15030900	-0.71389300	-3.22636400
H	-1.97983200	-1.78731800	-3.31088600
H	-1.11120000	-0.34973200	-5.06873200
H	-1.94745100	1.12773800	-4.35874500
O	-3.13936600	-0.05325700	3.97765400
O	4.48976100	4.75377900	0.50863200
O	4.32380900	-4.82728600	0.37491600
C	5.49018200	-4.81164400	1.18376000
H	5.25870900	-4.55243000	2.22561300
H	5.89551500	-5.82415900	1.14848200
H	6.24119900	-4.10880100	0.79933800
C	-2.98849400	-0.86585100	5.13178400
H	-3.87827200	-0.69533700	5.74018900
H	-2.92597700	-1.93139800	4.87340300
H	-2.09781600	-0.58650700	5.70985800
C	4.63286800	5.35390900	1.78700900
H	5.33790900	6.17653100	1.65698700
H	3.67878100	5.75157000	2.15769100
H	5.03600800	4.64714900	2.52469500
O	-5.74103800	0.75067700	0.89863000

C	-6.05407400	-0.15081800	1.95372700
H	-6.70632800	0.40099100	2.63293900
H	-6.58944200	-1.03547300	1.58392200
H	-5.15285200	-0.46187100	2.49604100
P	0.89331100	0.03791700	-0.49037100

(O) PdL

Total energy: -1507.88312295 Hartree

Free energy: -1507.569249 Hartree

Pd	0.00073100	0.00016700	3.17716200
C	1.48132400	-0.75900700	0.16539800
C	1.41929400	-1.51385300	-1.01096000
C	2.74215100	-0.54529700	0.75385200
C	2.57346400	-2.04276900	-1.59695000
H	0.46069700	-1.70019700	-1.48475600
C	3.89611700	-1.05476500	0.17809300
H	2.80643600	0.02146800	1.67914900
C	3.81966400	-1.81080800	-1.00306400
H	2.48542800	-2.62879600	-2.50405000
H	4.87108600	-0.89513700	0.62693500
C	-0.08361400	1.66195300	0.16533300
C	-0.90020600	2.64646100	0.75317300
C	0.60218500	1.98626800	-1.01024500
C	-1.03607100	3.90062100	0.17756200
H	-1.42391200	2.41829700	1.67795400
C	0.48303800	3.25034200	-1.59606700
H	1.24382700	1.24982000	-1.48362300
C	-0.34205800	4.21304700	-1.00282100
H	-1.66262500	4.66473600	0.62595900
H	1.03533900	3.46757000	-2.50259000
C	-1.39786400	-0.90359500	0.16556500
C	-1.84412500	-2.10165100	0.75472200
C	-2.02020600	-0.47273400	-1.01112000
C	-2.86264100	-2.84607200	0.17921200
H	-1.38600600	-2.44024300	1.68047500
C	-3.05559900	-1.20763100	-1.59688100

H	-1.70203000	0.45028500	-1.48541400
C	-3.47859500	-2.40228900	-1.00239900
H	-3.21258900	-3.76967900	0.62864200
H	-3.51867800	-0.83864100	-2.50430300
O	-0.53461300	5.47451800	-1.48234700
O	-4.47516600	-3.19936800	-1.48180200
O	5.00834400	-2.27485400	-1.48267600
C	4.99647000	-3.06157300	-2.66412800
H	4.59895000	-2.50138300	-3.52108600
H	6.03658800	-3.32638300	-2.86094200
H	4.40864300	-3.97993200	-2.53418800
C	0.15357500	5.85809200	-2.66310200
H	-0.13758600	6.89110100	-2.86013800
H	1.24271800	5.80885200	-2.53210800
H	-0.13156800	5.23361500	-3.52038700
C	-5.14992800	-2.79601200	-2.66371600
H	-5.89961200	-3.56412300	-2.86040200
H	-5.65094000	-1.82745800	-2.53446800
H	-4.46570000	-2.73262100	-3.52046900
P	0.00007500	-0.00023600	0.95908200