Supplementary material to:

Dramatic Mechanistic Switch in Sn/Au^{I} Group Exchanges: Transmetalation *vs.* Oxidative Addition

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Experimental Section

General section

All reactions were carried out under argon or nitrogen. Solvents were dried using a solvent purification system (SPS). NMR spectra were recorded on a Bruker AV 400 or a Varian 500/MR instrument equipped with a variable-temperature probe. Chemical shifts were reported in ppm from tetramethylsilane (^{1}H), CCl_3F (^{19}F), or 85% H_3PO_4 (^{31}P), with positive shifts downfield, at ambient probe temperature unless otherwise stated. The temperature for the NMR probe was calibrated using ethylene glycol as a temperature standard (T > 300K) and with a methanol standard (T < 300K). In the ^{19}F and ^{31}P spectra measured in non-deuterated solvents, a coaxial tube containing acetone-d_6 was used to maintain the lock ^{2}H signal. The chemical shifts found for the gold complexes are in good agreement with values reported in the literature for similar complexes. IR spectra in solution were measured with a ReactIR (Metler-Toledo) spectrometer, Combustion CHN analyses were made on a Perkin Elmer 2400 CHN microanalyzer. Weights for kinetic experiments and for the measurement of K_{eq} were measured in a "Cobos Precision Shimadzu" balance, with a precision of 0.01 mg. Unless specified, all compounds were used from commercial sources and used without further purification. The following compounds: $[Au(C_6F_5)(tht)]$,[1] $[Au(C_6F_5)(PMe_3)]$, [2] $[AuCl(PMe_3)]$, [3] $[AuPh(PPh_3)]$, [4] $[Au(C_6Cl_2F_3)(PMe_3)]$,[5] methyl-1-naphtyltri-n-butyltin,[6] 3,5-dichloro-2,4,6-trifluorofenyltri-n-butyltin,[7] and pentafluorophenyltri-n-butyl, [8] were prepared as reported in the literature. Stock solutions of n-Bu_3SnOTf in different concentrations were prepared in dry THF under argon atmosphere and subsequently dried with zeolites for three days before their use.

Synthesis and characterization of the complexes

$[AuI(PMe_3)]$. KI (2.15 g, 12.9 mmol) was added to a stirred solution of $[AuCl(PMe_3)]$ (200 mg, 0.65 mmol) in acetone (50 mL) at room temperature. After 24 h the solution was filtered and the solvent was evaporated. The solid obtained was dissolved in dichloromethane, filtered and crystallized from dichloromethane/pentane. Yield: 200 mg. (77 %). ^{1}H NMR ($CDCl_3$, 298 K): δ 1.75 (d, J = 7.8 Hz, 9H). ^{31}P NMR ($CDCl_3$, 298 K): δ 1.85 (s, 1P). ^{13}C NMR ($CDCl_3$, 298 K): δ 16.15 (d, J = 37 Hz). Cald. for C_3H_9AuIP: C, 9.00; H, 2.27. Found: C, 9.30; H, 2.16.

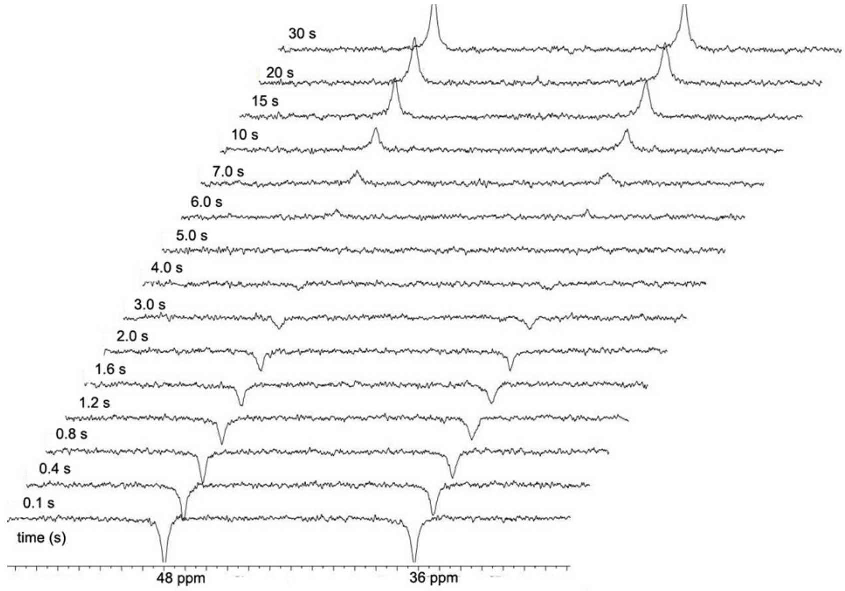
$[Au(C_6H_5)(PMe_3)]$. A two-necked flask was charged with $[AuCl(PMe_3)]$ (700 mg, 2.27 mmol) and 100 mL of THF. A 1M solution of phenylmagnesium bromide in THF (2.6 mL, 2.6 mmol) was added dropwise under stirring. The mixture was stirred during 4 hours and then three drops of water were added to quench the reaction. The solvents were evaporated and the residue was dissolved in dichloromethane, the solution was filtered through celite, concentrated and crystallized by addition of n-hexane. Yield 794.5 mg (95 %). ^{1}H NMR ($CDCl_3$, 298 K): δ 7.4-7.3 (m, *J* = 6.0 Hz, 2H) δ 7.15-7.05 (m, 2H), δ 6.90 (t, *J* = 7.4 Hz, 1H). ^{31}P NMR ($CDCl_3$, 298 K): δ 6.38 (s). ^{13}C NMR ($CDCl_3$, 298 K, quaternary carbons are not included): δ 15.87 (d, *J* = 31 Hz), δ 125.64 (s), δ 127.45 (d, *J* = 6 Hz), δ 139.52 (s). Cald. For $C_9H_{14}AuP$: C, 30.87; H, 4.03. Found: C, 30.45; H, 3.93.

[Au(2-MeC$_{10}$H$_6$)(PMe$_3$)]. A two-necked flask was charged with 280 µL (1.78 mmol) of 1-bromo-2-metylnaphtalene and 50 mL of THF. The mixture was cooled down to -78 ºC and 0.7 mL (1.0 mmol) of a 2.5 M solution of *n*-BuLi in hexane were added dropwise. The reaction was stirred for 1h and 500 mg (1.62 mmol) of [AuCl(PMe$_3$)] were subsequently added. The cooling bath was removed and the mixture was stirred at room temperature for 4 hours. Next, a few drops of EtOH were added. The solvents were evaporated and then a saturated aqueous solution of NH_4Cl (30 mL) was added. The aqueous layer was decanted and extracted with Et_2O (3x30 mL). All the organic layers were combined, washed with brine (3x60 mL) and dried over $MgSO_4$. The solvent was removed under reduced pressure and the resulting yellow solid was dissolved in CH_2Cl_2, filtered and the compound precipitated by slow addition of n-hexane under stirring. Yield 580 mg (86 %). ^{1}H NMR (acetone-d_6, 298 K): δ 8.48 (d, *J* = 8.04 Hz, 1H), δ 7.70 (d, *J* = 7.8 Hz, 1H), δ 7.55 (d, *J* = 8.0 Hz, 1H), δ 7.3-7.1 (m, 3H), δ 2.70 (s, 3H), δ 1.65 (d, *J* = 9.6Hz, 9H). ^{31}P NMR (acetone-d_6, 298 K): δ 9.49 (s). ^{13}C NMR (acetone-d_6, 298 K, quaternary carbons are not included): δ 15.51 (d, *J* = 32 Hz), δ 26.97 (s), δ 124.09 (s), δ 124.20 (s), δ 125.33 (s), 128.43 (s), δ 128.61 (d, *J* = 8 Hz), δ 134.20 (s). Cald. For $C_{14}H_{18}AuP$: C, 40.59; H, 4.38. Found: C, 40.38; H, 4.22.

[Au(C$_6$H$_5$)(PCy$_3$)]. A two-necked flask was charged with 400 mg (0.78 mmol) of [AuCl(PCy$_3$)] dissolved in 20 mL of THF. To this solution, 0.90 mL of a 1M solution (0.90 mmol) of phenylmagnesium bromide in THF were added dropwise. The reaction was stirred during 4 hours at room temperature and then three drops of water were added to hydrolyze any remaining organomagnesium. The solvents were evaporated yielding a white solid that was recrystallized by dissolving in CH_2Cl_2 filtration through a celite pad, and slow addition of *n*-hexane. Yield 226 mg (53 %). ^{1}H NMR ($CDCl_3$, 298 K): δ 7.40-7.30 (m, 2H), δ 7.15-7.00 (m, 2H), δ 6.88 (t, *J* = 7.4 Hz, 1H), δ 2.10-1.00 (m, 33 H). ^{31}P NMR ($CDCl_3$, 293 K): δ 57.1 (s). ^{13}C NMR ($CDCl_3$, 298 K, quaternary carbons are not included): δ 26.05 (s), δ 27.21 (d, *J* = 12 Hz), δ 30.69 (s), δ 33.24 (d, J = 23.64 Hz), δ 125.36 (s), δ 127. 43 (d, J = 6 Hz), δ 139.26 (s). Cald. for $C_{24}H_{38}AuP$: C, 51.99; H, 6.91. Found: C, 51.64; H, 6.77.

[Au(vinyl)(PMe_3)]. This complex could not be isolated in a pure form due to extensive decomposition, but it was prepared in solution in order to identify its NMR signals. [AuCl(PMe_3)] (1.00 g, 3.24 mmol) was dissolved in 30 mL of THF and the solution was cooled down to -20 ºC. To this solution, 3.2 mL of a solution 1M of vinylmagnesium bromide in THF (3.2 mmol) were added dropwise. The reaction was stirred during 0.5 hours and further 0.5 mL (0.5 mmol) of vinylmagnesium bromide were subsequently added. The solvents were evaporated, the residue was dissolved in $CDCl_3$, filtered, and the NMR was registered under nitrogen. ^{1}H NMR ($CDCl_3$, 298 K): δ 7.0-7.8 (m, 1H), δ 5.8-5.6 (m, 1H), δ 5.2-5.0 (m, 1H), δ 1.5-1.42 (d, J = 9.4 Hz 9H). ^{31}P NMR ($CDCl_3$, 298 K): δ 7.92 (s).

^{31}P NMR T_1 Inversion Recovery Experiment of a mixture of $PhAuPPh_3$ and $ClAuPPh_3$.



T_1 = 7.2 s for both complexes. Since the relaxation times are almost identical for both complexes, the integration of the ^{31}P NMR spectra is a reliable measurement of the relative concentration of the compounds in solution.

a) Reactions of aryl gold complexes with $SnBu_3X$.

$$AuRPMe_3 + SnBu_3X \rightleftharpoons AuXPMe_3 + SnBu_3R \qquad Keq = \frac{[AuXPMe_3][SnBu_3R]}{[AuRPMe_3][SnBu_3X]}$$

The equilibrium constants K_{eq} for the transmetalation reactions between $SnBu_3X$ (X = Cl, I) and [AuRL] (R = vinyl, phenyl, $C_6Cl_2F_3$: 3,5-dichloro-2,4,6-trifluorophenyl, C_6F_5: pentafluorophenyl, and $C_{11}H_9$: 2-methyl naphthyl; L = PMe_3, PCy_3, PPh_3), were measured by integration of the ^{31}P NMR signals of the initial and final products. In a typical experiment, a NMR tube (5mm) was charged under Ar with the gold complex (10 mg) and $XSnBu_3$ (2 eq. to 10 eq.), and THF was added to reach a fixed volume of 0.6 mL. Then, the tube was charged with an acetone-d_6 capillary for NMR registration. The samples reacted at room temperature and were checked periodically until verifying that no further changes in concentration were produced (from 1 to 48 h).

b) Reactions of gold halide complexes with $SnBu_3R$.

$$AuXPMe_3 + SnBu_3R \rightleftharpoons AuRPMe_3 + SnBu_3X \qquad Keq = \frac{[AuRPMe_3][SnBu_3X]}{[AuXPMe_3][SnBu_3R]}$$

The equilibrium constants K_{eq} for the transmetalation reactions between [XAuL] (X = Cl, I) and $SnBu_3R$ (R = vinyl, phenyl, $C_6Cl_2F_3$: 3,5-dichloro-2,4,6-trifluorophenyl, C_6F_5: pentafluorophenyl, and $C_{11}H_9$: 2-methyl naphthyl) with the ligands L = PMe_3, PCy_3, PPh_3, were measured by integration of the ^{31}P NMR signals of the initial and final products. In a typical experiment, a NMR tube (5mm) was charged under Ar with the gold complex (10 mg) and Bu_3SnR (10 eq.), and THF was added to reach a fixed volume of 0.6 mL. The tube was charged with an acetone-d_6 capillary for NMR registration. The samples reacted at room temperature and were checked periodically until verifying that no further changes in concentration were produced (from 1 to 48 h).

Table S1. K_{eq} for the Sn/Au transmetalation. The equilibria were measured in THF at room temperature and the constants were calculated when possible (otherwise the upper limit value is given).

$$AuRL + SnBu_3X \rightleftharpoons AuXL + SnBu_3R \qquad L_1 = PPh_3^{[a]}, L_2 = PMe_3, L_3 = PCy_3$$

Entry	R	K_{eq} (X = I)	K_{eq} (X = Cl)
1	Vinyl	$L_1 : > 10^{+5}$ $L_2 : > 10^{+5}$	$L_1 : > 10^{+5}$ $L_2 : 5$
2	C_6H_5	$L_1 : > 10^{+5}$ $L_2 : > 10^{+5}$	$L_1 : > 10^{+5}$ $L_2 : 1.1$ $L_3 : 0.6$
3	$C_6F_3Cl_2$	$L_1 : > 10^{+5}$ $L_2 : 0.7$	$L_1 : > 10^{+5}$ $L_2 : 4.3\cdot10^{-3}$
4	C_6F_5	$L_2 : 0.2$	$L_2 : > 10^{-6}$
5	$C_{11}H_9$	$L_1 : > 10^{+5}$ $L_2 : 25$	$L_1 : 2.6\cdot10^{-2}$ $L_2 : 2.2\cdot10^{-3}$

[a] Values for $L_1 = PPh_3$ are taken from Ref. 9.

Kinetic experiments

Kinetic experiments were monitored by ^{31}P NMR. A NMR tube (5mm), placed in a bath at –78 ˚C, was charged with [AuPh(PPh_3)], [AuPh(PMe_3)] or [AuPh(PCy_3)] and Bu_3SnCl, and a small amount of THF (about 0.5 mL) was added to dissolve the solids. Next, an additional amount of THF was added to reach a fixed volume of 0.6 mL. The tube was subsequently charged with an acetone-d_6 capillary for NMR lock and placed in a thermostated probe. ^{31}P NMR spectra were recorded at fixed time intervals of 6 or 15 min. Concentration-time data were obtained from the integrated areas of NMR signals of the gold complexes [AuPh(PPh_3)], [AuPh(PMe_3)], and [AuPh(PCy_3)]. The initial rate was obtained by linear fitting of the concentration-time curves in the interval 0-15% of consumption of the starting reagents.

In a typical experiment at 303 K, a NMR tube was charged with [AuPh(PMe_3)] = 0.05 mol L^{-1} and [Bu_3SnCl] = 0.95 mol L^{-1}.

Experimental rate constants for the transmetalation of [AuPh(PMe_3)], [AuPh(PPh_3)] or [AuPh(PCy_3)] with Bu_3SnCl.

Table S2. Values for the transmetalation reaction of [AuPhL] with Bu_3SnCl in THF at 303 K.

Gold compound	[AuPhL] / mol L^{-1}	Rate constant / L mol^{-1} s^{-1}
[AuPh(PMe_3)]	0.039	5.08(3) $x10^{-4}$
[AuPh(PPh_3)]	0.027	9.4(2) $x10^{-5}$
[AuPh(PCy_3)]	0.026	3.453(8) $x10^{-4}$

Experimental kinetic order in [AuPh(PMe_3)]

Table S3. Starting conditions for the transmetalation reaction of [AuPh(PMe_3)] with Bu_3SnCl in THF at 303 K.

[AuPh(PMe_3)] / mol L^{-1}	Initial rates (r_0) / mol L^{-1} s^{-1}
$1.32x10^{-2}$	3.0(6) $x10^{-6}$
$2.36x10^{-2}$	5.1(5) $x10^{-6}$
$4.88x10^{-2}$	9.8(8) $x10^{-6}$
$7.13x10^{-2}$	1.6(1) $x10^{-5}$
$8.98x10^{-2}$	2.40(9) $x10^{-5}$
[Bu_3SnCl]$_0$ = 0.95 mol L^{-1}	

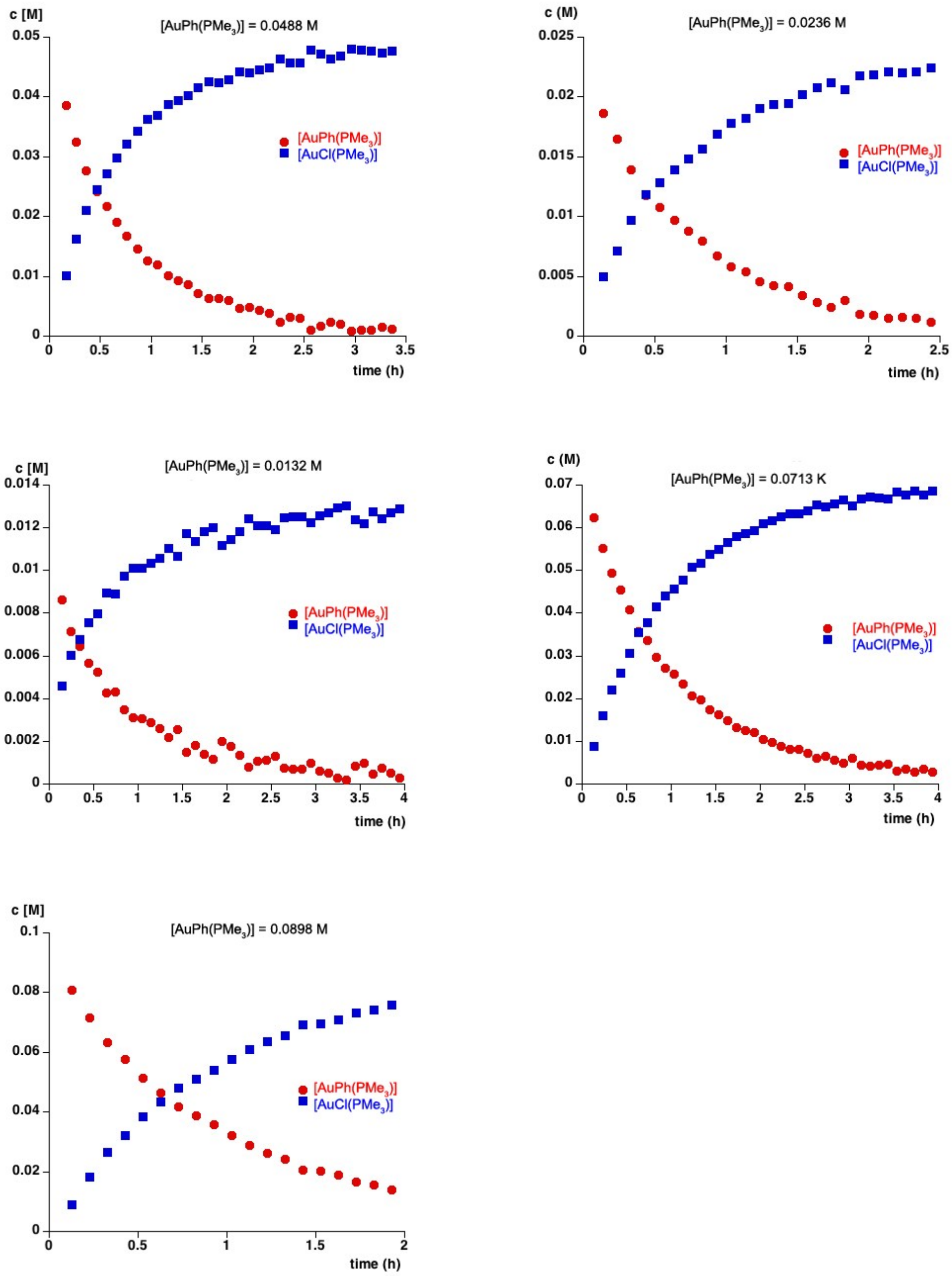


Figure S1. Representation of the concentrations of [AuPh(PMe$_3$)] and [AuCl(PMe$_3$)] *vs* time. Starting conditions: [Bu$_3$SnCl]$_0$ = 0.95 mol L^{-1} in THF at 303 K.

The experimental representation of $\ln(r_0)$ *vs* $\ln[AuPh(PMe_3)]$ for different concentrations of $[AuPh(PMe_3)]$ leads to a straight line with slope +1.05.

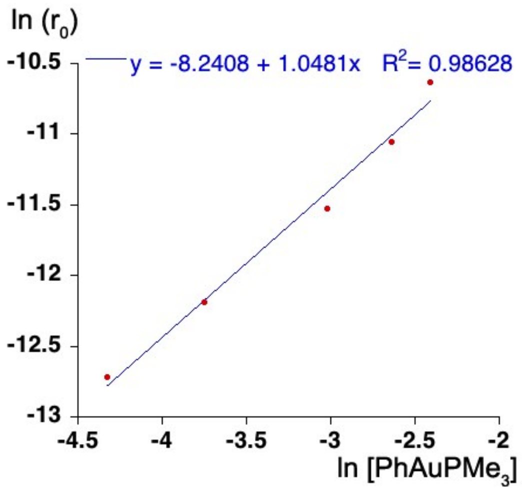


Figure S2. Plot of $\ln[r_0]$ *vs* $\ln[AuPh(PMe_3)]$.

Activation parameters for the transmetalation between $[AuPh(PMe_3)]$ and Bu_3SnCl

Table S4. Values of the rate constants for the transmetalation reaction between $[AuPh(PMe_3)]$ and Bu_3SnCl in THF at different temperatures.

T / K	**Rate constant / L mol^{-1} s^{-1}**
254	2.78(1) x10^{-5}
273	1.04(1) x10^{-4}
303	2.95(1) x10^{-4}
322	6.02(2) x10^{-4}
$[AuPh(PMe_3)]_0 = 0.07$ mol L^{-1}	
$[Bu_3SnCl]_0 = 0.95$ mol L^{-1}	

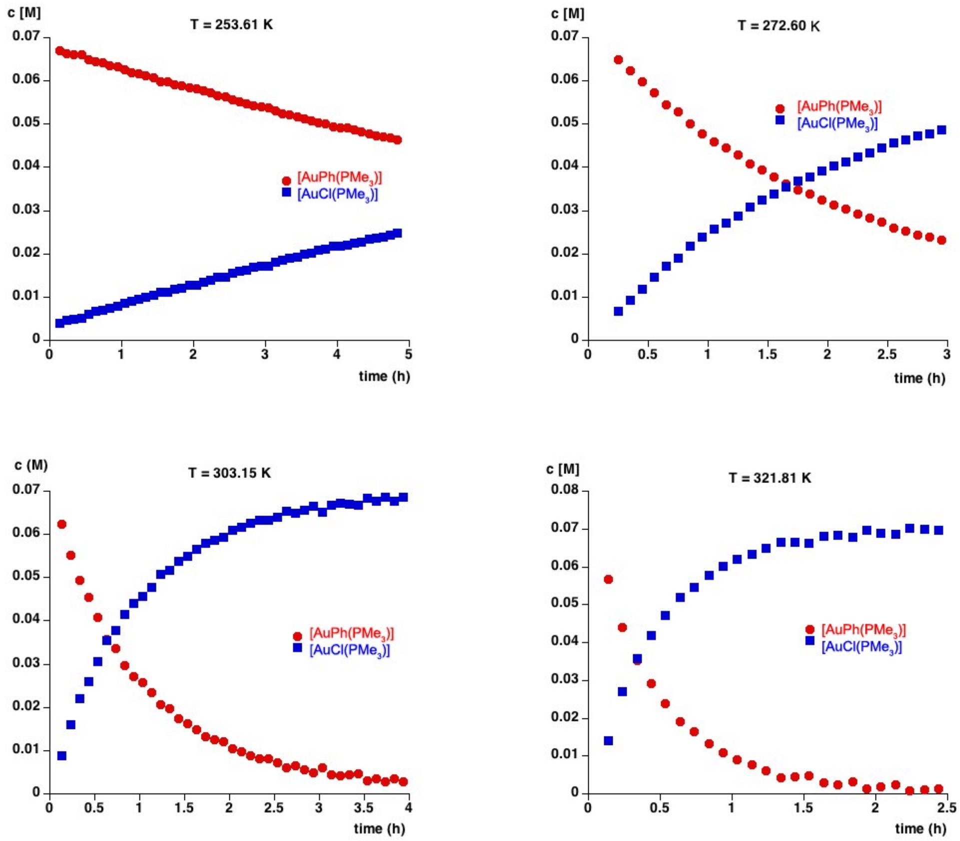


Figure S3. Representation of the concentrations of [AuPh(PMe_3)] and [AuCl(PMe_3)] as a function of time. Starting conditions: [Bu_3SnCl]$_0$ = 0.95 mol L^{-1} in THF at different temperatures.

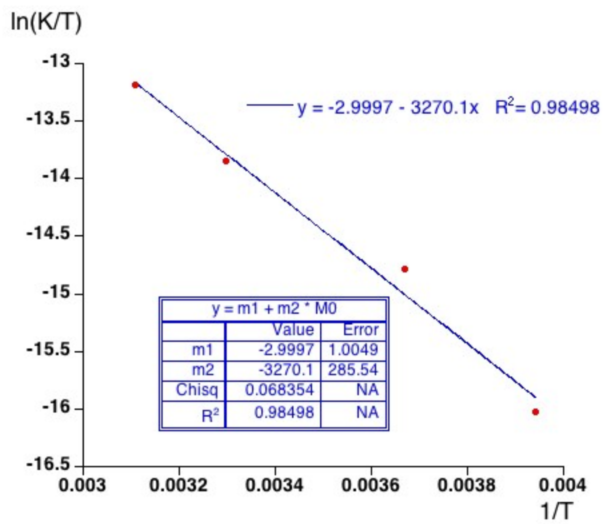


Figure S4. Eyring plot (data from Table S4).

With the data obtained in the representation shown in figure S4, the following activation parameters were determined: $\Delta H^{\ddagger} = 27(2)$ kJ mol^{-1} and $\Delta S^{\ddagger} = -223(23)$ J K^{-1} mol^{-1}.

Vinyl for aryl exchange

$$[AuPhL] + Bu_3Sn(vinyl) = Bu_3SnPh + [Au(vinyl)L] \ (L = PMe_3).$$

The kinetic experiment was monitored by ^{31}P NMR at 323 K. A NMR tube (5mm) was placed in a bath at –78 ˚C and charged with $Bu_3Sn(vinyl)$ (0.95 mol L^{-1}) and $[AuPh(PMe_3)]$ (0.048 mol L^{-1}). A small amount of THF (about 0.5 mL) was added to dissolve the solids. When the gold complex was completely dissolved, an additional amount of THF was added to reach a fixed volume of 0.60 mL. The tube then was charged with an acetone-d_6 capillary for NMR lock and placed in a thermostated probe. The rate constant obtained was k = (1.7 ±0.02) x10^{-6} ($\Delta G^{\ddagger}$ = 115.09 kJ mol^{-1}; = 27.49 kcal mol^{-1}). In the same reaction, after 48 hours in THF-d_8 at 323 K, the presence of a small amount of styrene was detected in the Gas Chromatography-Mass.

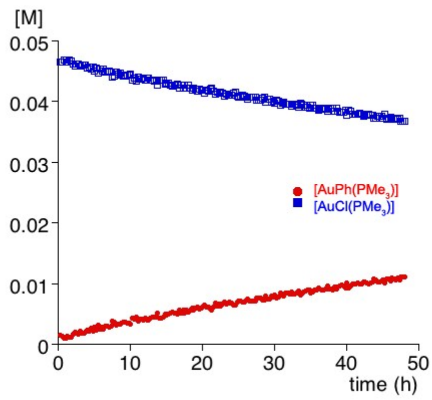


Figure S5. Observed concentration of $[Au(vinyl)(PMe_3)]$ and $[AuPh(PMe_3)]$ vs. time. Starting conditions: $[Bu_3SnCl]_0$ = 0.95 mol L^{-1} and $[AuPh(PMe_3)]$ (0.048 mol L^{-1}) at 323 K.

Computational Section

All the calculations were carried out by means of the Density Functional Theory using the dispersion corrected hybrid functional ωB97X-D,[10] as implemented in the Gaussian09 program.[11] We employed this methodology based on the satisfactory results obtained in our previous studies on related Pd/Au and Au/Sn transmetalations.[9,12] Geometry optimizations in vacuum were performed without imposing any constraint and using the double-ζ basis set 6-31G(d,p) to describe the C, H, P, and Cl atoms. For the Sn and Au metals, the effective core potential LANL2DZ[13] including d- (exponent 0.180) and f-polarization (exponent 1.050) functions, respectively, was employed. The nature of all the stationary points was further verified through vibrational frequency analysis. Furthermore, for transition states, geometry relaxations along the reaction coordinate were performed to confirm that they connect the corresponding reaction minima.

Solvent effects (THF, $\varepsilon = 7.43$) were introduced through single point calculations at the optimized gas-phase geometries using the *SMD* solvation model[14] and a larger basis set for C, H, P, and Cl atoms. This consisted in a triple-ζ 6-311G(d,p) for C, H, and P, and the same basis set plus diffuse functions for Cl. To model the changes in entropy in the condensed phase, entropic contributions were evaluated at the pressure of 301 atm. This pressure was calculated using the experimental density of THF at 298 K (ρ = 0. 889 g/mL)[15] and following the scheme described by Martin *et al*.[16-17] Gibbs energies in solution were obtained by adding to the potential energies in solution the gas-phase Gibbs energy corrections of the solute at the experimental temperature of 323 K and at 301 atm. Gibbs energies at the same temperature and at 1 atm were also computed and are presented in Table S5. We find, however, that the values at 301 atm are in a better agreement with the ones obtained experimentally, and therefore, we have adopted this methodology throughout this work.

Table S5. Relative Gibbs energies (in kcal/mol) in THF at 323K and the pressures of 1 and 301 atm for the species involved in the Ph/Cl and Ph/vinyl exchanges presented in Figures 1 and 2.

Exchange	**Species**	$\Delta G_{THF, 323K, 1atm}$	$\Delta G_{THF, 323K, 301atm}$
Ph/Cl	**I1**	5.9	2.2
	TS1	27.9	24.2
	I2	21.5	17.9
	TS2	21.8	18.1
	I3	6.2	2.5
Ph/vinyl	**I4**	4.2	0.5
	TS3	32.3	28.6
	I5	19.7	16.1
	TS4	32.5	28.9
	I6	3.2	-0.5

Optimized transition state structure for the oxidative addition of $SnClBu_3$ to $[AuPh(PMe_3)]$.

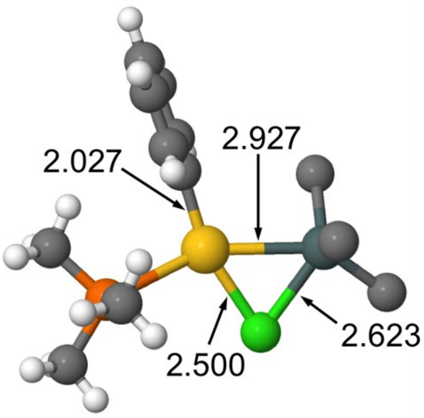


Figure S6. Optimized transition state structure for the oxidative addition of $SnClBu_3$ to $[AuPh(PMe_3)]$. Relevant bond distances are shown in Å. The corresponding $\Delta G_{THF, 323K, 301atm}$ is 34.2 kcal/mol,

Alternative transmetalation mechanism for the Ph/vinyl exchange between [AuPh(PMe$_3$)] and SnBu$_3$(vinyl).

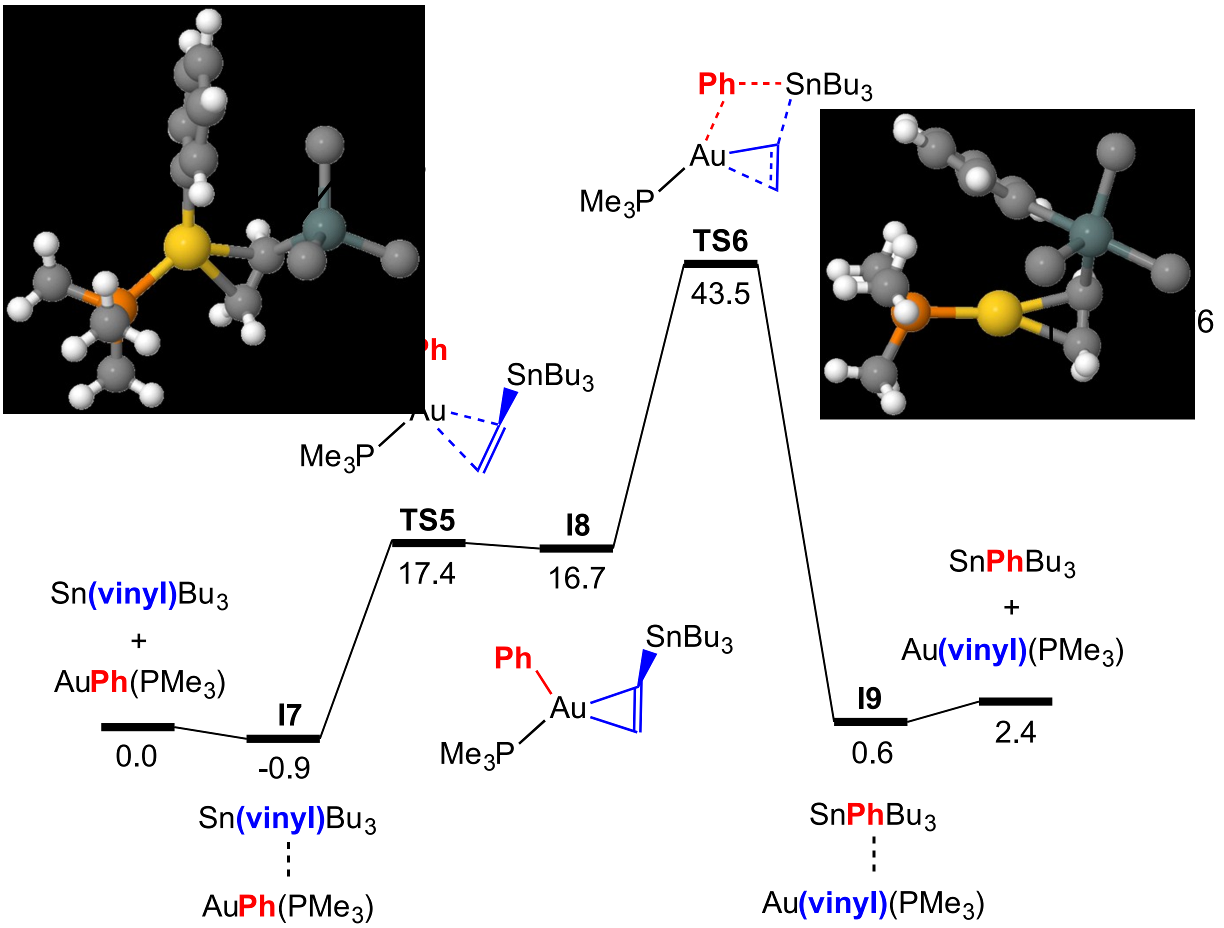
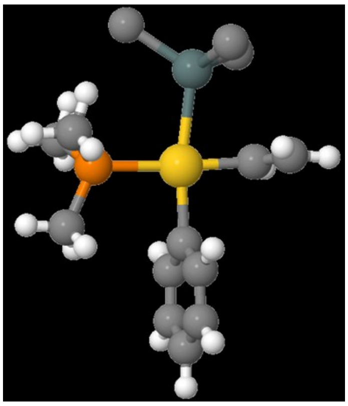
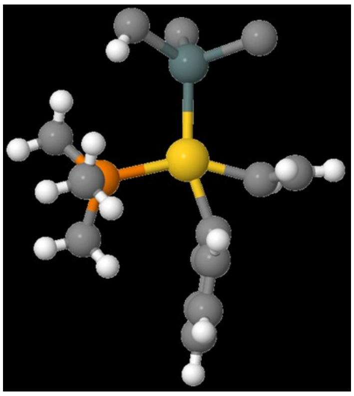


Figure S7. Calculated Gibbs energy profile in THF at 323K and 301 atm for the alternative transmetalation mechanism between [AuPh(PMe$_3$)] and Sn(vinyl)Bu$_3$ to produce [Au(vinyl)(PMe$_3$)] and SnPhBu$_3$.

Optimized relevant structures involved in the formation of the Ph-vinyl coupling product.



I5-*CIS*



TS4-*CIS*

Figure S8. Optimized geometries of one of the two possible *cis* isomers (**I5-*CIS***) of the intermediate **I5** and the corresponding transition state (**TS4-*CIS***) equivalent to **TS4**.

Table S6. Selected donor-acceptor interactions in the second order perturbative analysis of NBO for **TS1** and **TS3**. *BD*, *LP* and *LV* stand for Bonding, Lone Pair, and Lone Vacancy orbitals. Energies in kcal/mol.

	Donor	**Orbitals**	**Acceptor**	**Orbitals**	**E**
TS1	LP Au	Au s(7%) d(93%)	BD* Sn−C_{Ph}	85% Sn s(15%) p(85%) 15% C_{Ph} s(27%) p(73%)	17.3
	BD Sn−C_{Ph}	15% Sn s(15%) p(85%) 85% C_{Ph} s(27%) p(73%)	BD* Au−P	79% Au s(89%) d(11%) 21% P s(31%) p(69%)	144.7
TS3	LP Au	Au s(3%) d(97%)	BD* Sn−C_{vinyl}	79% Sn s(20%) p(80%) 21% C_{vinyl} s(31%) p(69%)	22.3
	BD Sn−C_{vinyl}	21% Sn s(20%) p (80%) 79% C_{vinyl} s(31%) p (69%)	BD* Au−C_{Ph}	78% Au s(93%) d(7%) 22% C_{Ph} s(26%) p(74%)	63.1

Table S7. Main contributions to the natural localized molecular orbitals (NLMO) involved in the donation-backdonation interactions in **TS1** and **TS3**. *BD* and *LP* stand for Bonding and Lone Pair.

	% from Parent NBO	Atomic Hybrid Contributions*	Occupancy
TS1	96% LP Au	96% Au s(7%) d(93%) 1% C_{Ph} s(26%) p(73%) d(1%) 2% Sn s(27%) p(73%)	2.00
	83% BD C_{Ph}−Sn	11% Au s(90%) d(10%) 3% P s(46%) p(54%) 70% C_{Ph} s(27%) p(73%) 13% Sn s(31%) p(69%)	2.00
TS3	91% LP Au	91% Au s(4%) d(96%) 5% Sn s(31%) p(69%) 2% C_{vinyl} s(25%) p(75%)	2.00
	91% BD Sn−C_{vinyl}	5% Au s(92%) p(1%) d(7%) 1% C_{Ph} s(29%) p(71%) 20% Sn s(36%) p(64%) 72% C_{vinyl} s(31%) p(69%)	2.00

*Note that these values correspond to the main contributions, so they do not necessarily add up to 100%.

Cartesian coordinates of all the calculated reaction intermediates and transition states

[AuPh(PMe$_3$)]

79	-0.142455	-0.007774	0.000676
6	-3.262221	1.671161	-0.049172
6	-3.293824	-0.856773	-1.414525
6	-3.295026	-0.775697	1.459839
1	-4.384848	-0.798021	-1.358850
1	-2.950623	-0.400245	-2.345712
1	-2.984954	-1.904702	-1.416446
1	-4.354685	1.614087	-0.048078
1	-2.926401	2.243365	0.818734
1	-2.925377	2.190049	-0.949544
1	-4.386005	-0.722386	1.398715
1	-2.984191	-1.821113	1.522679
1	-2.954909	-0.266319	2.364373
6	1.895119	-0.001817	0.000227
6	2.638513	-1.194309	-0.000715
6	2.627593	1.197521	0.000569
6	4.031956	-1.192619	-0.001360
6	4.020914	1.208893	-0.000044
6	4.729826	0.011353	-0.001022
1	4.554114	2.156015	0.000230
1	5.816211	0.016446	-0.001537
15	-2.508115	0.002463	0.000072
1	2.103368	2.150102	0.001321
1	2.122967	-2.151576	-0.001017
1	4.573874	-2.134790	-0.002124

[SnBu$_3$Cl]

17	-0.839996	0.903030	2.524907
50	-0.274614	-0.170965	0.485254
6	1.357340	-1.495151	0.911530
6	2.122024	-1.889077	-0.359758
1	0.968915	-2.385447	1.418120
1	2.024550	-0.993720	1.620990
6	3.273681	-2.860116	-0.088599
1	1.439872	-2.349414	-1.089325
1	2.524024	-0.991100	-0.849377
6	4.051534	-3.227458	-1.350767
1	3.952229	-2.411236	0.647701
1	2.871512	-3.767987	0.378129
1	4.860954	-3.929219	-1.130603
1	3.396866	-3.694915	-2.094207
1	4.494927	-2.338352	-1.811690
6	-2.076014	-1.140998	-0.155267
6	-3.122102	-0.161806	-0.701021
1	-2.478663	-1.694576	0.700427
1	-1.813670	-1.886105	-0.916919
6	-4.421696	-0.851869	-1.122692
1	-3.352832	0.598338	0.056890
1	-2.711883	0.381873	-1.563168
6	-5.455277	0.124445	-1.681221
1	-4.193433	-1.620146	-1.872596
1	-4.841019	-1.380565	-0.257536
1	-6.376944	-0.389811	-1.968354
1	-5.714600	0.887133	-0.939583
1	-5.069352	0.639964	-2.567140
6	0.357038	1.407010	-0.820621
6	1.632029	2.107728	-0.337009
1	-0.463124	2.126902	-0.919253
1	0.514074	0.970829	-1.815842
6	2.113319	3.199808	-1.294848
1	1.459869	2.548157	0.653492
1	2.439071	1.372642	-0.205501
6	3.389147	3.888975	-0.814829
1	2.280429	2.758143	-2.285824
1	1.315320	3.942655	-1.419990

1	3.715660	4.660738	-1.517753
1	3.235267	4.365159	0.159184
1	4.206458	3.167837	-0.705757

[AuCl(PMe_3)]

79	0.563245	0.000094	-0.000387
15	-1.714567	0.000323	0.000117
6	-2.468140	-0.820598	-1.448744
6	-2.465612	-0.845931	1.435351
6	-2.466881	1.665786	0.015252
1	-3.557454	-0.811863	1.380711
1	-2.132094	-1.885780	1.454713
1	-2.129756	-0.362299	2.355285
1	-3.559952	-0.791640	-1.389731
1	-2.137169	-0.317531	-2.359989
1	-2.130763	-1.858589	-1.489545
1	-3.558678	1.600542	0.014951
1	-2.132578	2.203718	0.905129
1	-2.132776	2.220278	-0.864410
17	2.888066	-0.000271	0.000619

$SnPhBu_3$

6	-1.157956	-1.409943	-0.779696
6	-2.537623	-1.347821	-1.015129
6	-0.535319	-2.662303	-0.878583
6	-3.270656	-2.489850	-1.331371
6	-1.261083	-3.808511	-1.194166
6	-2.632415	-3.723365	-1.420149
1	-0.756903	-4.767775	-1.266198
1	-3.200147	-4.615639	-1.666617
50	-0.034577	0.352991	-0.290598
1	0.535914	-2.754727	-0.709667
1	-3.057097	-0.393522	-0.956305
1	-4.339557	-2.415544	-1.509092
6	1.637831	0.522395	-1.642926
6	2.812825	1.313216	-1.056362
1	1.298971	0.981056	-2.579258
1	1.961195	-0.494073	-1.900542
6	4.020964	1.386373	-1.993361
1	2.494998	2.336252	-0.808921
1	3.130016	0.861415	-0.105951
6	5.192774	2.163626	-1.396758
1	4.340511	0.365809	-2.240401
1	3.712736	1.848270	-2.939947
1	6.042744	2.196488	-2.084726
1	4.906080	3.196513	-1.171082
1	5.535016	1.703488	-0.463542
6	-1.400146	2.016025	-0.392059
6	-2.367359	2.068603	0.798233
1	-1.962438	1.930614	-1.330766
1	-0.835118	2.953147	-0.460359
6	-3.427754	3.164537	0.667503
1	-2.876738	1.101801	0.919468
1	-1.804391	2.224067	1.728564
6	-4.386258	3.208908	1.855962
1	-2.928486	4.135376	0.554693
1	-3.993036	3.002536	-0.259378
1	-5.141807	3.990773	1.734945
1	-4.908965	2.253406	1.973096
1	-3.847444	3.405898	2.789008
6	0.788064	0.138056	1.691531
6	1.554241	-1.178958	1.861790
1	-0.019816	0.202050	2.429894
1	1.453564	0.989470	1.882892
6	2.210855	-1.331948	3.235611
1	0.872839	-2.024670	1.697133
1	2.333547	-1.264877	1.089352
6	2.935684	-2.666375	3.400661

1	2.915481	-0.504654	3.390241
1	1.441558	-1.229502	4.011629
1	3.404667	-2.751579	4.385289
1	2.240364	-3.505003	3.286940
1	3.720573	-2.782404	2.645125

THF

6	-1.173552	-0.412821	-0.110325
8	-0.015972	-1.244044	-0.033474
6	1.150044	-0.447349	0.151894
6	0.752343	0.975897	-0.233528
6	-0.711289	1.010471	0.214826
1	-1.587515	-0.476778	-1.125021
1	-1.925072	-0.786420	0.592166
1	1.465551	-0.495302	1.204123
1	1.950431	-0.859709	-0.468409
1	1.373461	1.733767	0.249590
1	0.824439	1.111825	-1.317728
1	-0.772896	1.196710	1.292150
1	-1.305891	1.771076	-0.296281

I1

79	-2.207717	0.717053	0.047889
15	-1.792416	2.886196	0.894226
6	-3.163735	4.077264	0.649140
6	-1.437090	2.995354	2.684091
6	-0.361361	3.707842	0.103376
1	-1.253358	4.031302	2.983332
1	-2.285908	2.598168	3.245524
1	-0.554578	2.390040	2.903572
1	-2.912350	5.058842	1.061471
1	-3.370908	4.174705	-0.419175
1	-4.064091	3.698367	1.138372
1	-0.230407	4.724339	0.485798
1	0.538343	3.124194	0.314425
1	-0.516400	3.741957	-0.977989
6	-2.477358	-1.144260	-0.754173
6	-3.148855	-2.175920	-0.076938
6	-1.968942	-1.457636	-2.027289
6	-3.303671	-3.444609	-0.633829
6	-2.112467	-2.724567	-2.590513
6	-2.782925	-3.725959	-1.893890
1	-1.703743	-2.928028	-3.576736
1	-2.902064	-4.713938	-2.329384
50	1.670182	-0.593647	0.377015
17	1.842768	1.261617	1.898785
1	-1.448611	-0.694286	-2.600612
1	-3.826205	-4.219245	-0.078592
1	-3.561652	-1.992423	0.912181
6	3.685126	-1.337083	0.235887
6	4.776129	-0.266920	0.360110
1	3.767222	-1.848345	-0.732505
1	3.820494	-2.107756	1.004111
6	6.187788	-0.838497	0.209049
1	4.626959	0.516132	-0.395490
1	4.691279	0.237200	1.330283
6	7.274653	0.226082	0.347023
1	6.338965	-1.621404	0.963448
1	6.275347	-1.332522	-0.767322
1	8.273807	-0.206144	0.239052
1	7.161840	1.003356	-0.416615
1	7.222748	0.714253	1.325816
6	0.375663	-1.972684	1.368627
6	0.221393	-3.302968	0.622669
1	-0.600929	-1.501239	1.512199
1	0.813836	-2.134072	2.361474
6	-0.570011	-4.330547	1.434497
1	-0.291562	-3.134883	-0.332622

1	1.207335	-3.729200	0.384227
6	-0.726293	-5.664953	0.710257
1	-0.073408	-4.486365	2.401418
1	-1.558648	-3.910444	1.652689
1	-1.316865	-6.372174	1.300553
1	-1.229505	-5.521993	-0.251179
1	0.248827	-6.124743	0.514545
6	1.101857	0.349358	-1.461636
6	2.124488	1.365374	-1.974707
1	0.130298	0.829693	-1.300049
1	0.931737	-0.441618	-2.201989
6	1.639237	2.100179	-3.226418
1	2.349937	2.103551	-1.192887
1	3.075791	0.864350	-2.199676
6	2.643642	3.127140	-3.744129
1	1.419837	1.364650	-4.010723
1	0.685020	2.594252	-2.999604
1	2.272544	3.633432	-4.639858
1	2.849328	3.890907	-2.986448
1	3.595832	2.649979	-3.999030

TS1

79	1.916686	-0.618601	0.160930
15	3.553438	1.053494	0.360479
6	4.896703	0.866522	1.588488
6	4.394447	1.242835	-1.249359
6	2.856142	2.711188	0.671282
1	5.102739	2.075926	-1.229209
1	4.920784	0.319879	-1.503433
1	3.619288	1.423355	-1.999699
1	5.607911	1.695013	1.525674
1	4.464922	0.834404	2.591475
1	5.420898	-0.075373	1.410880
1	3.627420	3.479835	0.567541
1	2.061159	2.871797	-0.063280
1	2.428336	2.758790	1.675210
6	0.547796	-2.124929	-0.338334
6	0.337419	-2.362223	-1.711153
6	0.334086	-3.198503	0.552178
6	-0.078566	-3.610188	-2.171573
6	-0.060859	-4.446894	0.092822
6	-0.275491	-4.650880	-1.271087
1	-0.211494	-5.260842	0.795417
1	-0.601318	-5.623400	-1.628300
50	-1.019832	-0.151402	0.091984
17	0.619112	1.178107	-1.950755
1	0.468723	-3.043647	1.618039
1	-0.247471	-3.766597	-3.232341
1	0.490911	-1.547514	-2.414963
6	-2.402014	-0.249299	-1.550053
6	-3.124268	1.076147	-1.805599
1	-3.118299	-1.047830	-1.317606
1	-1.841272	-0.547393	-2.439337
6	-4.117425	0.998126	-2.967568
1	-3.666053	1.399469	-0.904263
1	-2.381377	1.853734	-2.020274
6	-4.821230	2.328563	-3.228533
1	-3.582333	0.678225	-3.870347
1	-4.861951	0.219218	-2.756697
1	-5.536284	2.251988	-4.053220
1	-5.369644	2.662713	-2.340762
1	-4.096422	3.108912	-3.482863
6	-1.990400	-1.372399	1.611566
6	-3.335685	-0.745044	1.992392
1	-1.353268	-1.480216	2.498346
1	-2.144497	-2.377343	1.202881
6	-4.160176	-1.600281	2.959331
1	-3.181706	0.245225	2.444826

1	-3.938051	-0.569989	1.087981
6	-5.502298	-0.965801	3.319251
1	-4.325018	-2.586214	2.506528
1	-3.574885	-1.775461	3.871069
1	-6.079399	-1.600301	3.998518
1	-5.359766	0.004757	3.806735
1	-6.108133	-0.798439	2.422099
6	-0.680554	1.674431	1.209544
6	-1.134553	2.978855	0.555382
1	0.389279	1.721484	1.434160
1	-1.190981	1.520129	2.168963
6	-0.788689	4.210562	1.396476
1	-0.670500	3.068569	-0.433369
1	-2.219492	2.958486	0.387002
6	-1.250733	5.515225	0.750445
1	-1.238751	4.110078	2.393059
1	0.298061	4.242904	1.553258
1	-0.990730	6.383697	1.363522
1	-0.789558	5.647080	-0.234032
1	-2.336787	5.518167	0.608431

I2

79	-1.719975	-0.569288	-0.011547
15	-3.678752	0.532688	-0.560042
6	-4.757250	-0.087568	-1.902122
6	-4.753955	0.620627	0.912157
6	-3.362502	2.278746	-0.977951
1	-5.630094	1.247609	0.722690
1	-5.074533	-0.384313	1.196161
1	-4.151709	1.042127	1.722058
1	-5.654794	0.530103	-2.001441
1	-4.203836	-0.076214	-2.843958
1	-5.047326	-1.118307	-1.686272
1	-4.300562	2.833972	-1.068097
1	-2.747219	2.692510	-0.173456
1	-2.807759	2.341090	-1.916723
6	0.122972	-1.819807	0.433812
6	-0.225866	-2.126522	1.777981
6	-0.201517	-2.793453	-0.546439
6	-0.815079	-3.337597	2.116466
6	-0.794711	-4.011531	-0.203959
6	-1.086945	-4.284439	1.125635
1	-1.020540	-4.740463	-0.975480
1	-1.539993	-5.233534	1.395647
50	1.683403	-0.333799	-0.012025
17	-1.198236	1.420687	1.862533
1	0.062037	-2.613764	-1.586330
1	-1.062947	-3.545752	3.152186
1	-0.038721	-1.384333	2.549122
6	2.257417	0.696375	1.777737
6	2.388710	2.214311	1.617973
1	3.199505	0.257897	2.130802
1	1.486568	0.486702	2.525684
6	2.766373	2.910945	2.925920
1	3.136486	2.460589	0.849427
1	1.429026	2.617167	1.275837
6	2.900512	4.424191	2.769118
1	1.995927	2.683789	3.672618
1	3.706855	2.491279	3.308185
1	3.157208	4.906023	3.717386
1	3.680521	4.677832	2.042383
1	1.961400	4.861472	2.414240
6	3.296617	-1.606255	-0.681324
6	4.576389	-0.825707	-1.001403
1	2.963192	-2.161138	-1.567925
1	3.495154	-2.356368	0.094319
6	5.727627	-1.714771	-1.479220
1	4.373891	-0.068795	-1.772873

1	4.907039	-0.267471	-0.113781
6	7.000140	-0.930044	-1.792610
1	5.936935	-2.469919	-0.710873
1	5.403789	-2.267136	-2.370869
1	7.801472	-1.588487	-2.140745
1	6.818745	-0.181880	-2.571949
1	7.363562	-0.401156	-0.905013
6	1.092362	0.828178	-1.734231
6	0.540963	2.235139	-1.483536
1	0.339062	0.222909	-2.258584
1	1.958534	0.873517	-2.406968
6	-0.043341	2.869556	-2.746837
1	-0.223418	2.211564	-0.696766
1	1.340239	2.880708	-1.098864
6	-0.555503	4.289755	-2.514867
1	0.716512	2.875147	-3.539196
1	-0.858270	2.231982	-3.119762
1	-0.996068	4.715001	-3.421909
1	-1.315596	4.309482	-1.726895
1	0.258398	4.949485	-2.196775

TS2

79	-2.029604	-0.149759	0.145917
6	-4.373686	1.126491	-2.296063
6	-4.923137	1.654209	0.497243
6	-2.729246	2.986112	-0.804190
1	-5.547642	2.493110	0.176441
1	-5.534450	0.752734	0.579876
1	-4.487197	1.865968	1.476703
1	-5.040318	1.963061	-2.526337
1	-3.610503	1.045463	-3.073348
1	-4.947079	0.196930	-2.280570
1	-3.439061	3.774045	-1.072028
1	-2.270227	3.202311	0.164311
1	-1.933103	2.936011	-1.550960
6	-0.397193	-1.909245	-0.012339
6	-0.931518	-2.467501	1.174143
6	-0.799884	-2.496169	-1.236749
6	-1.803380	-3.556939	1.134051
6	-1.657430	-3.591013	-1.274940
6	-2.155901	-4.122945	-0.087410
1	-1.937092	-4.028794	-2.228098
1	-2.825678	-4.977172	-0.115342
50	1.343318	-0.578521	0.001786
17	-1.015216	0.904630	2.324049
15	-3.553636	1.359631	-0.676651
1	-2.198852	-3.963685	2.059216
1	-0.659229	-2.032713	2.132180
1	-0.406300	-2.102130	-2.171128
6	0.890465	1.349553	-0.854243
6	2.100407	2.062008	-1.464343
1	0.438681	1.951621	-0.058619
1	0.117617	1.204037	-1.622398
6	1.748157	3.422941	-2.069736
1	2.874915	2.207799	-0.698477
1	2.558355	1.435208	-2.242464
6	2.952132	4.133240	-2.685198
1	0.971451	3.282262	-2.834023
1	1.302166	4.053665	-1.290294
1	2.674194	5.100581	-3.114060
1	3.727265	4.311383	-1.932193
1	3.398259	3.529115	-3.482663
6	2.233154	-0.471782	1.948502
6	2.861901	0.903951	2.197208
1	2.984730	-1.264888	2.045402
1	1.448412	-0.654044	2.688331
6	3.477476	1.040193	3.590906
1	3.640140	1.109338	1.446681

1	2.092471	1.677170	2.074016
6	4.096914	2.416056	3.828618
1	2.698781	0.849090	4.339297
1	4.239269	0.261095	3.727535
1	4.540759	2.492397	4.825833
1	4.884036	2.624457	3.095221
1	3.341206	3.203347	3.736906
6	2.727627	-1.548857	-1.351244
6	4.177817	-1.109020	-1.113158
1	2.436466	-1.332171	-2.387345
1	2.639415	-2.635282	-1.226013
6	5.184497	-1.796515	-2.038684
1	4.268813	-0.021066	-1.240762
1	4.462369	-1.310334	-0.070886
6	6.625610	-1.360030	-1.781767
1	5.097880	-2.883333	-1.911908
1	4.914053	-1.587547	-3.081880
1	7.326036	-1.874367	-2.446414
1	6.744260	-0.282576	-1.939464
1	6.922071	-1.576710	-0.749770

I3

79	-2.250822	-1.059985	-0.187730
6	-4.602654	1.406424	0.321489
6	-4.577580	-0.667328	2.339826
6	-2.495994	1.336586	2.287181
1	-5.157608	0.012918	2.969969
1	-5.256771	-1.294479	1.758128
1	-3.966129	-1.317018	2.970089
1	-5.184989	2.005689	1.027317
1	-3.994882	2.061828	-0.307148
1	-5.277097	0.835007	-0.320034
1	-3.142678	1.961621	2.909761
1	-1.859432	0.718724	2.924607
1	-1.860551	1.969144	1.662216
6	-0.214836	2.003239	-0.846095
6	-1.054269	1.627177	-1.905367
6	-0.475912	3.225331	-0.209875
6	-2.115551	2.436228	-2.308906
6	-1.538516	4.038264	-0.603988
6	-2.358943	3.644917	-1.659104
1	-1.716363	4.983741	-0.099507
1	-3.179099	4.281516	-1.978498
50	1.455104	0.776070	-0.256141
17	-0.955426	-2.392806	-1.614533
15	-3.489100	0.259108	1.199827
1	-2.749153	2.123295	-3.133707
1	-0.884604	0.687512	-2.426144
1	0.164997	3.562344	0.603340
6	0.958293	-0.513229	1.401838
6	2.173026	-0.896647	2.253184
1	0.488190	-1.414809	0.993033
1	0.202238	-0.017322	2.024143
6	1.813774	-1.797719	3.437238
1	2.914359	-1.414959	1.629119
1	2.674198	0.005211	2.632334
6	3.026715	-2.186399	4.280390
1	1.074828	-1.282461	4.065501
1	1.319195	-2.700680	3.058064
1	2.744604	-2.832202	5.117302
1	3.765175	-2.724908	3.676953
1	3.519282	-1.298933	4.692536
6	2.122239	-0.394583	-1.925291
6	2.816569	-1.690290	-1.490337
1	2.789755	0.210639	-2.550618
1	1.243240	-0.641013	-2.530711
6	3.203598	-2.580918	-2.672405
1	3.719138	-1.460862	-0.904346

1	2.150034	-2.259917	-0.829634
6	3.907373	-3.866078	-2.242096
1	2.294197	-2.826384	-3.234328
1	3.849772	-2.012883	-3.354604
1	4.170731	-4.487538	-3.103425
1	4.830684	-3.645769	-1.694400
1	3.264282	-4.461163	-1.585014
6	3.026261	2.097328	0.421450
6	4.416784	1.464456	0.278502
1	2.842546	2.358208	1.471887
1	2.981007	3.036059	-0.144070
6	5.549732	2.361295	0.782508
1	4.455447	0.510343	0.822945
1	4.603683	1.213548	-0.774855
6	6.930193	1.731334	0.606434
1	5.509300	3.321196	0.251761
1	5.378521	2.589515	1.842551
1	7.722011	2.387830	0.979218
1	7.000069	0.780811	1.146227
1	7.134476	1.526636	-0.450032

Sn(vinyl)Bu$_3$

6	-0.761953	1.008301	2.362452
6	-0.117978	0.755007	3.504803
50	-0.301853	-0.010406	0.539426
1	0.671695	0.007734	3.571112
1	-0.345674	1.277964	4.433195
1	-1.539575	1.773186	2.383319
6	1.273172	-1.429667	0.928410
6	1.811287	-2.062233	-0.360737
1	0.905174	-2.208220	1.607357
1	2.084081	-0.914257	1.458457
6	2.936402	-3.071612	-0.120367
1	0.995611	-2.565390	-0.899525
1	2.178088	-1.278098	-1.038465
6	3.458847	-3.700046	-1.410780
1	3.758334	-2.570319	0.406976
1	2.573218	-3.856556	0.555199
1	4.260264	-4.417736	-1.212532
1	2.659130	-4.229698	-1.940048
1	3.853113	-2.935414	-2.088870
6	-2.055625	-0.991814	-0.241605
6	-3.188657	-0.021398	-0.596028
1	-2.404044	-1.727536	0.493112
1	-1.759784	-1.561359	-1.132031
6	-4.420818	-0.716063	-1.181260
1	-3.492246	0.542637	0.297138
1	-2.830277	0.726562	-1.317321
6	-5.545941	0.256991	-1.528249
1	-4.122849	-1.273648	-2.078541
1	-4.784014	-1.462488	-0.463222
1	-6.412110	-0.262691	-1.948138
1	-5.881604	0.801884	-0.639260
1	-5.211710	0.997151	-2.263281
6	0.441650	1.406289	-0.907939
6	1.777611	2.026976	-0.483427
1	-0.308038	2.192150	-1.061780
1	0.552383	0.893775	-1.871832
6	2.322733	3.043735	-1.489367
1	1.667678	2.517139	0.493901
1	2.528475	1.236695	-0.338660
6	3.651384	3.658855	-1.053668
1	2.442574	2.553862	-2.464323
1	1.576866	3.835866	-1.634486
1	4.015721	4.387328	-1.784059
1	3.548325	4.171598	-0.091296
1	4.421163	2.888227	-0.936808

[Au(vinyl)(PMe_3)]

79	0.033969	-0.619438	0.000000
6	0.358186	2.615321	1.437797
6	0.358186	2.615321	-1.437797
6	-2.102621	2.225500	0.000000
1	0.162471	3.689745	-1.374373
1	1.436252	2.443183	-1.477746
1	-0.082004	2.216919	-2.354852
1	0.162471	3.689745	1.374373
1	-0.082004	2.216919	2.354852
1	1.436252	2.443183	1.477746
1	-2.208958	3.314359	0.000000
1	-2.592789	1.811827	-0.884337
1	-2.592789	1.811827	0.884337
15	-0.341232	1.721098	0.000000
6	0.358186	-2.616768	0.000000
6	1.554589	-3.217319	0.000000
1	2.490593	-2.662217	0.000000
1	1.653560	-4.303609	0.000000
1	-0.507272	-3.285079	0.000000

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79	2.405491	0.377413	0.120116
15	3.470850	-1.730547	0.118110
6	4.235464	-2.212566	-1.473206
6	4.832359	-1.922724	1.329583
6	2.367091	-3.141646	0.493566
1	5.282399	-2.918040	1.271483
1	5.596796	-1.166537	1.136008
1	4.439854	-1.759386	2.336059
1	4.712126	-3.194647	-1.403392
1	3.455791	-2.236062	-2.237440
1	4.978390	-1.465581	-1.761619
1	2.903313	-4.093265	0.434434
1	1.950373	-3.020082	1.496221
1	1.544182	-3.136621	-0.225222
6	1.437197	2.175271	0.130793
6	0.916114	2.726453	1.314446
6	1.243176	2.918432	-1.046123
6	0.241886	3.946818	1.325840
6	0.568396	4.137669	-1.046300
6	0.065407	4.658424	0.142710
1	0.433226	4.681513	-1.977533
1	-0.463641	5.606979	0.146029
50	-1.371865	-0.944573	-0.854117
1	-0.148431	4.342915	2.259737
1	1.035969	2.193270	2.254974
1	1.628519	2.540025	-1.990535
6	0.942971	-0.995741	-2.897014
1	0.946105	0.090168	-2.814128
1	1.646702	-1.411264	-3.619459
6	0.125312	-1.759631	-2.165112
1	0.182415	-2.839941	-2.320031
6	-0.762730	-0.886201	1.216597
6	-1.899708	-1.069085	2.225367
1	-0.284036	0.086762	1.370704
1	0.014991	-1.641114	1.384482
6	-1.417723	-0.992857	3.676006
1	-2.664959	-0.296066	2.069132
1	-2.404829	-2.032076	2.065531
6	-2.542335	-1.171103	4.693829
1	-0.647886	-1.759788	3.836048
1	-0.922934	-0.025854	3.832958
1	-2.168349	-1.110451	5.720235
1	-3.308200	-0.397705	4.570791
1	-3.031988	-2.143411	4.571507
6	-3.123142	-2.203528	-1.023302
6	-4.395898	-1.527708	-0.497008

1	-2.952274	-3.146190	-0.487772
1	-3.254479	-2.469663	-2.079791
6	-5.652753	-2.387299	-0.651898
1	-4.272926	-1.274001	0.564444
1	-4.555625	-0.571970	-1.015730
6	-6.903280	-1.717722	-0.085090
1	-5.802251	-2.613882	-1.715430
1	-5.490593	-3.351570	-0.152922
1	-7.790949	-2.343621	-0.216100
1	-6.788120	-1.518893	0.985909
1	-7.093060	-0.759095	-0.579973
6	-1.910322	1.027402	-1.516388
6	-2.492579	1.884706	-0.386522
1	-2.640828	0.917781	-2.328402
1	-1.032053	1.527017	-1.938381
6	-3.035961	3.227940	-0.876662
1	-3.303948	1.347712	0.128400
1	-1.715355	2.069779	0.365632
6	-3.564644	4.100057	0.259111
1	-2.233788	3.756762	-1.404363
1	-3.831875	3.048990	-1.612122
1	-3.947513	5.056090	-0.111724
1	-4.379253	3.599138	0.794594
1	-2.770084	4.310963	0.982480

TS3

79	1.549215	-0.310047	-0.027210
15	3.757032	-1.499752	0.463745
6	4.615834	-1.811091	-1.128949
6	5.009870	-0.570659	1.430700
6	3.773737	-3.163388	1.246243
1	5.974308	-1.086608	1.468378
1	5.138875	0.414745	0.975780
1	4.639168	-0.422148	2.448048
1	5.573388	-2.322130	-0.990283
1	3.967516	-2.420375	-1.765062
1	4.785038	-0.855930	-1.632773
1	4.781138	-3.588027	1.299535
1	3.359478	-3.094414	2.255369
1	3.134826	-3.830866	0.661617
6	1.598532	1.767799	0.027833
6	1.434587	2.493442	1.219333
6	1.719658	2.524011	-1.151139
6	1.372760	3.886584	1.235402
6	1.665364	3.916745	-1.145946
6	1.485329	4.607091	0.049896
1	1.752010	4.463782	-2.081392
1	1.432806	5.691998	0.056725
50	-1.197160	-0.691412	-0.229837
1	1.233271	4.409634	2.178045
1	1.334236	1.962182	2.163563
1	1.838612	2.018007	-2.107007
6	0.718036	-2.613532	-1.855916
1	0.692723	-1.877391	-2.658124
1	0.882797	-3.645820	-2.165007
6	0.552540	-2.263154	-0.566119
1	0.555636	-3.079129	0.160266
6	-1.464287	0.187418	1.725887
6	-2.925165	0.301585	2.168545
1	-0.992803	1.175406	1.692399
1	-0.892170	-0.404199	2.451743
6	-3.084309	0.958543	3.542171
1	-3.496713	0.886417	1.433467
1	-3.393793	-0.692018	2.194107
6	-4.542106	1.074033	3.982848
1	-2.517264	0.378309	4.281612
1	-2.623201	1.953677	3.514528
1	-4.629192	1.547108	4.965502

1	-5.120734	1.673681	3.271878
1	-5.013857	0.087189	4.043709
6	-2.671482	-2.276358	-0.389643
6	-4.067399	-1.748372	-0.739868
1	-2.703985	-2.825880	0.560101
1	-2.331268	-2.986631	-1.151756
6	-5.124575	-2.851272	-0.842259
1	-4.398143	-1.015454	0.008567
1	-4.031846	-1.205410	-1.694554
6	-6.507179	-2.317502	-1.212374
1	-4.799636	-3.589788	-1.586243
1	-5.177680	-3.384188	0.115872
1	-7.247499	-3.120971	-1.269474
1	-6.857959	-1.591448	-0.470945
1	-6.485306	-1.812368	-2.183993
6	-1.492441	0.738051	-1.817049
6	-1.775018	2.133579	-1.247054
1	-2.299572	0.414359	-2.483865
1	-0.570015	0.762984	-2.408468
6	-1.780763	3.228572	-2.313956
1	-2.740821	2.134345	-0.721413
1	-1.015005	2.390652	-0.500166
6	-2.017763	4.617044	-1.724792
1	-0.811359	3.212667	-2.828001
1	-2.542854	3.002623	-3.071564
1	-2.006312	5.389766	-2.499649
1	-2.986133	4.669538	-1.214647
1	-1.238690	4.857684	-0.993942

I5

79	1.382321	-0.456922	0.281585
15	3.839089	-0.975875	0.325617
6	4.538390	-0.719495	-1.347748
6	4.865187	0.111377	1.382341
6	4.346973	-2.677824	0.765671
1	5.934101	-0.059083	1.224124
1	4.618043	1.150377	1.147746
1	4.623340	-0.068697	2.432874
1	5.617588	-0.897278	-1.369635
1	4.045876	-1.395826	-2.051183
1	4.328961	0.309023	-1.653587
1	5.411263	-2.852458	0.584003
1	4.124884	-2.855115	1.821009
1	3.745530	-3.376439	0.178568
6	1.807943	1.549862	-0.114250
6	1.957822	2.498152	0.908078
6	1.990374	2.001613	-1.430395
6	2.274131	3.827789	0.634093
6	2.307041	3.329437	-1.714545
6	2.449503	4.250460	-0.680799
1	2.436498	3.646139	-2.746094
1	2.688044	5.287482	-0.896732
50	-1.163931	0.081849	0.023125
1	2.375917	4.539288	1.449312
1	1.812245	2.200322	1.944606
1	1.869363	1.305864	-2.259205
6	0.565870	-3.352729	-0.319455
1	0.657852	-3.139015	-1.383983
1	0.291373	-4.377366	-0.067920
6	0.758169	-2.415340	0.615586
1	0.610638	-2.728508	1.653468
6	-2.245558	-0.870226	1.630200
6	-3.720756	-0.470352	1.726914
1	-1.731545	-0.658004	2.575409
1	-2.151219	-1.950057	1.463872
6	-4.487566	-1.244879	2.802093
1	-3.805594	0.604209	1.939541

1	-4.220845	-0.623822	0.759637
6	-5.961401	-0.852008	2.882997
1	-4.400171	-2.319396	2.596502
1	-4.004094	-1.079471	3.773555
1	-6.486340	-1.414418	3.660977
1	-6.072355	0.214338	3.108041
1	-6.469736	-1.041942	1.931408
6	-1.544686	2.206894	-0.014584
6	-2.957323	2.574335	-0.478873
1	-0.794645	2.655586	-0.675677
1	-1.349184	2.615812	0.983978
6	-3.179942	4.085816	-0.580889
1	-3.160804	2.123912	-1.460663
1	-3.706785	2.151909	0.204202
6	-4.592187	4.450873	-1.034680
1	-2.973533	4.544461	0.394533
1	-2.443797	4.505843	-1.278036
1	-4.722352	5.534077	-1.117419
1	-4.814023	4.011591	-2.013418
1	-5.340588	4.076672	-0.327552
6	-1.777615	-0.807266	-1.853318
6	-2.554139	-2.115990	-1.677166
1	-0.866472	-0.992612	-2.435270
1	-2.370048	-0.081145	-2.423406
6	-2.856467	-2.819455	-3.001921
1	-1.981252	-2.799237	-1.037550
1	-3.499172	-1.925882	-1.149491
6	-3.599475	-4.141272	-2.816389
1	-3.442790	-2.149729	-3.644379
1	-1.910199	-2.999620	-3.528895
1	-3.792856	-4.632850	-3.774627
1	-3.016756	-4.830888	-2.196103
1	-4.563260	-3.984162	-2.320017

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79	1.445832	-0.126898	0.153460
15	1.950607	2.146179	-0.423378
6	1.303418	2.632755	-2.064186
6	1.324125	3.417003	0.732663
6	3.735142	2.515116	-0.551530
1	1.594992	4.422197	0.397029
1	0.238598	3.336369	0.811780
1	1.758082	3.238762	1.719646
1	1.565459	3.667899	-2.300943
1	1.732619	1.968968	-2.818833
1	0.218379	2.515126	-2.083427
1	3.901458	3.551200	-0.859920
1	4.213063	2.327818	0.412242
1	4.187036	1.828816	-1.271256
6	3.508831	-0.623974	0.309859
6	4.258392	-0.300534	1.447391
6	4.177814	-1.256826	-0.743239
6	5.621766	-0.583525	1.528155
6	5.542530	-1.535885	-0.676483
6	6.270959	-1.197811	0.460936
1	6.037158	-2.024389	-1.512147
1	7.333219	-1.416234	0.518343
50	-1.217507	0.066786	0.016046
1	6.177214	-0.325719	2.426375
1	3.777506	0.184077	2.296503
1	3.627456	-1.549996	-1.635603
6	0.651654	-3.016945	-0.295371
1	0.599831	-2.841219	-1.367196
1	0.473763	-4.039149	0.032743
6	0.919614	-2.051017	0.583294
1	0.945781	-2.300404	1.644444
6	-2.141417	-0.894370	1.722546
6	-3.620517	-0.561088	1.930797

1	-1.567391	-0.635804	2.621248
1	-2.010944	-1.973486	1.578207
6	-4.259553	-1.318238	3.097564
1	-3.741673	0.517756	2.102499
1	-4.189640	-0.783069	1.016526
6	-5.739453	-0.988398	3.282922
1	-4.137471	-2.396059	2.931182
1	-3.708951	-1.087000	4.018609
1	-6.172616	-1.535066	4.125806
1	-5.883120	0.081660	3.469092
1	-6.312874	-1.246551	2.385777
6	-2.073177	2.079363	-0.056536
6	-3.504778	2.127953	-0.602656
1	-1.439227	2.743130	-0.659220
1	-2.054985	2.487693	0.963732
6	-4.094132	3.540448	-0.640729
1	-3.534138	1.706772	-1.616658
1	-4.159772	1.488853	0.003278
6	-5.530496	3.572711	-1.159807
1	-4.055542	3.971998	0.367938
1	-3.457687	4.177335	-1.269567
1	-5.929193	4.591282	-1.183778
1	-5.590682	3.165156	-2.174782
1	-6.188401	2.970264	-0.524235
6	-1.880055	-0.969172	-1.774836
6	-2.655965	-2.257419	-1.483520
1	-0.987868	-1.203497	-2.369036
1	-2.489407	-0.290947	-2.384778
6	-3.028694	-3.039079	-2.745393
1	-2.059141	-2.906226	-0.829185
1	-3.573229	-2.026222	-0.924283
6	-3.792023	-4.327288	-2.443141
1	-3.628542	-2.397544	-3.404175
1	-2.110683	-3.275061	-3.299581
1	-4.041187	-4.872025	-3.358839
1	-3.197666	-4.992631	-1.807674
1	-4.727930	-4.114577	-1.915024

TS4

79	1.534733	-0.765749	0.265625
15	4.023204	-0.196748	0.010870
6	4.462422	-0.018639	-1.764330
6	4.642990	1.382747	0.713697
6	5.247722	-1.429610	0.605527
1	5.705128	1.536009	0.497489
1	4.061850	2.205739	0.289499
1	4.491132	1.386927	1.795984
1	5.523393	0.210795	-1.903620
1	4.220763	-0.945567	-2.290652
1	3.860926	0.787688	-2.192463
1	6.276932	-1.137479	0.374003
1	5.140705	-1.548271	1.686703
1	5.030283	-2.394404	0.140287
6	1.006634	1.467174	-0.034080
6	1.177009	2.290008	1.093996
6	1.350643	2.011808	-1.286127
6	1.679065	3.583770	0.982324
6	1.861593	3.301007	-1.404726
6	2.024904	4.091864	-0.267822
1	2.123526	3.695123	-2.382434
1	2.414208	5.101279	-0.358436
50	-1.030217	0.270895	-0.034318
1	1.800701	4.197014	1.870322
1	0.912069	1.909639	2.078206
1	1.213888	1.413115	-2.184660
6	0.560280	-3.619686	-0.339396
1	0.375512	-3.350011	-1.378523
1	0.345720	-4.657665	-0.081288

6	1.023062	-2.745067	0.562762
1	1.157865	-3.142601	1.573584
6	-1.730429	-0.646826	1.787174
6	-3.200181	-0.370746	2.110456
1	-1.085591	-0.303345	2.605969
1	-1.540002	-1.720037	1.678801
6	-3.664899	-1.032523	3.410321
1	-3.375495	0.712033	2.180502
1	-3.838652	-0.726042	1.289018
6	-5.128195	-0.742140	3.737828
1	-3.508394	-2.115699	3.332665
1	-3.024947	-0.688998	4.233334
1	-5.436299	-1.230799	4.666964
1	-5.298529	0.333833	3.853358
1	-5.788073	-1.097349	2.938872
6	-2.121096	2.134850	-0.240867
6	-3.533782	1.947807	-0.802622
1	-1.535641	2.794625	-0.892851
1	-2.160932	2.626335	0.739744
6	-4.292884	3.264849	-0.986724
1	-3.486183	1.432568	-1.772500
1	-4.121986	1.292800	-0.144918
6	-5.687918	3.072484	-1.578717
1	-4.368090	3.772451	-0.016524
1	-3.703067	3.926880	-1.633736
1	-6.206684	4.027570	-1.704444
1	-5.633234	2.589312	-2.560332
1	-6.304952	2.438296	-0.932875
6	-1.452217	-0.865914	-1.820401
6	-2.477068	-1.971862	-1.545501
1	-0.520456	-1.304927	-2.193343
1	-1.821877	-0.183930	-2.596100
6	-2.795802	-2.815526	-2.781175
1	-2.097920	-2.631095	-0.753966
1	-3.411675	-1.534571	-1.164259
6	-3.817243	-3.916250	-2.502522
1	-3.165190	-2.158736	-3.579632
1	-1.864577	-3.260816	-3.154910
1	-4.038735	-4.496655	-3.403230
1	-3.447056	-4.608899	-1.739139
1	-4.759089	-3.492966	-2.136399

TS4-CIS

79	-1.276279	0.053550	0.095170
15	-1.950187	-2.285515	0.434581
6	-2.165759	-3.146579	-1.167483
6	-0.824370	-3.377768	1.375488
6	-3.580653	-2.476623	1.248133
1	-1.223865	-4.391735	1.469594
1	0.140786	-3.409446	0.862833
1	-0.665232	-2.954666	2.370446
1	-2.514695	-4.174382	-1.032150
1	-2.893278	-2.592736	-1.766662
1	-1.211963	-3.152553	-1.700796
1	-3.892079	-3.523754	1.305377
1	-3.529837	-2.055692	2.255327
1	-4.318080	-1.898403	0.683293
6	-3.275351	0.866033	-0.050589
6	-3.916435	1.148927	1.159146
6	-4.055611	0.494223	-1.155350
6	-5.302803	1.047721	1.270130
6	-5.434550	0.383738	-1.040775
6	-6.066119	0.657132	0.175390
1	-6.024764	0.088084	-1.903595
1	-7.144772	0.574604	0.261601
50	1.384072	-0.050975	0.054178
1	-5.784567	1.271074	2.217596
1	-3.329053	1.450147	2.023574

1	-3.576113	0.306352	-2.112938
6	-1.570160	2.613345	-1.580165
1	-1.596566	2.029880	-2.495651
1	-1.425962	3.684758	-1.684637
6	-1.709471	2.063436	-0.364979
1	-1.687421	2.706066	0.513136
6	2.454041	0.299624	1.913331
6	3.974796	0.256664	1.737552
1	2.140154	-0.441301	2.659921
1	2.148792	1.277883	2.306219
6	4.752237	0.545077	3.024830
1	4.280012	-0.728778	1.356833
1	4.281873	0.981507	0.969770
6	6.267128	0.499038	2.832894
1	4.456509	1.530594	3.407140
1	4.453635	-0.181753	3.791492
1	6.798615	0.698637	3.768411
1	6.586529	-0.483867	2.469045
1	6.591491	1.243207	2.097462
6	2.180690	-1.953579	-0.674582
6	3.424719	-1.825941	-1.559073
1	1.392457	-2.485064	-1.226282
1	2.414739	-2.575635	0.201769
6	3.984140	-3.171614	-2.028407
1	3.192176	-1.211008	-2.439423
1	4.213568	-1.282554	-1.020346
6	5.216293	-3.032630	-2.920599
1	4.231042	-3.781091	-1.149005
1	3.197175	-3.716963	-2.566474
1	5.597851	-4.007874	-3.238336
1	4.984471	-2.454424	-3.821785
1	6.024521	-2.512787	-2.394648
6	2.082232	1.518103	-1.273352
6	1.973227	2.891349	-0.602604
1	1.443200	1.500308	-2.166036
1	3.108609	1.335982	-1.613982
6	2.166741	4.059307	-1.571799
1	0.986868	2.999103	-0.130311
1	2.710347	2.968746	0.209564
6	2.044955	5.424334	-0.897335
1	3.146584	3.968542	-2.058321
1	1.417077	3.975202	-2.369665
1	2.174317	6.242123	-1.613116
1	1.061009	5.541257	-0.429112
1	2.799579	5.543544	-0.111995

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79	-2.095101	-1.188858	-0.283625
15	-3.392304	0.318627	1.015275
6	-2.535981	1.694810	1.861570
6	-4.720202	1.173164	0.089048
6	-4.283546	-0.522969	2.378307
1	-5.342724	1.775484	0.757331
1	-4.255400	1.824194	-0.655244
1	-5.341358	0.437318	-0.426554
1	-3.248647	2.299912	2.429904
1	-1.778978	1.295073	2.540386
1	-2.036169	2.319682	1.118236
1	-4.890852	0.181485	2.954212
1	-4.926132	-1.303600	1.964340
1	-3.554346	-0.997785	3.039366
6	-0.044529	2.426183	-0.748313
6	-1.015262	2.016845	-1.673759
6	-0.185013	3.698001	-0.176257
6	-2.092199	2.837474	-2.005189
6	-1.260727	4.524185	-0.500003
6	-2.220542	4.091623	-1.412313
1	-1.350845	5.504113	-0.040320

1	-3.057746	4.734207	-1.668569
50	1.512714	1.052633	-0.189752
1	-2.826392	2.498882	-2.731177
1	-0.937356	1.040605	-2.147465
1	0.550809	4.055960	0.541052
6	-0.406232	-3.610692	-0.917277
1	-0.388685	-3.859049	0.142426
1	0.136877	-4.294268	-1.571153
6	-1.053189	-2.536252	-1.389329
1	-0.998759	-2.393704	-2.473070
6	1.781220	-0.318925	-1.818475
6	3.042996	-1.183319	-1.717202
1	1.782511	0.242772	-2.760766
1	0.898463	-0.967146	-1.833902
6	3.101691	-2.262080	-2.800768
1	3.941696	-0.553130	-1.780699
1	3.088785	-1.676328	-0.736662
6	4.356555	-3.128128	-2.718741
1	2.206888	-2.890619	-2.709039
1	3.043037	-1.783480	-3.786966
1	4.365027	-3.897413	-3.496494
1	5.262363	-2.523171	-2.836684
1	4.420662	-3.632785	-1.748545
6	3.365756	2.067716	0.247031
6	4.290631	1.195370	1.107429
1	3.170444	3.021092	0.753272
1	3.858056	2.316191	-0.700991
6	5.654849	1.833775	1.378183
1	3.805336	0.971999	2.067935
1	4.450035	0.221954	0.621943
6	6.556323	0.959248	2.247888
1	6.148961	2.037948	0.419750
1	5.505462	2.808668	1.860120
1	7.528909	1.429795	2.419560
1	6.096841	0.772592	3.224584
1	6.732903	-0.012688	1.774621
6	0.879278	-0.020340	1.572450
6	1.384590	-1.465483	1.623857
1	-0.216428	-0.028101	1.548360
1	1.173755	0.527398	2.476496
6	0.702885	-2.295063	2.713303
1	1.203216	-1.957741	0.660086
1	2.472439	-1.476831	1.782102
6	1.266398	-3.710607	2.820557
1	0.799887	-1.782583	3.679815
1	-0.372699	-2.339418	2.490131
1	0.742678	-4.297884	3.580758
1	1.175491	-4.238806	1.865581
1	2.329328	-3.689264	3.084806

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79	-2.384398	0.428161	0.008294
15	-3.393461	-1.698345	0.271640
6	-4.876194	-1.727385	1.347516
6	-3.971004	-2.460433	-1.288971
6	-2.307604	-2.985093	0.987737
1	-4.444558	-3.429537	-1.106783
1	-4.682125	-1.792853	-1.780756
1	-3.108572	-2.596411	-1.945522
1	-5.296854	-2.734401	1.421586
1	-4.602249	-1.374536	2.344661
1	-5.629160	-1.047207	0.942309
1	-2.838625	-3.935586	1.093861
1	-1.448693	-3.115965	0.324569
1	-1.943622	-2.656817	1.964065
6	-1.431909	2.213552	-0.240257
6	-1.274223	2.800009	-1.507892
6	-0.823770	2.876033	0.840137

6	-0.537003	3.967912	-1.692207
6	-0.079664	4.041464	0.665375
6	0.068905	4.591611	-0.605049
1	0.383890	4.521324	1.523513
1	0.648183	5.499493	-0.745992
50	1.371238	-1.015122	-0.707363
1	-0.428309	4.389653	-2.687715
1	-1.722091	2.328186	-2.378978
1	-0.921545	2.469920	1.844046
6	-0.210480	-3.114290	-2.352478
1	0.532041	-3.844251	-2.032333
1	-0.981627	-3.499370	-3.020939
6	-0.164010	-1.834741	-1.968091
1	-0.941702	-1.165418	-2.343411
6	1.878868	0.974614	-1.340400
6	3.259260	1.443631	-0.867893
1	1.103774	1.640392	-0.947210
1	1.810105	1.037463	-2.432836
6	3.529652	2.912786	-1.199047
1	3.353010	1.312225	0.219259
1	4.046865	0.819994	-1.314525
6	4.898755	3.389655	-0.719323
1	3.441590	3.058582	-2.283457
1	2.738574	3.522123	-0.745304
1	5.059246	4.447803	-0.947006
1	4.999727	3.262673	0.364228
1	5.705197	2.819641	-1.194131
6	3.090097	-2.321289	-0.801374
6	4.078900	-2.060086	0.342404
1	3.590113	-2.195140	-1.769123
1	2.749364	-3.364484	-0.764618
6	5.283089	-3.004804	0.333284
1	4.443059	-1.024649	0.294561
1	3.566152	-2.151324	1.310512
6	6.267896	-2.728261	1.467844
1	4.924033	-4.040244	0.398150
1	5.796830	-2.918642	-0.632693
1	7.109873	-3.426610	1.448003
1	6.673064	-1.713101	1.397246
1	5.778735	-2.822262	2.443535
6	0.740966	-0.951283	1.358697
6	1.296520	0.265071	2.105723
1	1.023207	-1.883238	1.864461
1	-0.353597	-0.904976	1.366311
6	0.621497	0.497465	3.458097
1	2.380052	0.153140	2.253396
1	1.161138	1.170209	1.500598
6	1.143206	1.743935	4.169629
1	-0.460936	0.592928	3.292303
1	0.758744	-0.385712	4.095658
1	0.641658	1.903550	5.128776
1	2.218569	1.663656	4.361807
1	0.984407	2.635950	3.553456

TS5

79	-2.068527	-0.137467	-0.493499
15	-4.126137	-0.864455	0.548403
6	-4.032623	-0.654841	2.368710
6	-5.568273	0.171526	0.090547
6	-4.786770	-2.570368	0.371139
1	-6.460010	-0.097372	0.665271
1	-5.316757	1.219576	0.269221
1	-5.775172	0.050256	-0.975612
1	-4.985127	-0.887508	2.854589
1	-3.252614	-1.307985	2.767989
1	-3.753948	0.379285	2.585586
1	-5.716812	-2.708269	0.931604
1	-4.971621	-2.774745	-0.686510

1	-4.040547	-3.284343	0.728682
6	-1.309953	1.809605	-0.302326
6	-1.165402	2.694805	-1.383650
6	-0.819933	2.259783	0.936189
6	-0.549981	3.938267	-1.246511
6	-0.191211	3.495894	1.083998
6	-0.047979	4.342559	-0.012141
1	0.189230	3.795983	2.057642
1	0.442998	5.305365	0.095430
50	1.385272	-0.828803	-0.636457
1	-0.449155	4.589686	-2.110934
1	-1.523125	2.403052	-2.368701
1	-0.905369	1.621448	1.814255
6	-1.341915	-2.267599	-1.349566
1	-1.218285	-2.866978	-0.449282
1	-2.117625	-2.605775	-2.034678
6	-0.407666	-1.327299	-1.723734
1	-0.523568	-0.901369	-2.722521
6	2.038799	1.131424	-1.213205
6	3.497721	1.452933	-0.874349
1	1.375179	1.838811	-0.707121
1	1.859650	1.265585	-2.286805
6	3.854877	2.910927	-1.173857
1	3.691182	1.260876	0.190539
1	4.177836	0.791447	-1.429687
6	5.299702	3.257846	-0.820359
1	3.673103	3.111875	-2.237495
1	3.165201	3.559391	-0.618949
1	5.524918	4.307205	-1.033465
1	5.494644	3.083799	0.243596
1	6.002982	2.641149	-1.390806
6	2.939629	-2.283562	-1.019106
6	4.035870	-2.236294	0.053363
1	3.374645	-2.104401	-2.009937
1	2.490779	-3.284049	-1.053993
6	5.136275	-3.280181	-0.151203
1	4.495767	-1.238572	0.077460
1	3.591955	-2.383304	1.048461
6	6.217021	-3.222488	0.926913
1	4.681061	-4.278777	-0.168874
1	5.590243	-3.133115	-1.139606
1	6.988413	-3.981560	0.765909
1	6.707636	-2.243283	0.938378
1	5.786882	-3.387568	1.920851
6	0.964314	-0.881381	1.481526
6	1.749315	0.189690	2.247088
1	1.179632	-1.878030	1.886221
1	-0.112369	-0.713136	1.612181
6	1.336421	0.312668	3.714402
1	2.826263	-0.025860	2.193460
1	1.608920	1.165354	1.764134
6	2.090260	1.419299	4.448799
1	0.256664	0.509807	3.760581
1	1.493882	-0.649160	4.219756
1	1.775325	1.500469	5.493484
1	3.169672	1.233101	4.437509
1	1.918532	2.389253	3.969398

I8

79	-1.923913	-0.601839	-0.527503
15	-4.070003	-0.613457	0.633895
6	-3.924180	0.196960	2.270392
6	-5.245455	0.473495	-0.255799
6	-5.059877	-2.118377	0.993632
1	-6.166831	0.630670	0.312627
1	-4.749473	1.431479	-0.432424
1	-5.488532	0.030328	-1.224713
1	-4.902594	0.340240	2.738364

1	-3.293892	-0.410549	2.924795
1	-3.437630	1.165126	2.126860
1	-5.996658	-1.877971	1.506328
1	-5.283442	-2.633181	0.055999
1	-4.469370	-2.792597	1.618894
6	-1.568614	1.485439	-0.391187
6	-1.642991	2.369527	-1.479687
6	-1.113222	2.034151	0.820399
6	-1.263859	3.707702	-1.375534
6	-0.722672	3.367738	0.937546
6	-0.790864	4.212628	-0.166897
1	-0.357767	3.744519	1.890233
1	-0.484077	5.251292	-0.085484
50	1.489631	-0.884262	-0.536844
1	-1.323946	4.356766	-2.245553
1	-1.982514	2.003196	-2.446386
1	-1.027646	1.399636	1.702112
6	-1.162679	-2.618344	-1.033574
1	-0.965964	-3.140501	-0.098789
1	-1.828098	-3.143731	-1.716038
6	-0.265939	-1.642388	-1.518734
1	-0.355291	-1.400931	-2.580276
6	1.833897	1.085286	-1.323790
6	3.212655	1.684543	-1.032602
1	1.049310	1.730235	-0.915665
1	1.660960	1.050165	-2.407108
6	3.356473	3.107062	-1.578653
1	3.394369	1.705688	0.051119
1	4.005135	1.053268	-1.459549
6	4.714252	3.734702	-1.270709
1	3.193479	3.088762	-2.664063
1	2.552232	3.725548	-1.160266
1	4.796854	4.741952	-1.690240
1	4.876785	3.808578	-0.189850
1	5.529508	3.132313	-1.686725
6	3.247824	-2.108267	-0.835814
6	4.323932	-1.798000	0.213214
1	3.643237	-1.931759	-1.843621
1	2.973062	-3.169103	-0.790123
6	5.601554	-2.623318	0.044746
1	4.586940	-0.731116	0.177316
1	3.921854	-1.970844	1.221690
6	6.656412	-2.308006	1.103763
1	5.345816	-3.690178	0.082169
1	6.015270	-2.442876	-0.955674
1	7.561618	-2.905860	0.962464
1	6.943991	-1.251581	1.066410
1	6.273792	-2.510064	2.110116
6	1.109320	-0.794502	1.588696
6	1.750444	0.435987	2.240435
1	1.466440	-1.711586	2.073122
1	0.021557	-0.767416	1.734629
6	1.342802	0.633686	3.701180
1	2.845598	0.359080	2.180614
1	1.477833	1.339789	1.679533
6	1.982035	1.869718	4.330350
1	0.248467	0.717777	3.753908
1	1.609177	-0.261544	4.278170
1	1.671408	2.001883	5.371079
1	3.074806	1.796017	4.313569
1	1.704345	2.774722	3.778773

TS6

79	-2.073778	-0.949564	-0.589349
15	-3.700427	-0.317166	0.943507
6	-4.682407	1.115738	0.394403
6	-4.928305	-1.607223	1.356529
6	-2.997885	0.184264	2.550550
1	-5.655052	-1.231300	2.082563
1	-5.449378	-1.916663	0.447858
1	-4.415742	-2.476997	1.773424
1	-5.410785	1.401140	1.158749
1	-4.001067	1.948220	0.197888
1	-5.202145	0.866921	-0.533436
1	-3.791878	0.466688	3.247642
1	-2.412401	-0.637522	2.969063
1	-2.332683	1.033955	2.381215
6	-0.557512	1.639534	-0.559145
6	-1.302301	2.085791	-1.666378
6	-0.778447	2.347581	0.638500
6	-2.199000	3.155012	-1.595262
6	-1.667020	3.418257	0.733247
6	-2.384155	3.829062	-0.391028
1	-1.793860	3.941610	1.678384
1	-3.071815	4.667915	-0.329891
50	1.191265	0.077981	-0.636705
1	-2.742948	3.470035	-2.482490
1	-1.171710	1.599802	-2.632707
1	-0.216697	2.068980	1.531475
6	-0.696548	-2.338800	-1.839027
1	-0.262223	-2.945743	-1.042816
1	-1.304962	-2.888715	-2.560049
6	-0.289255	-1.038366	-2.031776
1	-0.685039	-0.586103	-2.948168
6	2.491611	1.844852	-0.788398
6	3.985025	1.635142	-0.547185
1	2.086560	2.570782	-0.071183
1	2.326990	2.294068	-1.778003
6	4.814653	2.917272	-0.661457
1	4.141994	1.208189	0.453636
1	4.381881	0.892808	-1.252920
6	6.305969	2.686491	-0.421802
1	4.662893	3.355408	-1.656765
1	4.434129	3.655379	0.056671
1	6.877688	3.616358	-0.502311
1	6.481753	2.269317	0.575967
1	6.713470	1.976982	-1.150505
6	2.695348	-1.457090	-1.265320
6	3.673397	-1.903954	-0.175357
1	3.260949	-1.055413	-2.119191
1	2.163246	-2.337015	-1.651037
6	4.729528	-2.902772	-0.658504
1	4.193370	-1.036284	0.251745
1	3.119911	-2.356966	0.660686
6	5.691103	-3.341798	0.444862
1	4.225647	-3.780947	-1.083524
1	5.294573	-2.448347	-1.482822
1	6.436860	-4.053419	0.076410
1	6.226150	-2.481050	0.861136
1	5.150180	-3.820966	1.268819
6	0.845547	-0.577211	1.420424
6	1.844665	0.010759	2.423273
1	0.885459	-1.673912	1.461804
1	-0.173954	-0.290431	1.712417
6	1.503644	-0.303548	3.882028
1	2.852331	-0.364971	2.201751
1	1.906009	1.102499	2.305746
6	2.524611	0.255860	4.870944
1	0.508043	0.104476	4.106817
1	1.423041	-1.391528	4.005713

1	2.246798	0.042471	5.907797
1	3.515026	-0.177053	4.694279
1	2.617375	1.342212	4.764684

I9

79	-2.181688	-1.175031	-0.300326
15	-3.479084	0.194900	1.134934
6	-4.616432	1.354773	0.294804
6	-4.573475	-0.748400	2.262790
6	-2.529882	1.275248	2.264603
1	-5.164547	-0.082274	2.898077
1	-5.243871	-1.375972	1.670873
1	-3.962168	-1.401381	2.890272
1	-5.207605	1.925650	1.017004
1	-4.022932	2.039355	-0.315750
1	-5.284701	0.792870	-0.361922
1	-3.195991	1.874499	2.892343
1	-1.889510	0.657786	2.898965
1	-1.897744	1.935620	1.666129
6	-0.279097	2.194562	-0.671384
6	-1.143251	1.884249	-1.730541
6	-0.477747	3.412586	-0.005582
6	-2.168456	2.749363	-2.107650
6	-1.507190	4.279995	-0.369609
6	-2.353999	3.949668	-1.424952
1	-1.640428	5.218629	0.160524
1	-3.149181	4.628494	-1.718757
50	1.350748	0.880741	-0.167367
1	-2.821802	2.485628	-2.934379
1	-1.018316	0.951926	-2.275656
1	0.183748	3.700922	0.809532
6	-0.259296	-3.364783	-1.086952
1	-0.117284	-3.599812	-0.032967
1	0.311023	-3.980361	-1.784267
6	-1.070228	-2.381890	-1.501445
1	-1.125170	-2.243904	-2.585746
6	3.018016	2.126383	0.419767
6	4.375329	1.448316	0.192118
1	2.906379	2.386056	1.480560
1	2.972153	3.070647	-0.136415
6	5.565093	2.302387	0.636207
1	4.413224	0.489806	0.728191
1	4.493480	1.200004	-0.871870
6	6.910780	1.621240	0.394611
1	5.534303	3.263209	0.106570
1	5.454630	2.536692	1.702943
1	7.743691	2.245516	0.731568
1	6.969324	0.667021	0.929280
1	7.059072	1.412381	-0.670366
6	1.850748	-0.288045	-1.898749
6	2.645946	-1.547900	-1.544009
1	2.401949	0.329652	-2.617797
1	0.910195	-0.583292	-2.378925
6	2.905234	-2.448180	-2.752650
1	3.606611	-1.279113	-1.081502
1	2.090732	-2.128407	-0.795805
6	3.625533	-3.742851	-2.383923
1	1.941418	-2.682677	-3.222146
1	3.487543	-1.893856	-3.500176
1	3.814938	-4.363732	-3.264736
1	4.589515	-3.536457	-1.905895
1	3.026463	-4.332010	-1.680800
6	0.938921	-0.464045	1.469229
6	2.208037	-0.912340	2.201191
1	0.424441	-1.332059	1.042125
1	0.238796	0.002680	2.172092
6	1.939068	-1.955289	3.288038
1	2.924096	-1.336222	1.482917

1	2.711984	-0.045450	2.651328	1	2.989034	-3.141500	4.788260
6	3.205458	-2.390640	4.022666	1	3.932064	-2.822470	3.325895
1	1.214545	-1.547722	4.005635	1	3.686322	-1.538026	4.514573
1	1.457129	-2.827864	2.828860				

SI References

(1) P. Espinet, A. M. Echavarren, A. Rosellón, M. Livendahl, T. Lauterbach, *Organic Letters*, 2010, **12**, 3006.
(2) J. M. López-de-Luzuriaga, M. Monge, M. E. Olmos, D. Pascual, T. Lasanta, *Chem. Commun*, 2011, **47**, 6795.
(3) A. Isab, M. Fettouhi, S. Ahmad, L. Ouahab, *Polyhedron*, 2003, **22**, 1349.
(4) M. Peña-López, M. Ayán-Varela, L. A. Sarandeses, J. Sestelo, *Chem. Eur. J.* 2010, **16**, 9905.
(5) T. Lasanta, J. M. López-de-Luzuriaga, M. Monge, M. E. Olmos, D. Pascual, *Chem. Eur. J.* 2013, **19**, 4754.
(6) C. Weisemann, G. Schmidtberg, H. J. Brune, *Organomet. Chem,* 1988, **361** (3), 299.
(7) A. L. Casado, A. M. Gallego, P. Espinet, *J. Am. Chem. Soc.* 2000, **122**, 11711.
(8) G. B. Deacon, B. M. Gatehouse, K. T. Nelson-Reed, *J. Organomet. Chem*, 1989, **359**, 267.
(9) J. delPozo, D. Carrasco, M. H. Pérez-Temprano, M. García-Melchor, R. Álvarez, J. A. Casares, P. Espinet, *Angew. Chem. Int. Ed.* 2013, **52**, 2189.
(10) Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-20.
(11) Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
(12) Pérez-Temprano, M. H.; Casares, J. A.; de Lera, A. R.; Álvarez, R.; Espinet, P. *Angew. Chem. Int. Ed.* **2012**, *51*, 4917–4920.
(13) (a) Hay, P. J.; Wadt, W. R.; *J. Chem. Phys.* **1985**, *82*, 270-283; (b) Hay, P. J.; Wadt, W. R.; *J. Chem. Phys.* **1985**, *82*, 299-310.
(14) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B*, **2009**, *113*, 6378–6396.
(15) http://www.sigmaaldrich.com/chemistry/solvents/tetrahydrofuran-center.html
(16) Martin, R. L.; Hay, P. J.; Pratt, L. R. *J. Phys. Chem. A*, **1998**, *102*, 3565–3573. For examples of this approach, see refs. 17 and 18.
(17) Sieffert, N.; Bühl, M. *J. Am. Chem. Soc.* **2010**, *132*, 8056–8070.