Supporting Information

A Combined Experimental and Theoretical Mechanistic Investigation of the Barbier Allylation in Aqueous Media

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General procedures

THF was distilled from Na/benzophenone under nitrogen. Solvents used for chromatography were of HPLC grade. Zinc dust (8.0 g, 122 mmol, Fluka 00618, ≥99.0%) was activated by stirring with 2 M HCl (150 mL) for 10 min, then filtered and washed successively with water (75 mL), methanol (75 mL) and ether (75 mL) and dried with a heatgun under high vacuum for 10 min to leave a fine, light grey powder. Antimony was prepared by a revised procedure[1]: $SbCl_3$ (2.32 g, 10.2 mmol) was suspended in water (50 mL) and stirred with $NaBH_4$ (1.15 g, 30.4 mmol) under argon for 5 min. The precipitated metal was isolated by filtration and washed successively with water (50 mL), methanol (50 mL) and ether (50 mL) and dried with a heatgun under high vacuum for 10 min to leave a fine black powder. Indium powder (Aldrich 264032, -100 mesh, 99.99%), tin powder (Aldrich 265632, -325 mesh, 99.8%), bismuth powder (Aldrich 26562, -100 mesh, 99.5%) and magnesium powder (Strem 931298, 99%) were used as received. *p*-Tolualdehyde and *p*-anisaldehyde were purified by fractional distillation before use.

Thin layer chromatography was performed on aluminum plates coated with silica gel 60. Visualization was done by UV-radiation and/or heating after dipping in a solution of cerium(IV)sulfate (2.5 g) and ammonium molybdate (6.25 g) in 10% aqueous sulfuric acid (250 mL). Flash chromatography was performed with 60 Å silica gel (35-70 μm). NMR spectroscopy was carried out in $CDCl_3$ with residual $CHCl_3$ (δ_H = 7.26 ppm) and $CDCl_3$ (δ_C = 77.0 ppm) as the internal standards, while IR spectra were obtained for thin films on AgCl plates.

Reaction progress was monitored by taking out samples of 100 μL and diluting with 0.9 mL of THF. Excess metal powder was removed by centrifugation. All samples were stored at 5 ºC immediately after being taken out. Analysis was performed by gas chromatography with a 30 m × 0.25 mm × 0.25 μm Supelco Equity-1 capillary column. Retention times for all compounds are shown below. The homoallylic alcohols were prepared according to the general procedure for the competitive zinc allylation. The corresponding pinacols were prepared as a mixture of isomers according to a literature procedure.[2]

The secondary kinetic isotope effect (SDKIE) was determined for each metal by a competition experiment using *d*-benzaldehyde and *p*-tolualdehyde, thus allowing straightforward separation by GC. The SDKIE could then be determined by comparison to the value determined in the competition experiment with *p*-tolualdehyde and benzaldehyde.

General procedure for competitive zinc allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in anhydrous THF (5.0 mL). A sample was taken out for analysis and allylbromide (173 μL, 2.0 mmol) was added. Another sample was taken out for analysis and saturated aqueous NH_4Cl (5.0 mL) was added. Portions of activated zinc dust (~ 13 mg, 0.2 mmol) were added at 5 min intervals on a water bath at room temperature until 2 equivalents of zinc was reached. Before each addition of zinc the vigorous stirring was discontinued and a sample was taken out for analysis.

General procedure for indium allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in THF (7.0 mL) and deionized H_2O (3.0 mL). A sample was taken out for analysis and allylbromide (130 μL, 1.5 mmol) was added. Another sample was taken out for analysis and indium powder (172 mg, 1.5 mmol) was added. Samples were then taken out every 20-30 min until the reaction had gone to completion (~5 h).

For indium direct determination of the kinetic isotope effect was accomplished by reacting a mixture of benzaldehyde and *d*-benzaldehyde following the procedure specified above. Samples were analyzed by GC-MS using a HP-5MS column (30 m × 0.25 mm × 0.25 μm) and the temperature program was 100 ºC (hold 5 min) and then a ramp (40 ºC /min) to 300 ºC. Single ion monitoring was selected (M = 105, 106, 128), which allowed the use of the molecular ion of each benzaldehyde to be quantified relative to the molecular ion of the internal standard (naphthalene, M = 128).

General procedure for tin allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in THF (7.0 mL) and deionized H_2O (3.0 mL) in a two-necked flask fitted with a reflux condenser. A sample was taken out for analysis and allylbromide (173 μL, 2.0 mmol) was added. Another sample was taken out for analysis followed by addition of tin powder (119 mg, 1.0 mmol) and heating the suspension on an oil bath to 60 ºC. After approximately 40 min where the allylation initiated samples were taken out at the following intervals: 30, 5, 2×2.5, 5×2, 2×3, 4, 2×5, 8, 12, 2×15, 2×30 min.

General procedure for antimony allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in THF (7.0 mL) and 0.5 M aqueous HCl (3.0 mL). A sample was taken out for analysis and allylbromide (216 μL, 2.5 mmol) was added. Another sample was taken out for analysis and activated antimony powder (244 mg, 2.0 mmol) was added. Samples were then taken out every hour until the reaction had gone to completion (~12-16 h). The reaction was run under an argon atmosphere.

General procedure for bismuth allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in THF (5.0 mL) and deionized H_2O (5.0 mL) in a two-necked flask fitted with a reflux condenser. A sample was taken out for analysis and allylbromide (173 μL, 2.0 mmol) was added. Another sample was taken out for analysis followed by addition of bismuth powder (418 mg, 2.0 mmol) and heating the suspension on an oil bath to 60 ºC. After approximately 40 min where the allylation initiated samples were taken out at the following intervals: 30, 5, 2×2.5, 5×2, 2×3, 4, 2×5, 8, 12, 2×15, 2×30 min.

General procedure for competitive magnesium allylation used for the Hammett plot

Benzaldehyde (0.5 mmol), the *p*-substituted benzaldehyde (0.5 mmol) and naphthalene (0.25 mmol) were dissolved in DMF (8.0 mL). A sample was taken out for analysis and allylbromide (457 μL, 5.0 mmol) was added. Another sample was taken out for analysis and 0.1 M aqueous NH_4Cl (2.0 mL) was added. Magnesium powder (486 mg, 20 mmol) was then added and the slurry was stirred at rt. Samples were drawn at regular time intervals and filtered through a small plug of cotton, which was washed with 0.8 mL of DMF. The samples were analyzed immediately by GC using a 15 m × 0.10 mm × 0.10 μm Supelco Equity-1 capillary column (FastGC). The temperature program was 100 ºC (hold 5 min) and then a ramp (20 ºC /min) to 300 ºC.

General procedure for the preparation of the corresponding pinacols

Benzaldehyde (5 mmol) was dissolved in methanol (10 mL) and aluminum powder (0.27 g, 10 mmol) was added followed by KOH (2.53 g, 45 mmol). After 10 min where the vigorous reaction had subsided, the slurry was filtrated and 50 mL of H_2O was added. Extraction with 3 × 50 mL of ethyl acetate, drying with Na_2SO_4 and concentration in vacuo left a white, crude solid of the mixed pinacols in quantitative yield.

General method for GC-analysis (Method A):

Temperature (ºC)	Hold Time (min.)
100.0	12.0 (ramp 20)
200.0	10.0 (ramp 20)
300.0	5.0

Retention times for reaction components (Method A):

	Aldehyde	Benzylalcohol	Pinacols(*dl/ meso*)	Homoallyl
-CN	11.40	16.08	-	18.13
$-CF_3$	3.80	6.47	21.67/ 22.09	13.70
-COOMe	15.47	17.29	-	19.44

-Cl	8.48	12.46	30.34/ 30.57	18.81
-H	4.01	5.15	22.04/ 21.06	12.51
-^{t}Bu	14.88	15.56	31.98/ 32.16	18.00
-OMe	12.98	13.94	31.16/ 31.35	17.18
-OBu	17.73	17.86	-	20.37

Method for *p*-Tolualdehyde GC-analysis (Method B):

Temperature (ºC)	Hold Time (min.)
120.0	10.0
200.0	10.0
300.0	5.0

Retention times for reaction components (Method B):

	Aldehyde	Benzylalcohol	Pinacols(*dl*/ *meso*)	Homoallyl
-H	3.10	3.52	18.72/ 17.73	6.84
-Me	4.18	4.72	23.02/ 23.58	10.38

4-(1-Hydroxybut-3-enyl)benzonitrile

R_f = 0.30 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.33-2.55 (m, 2H), 2.59 (bs, 1H), 4.77 (dd, 1H, *J* = 5.0, 7.8 Hz), 5.09-5.19 (m, 2H), 5.68-5.82 (m, 1H), 7.42-7.48 (m, 2H), 7.57-7.62 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.6, 72.2, 110.8, 118.8, 119.2, 126.4, 132.1, 133.3, 149.2. IR (neat, cm^{-1}): br 3460, 3076, 2907, 2228, 1641, 1608, 1504, 1414, 1055, 921, 843. MS *m/z*: 173. Anal. Calcd for $C_{11}H_{11}NO$: C, 76.28; H, 6.40; N, 8.09. Found: C, 76.02; H, 6.44; N, 7.94.

1-(4-(Trifluoromethyl)phenyl)but-3-en-1-ol

R_f = 0.47 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.19 (bs, 1H), 2.39-2.59 (m, 2H), 4.79 (dd, 1H, *J* = 4.8, 7.9 Hz), 5.14-5.22 (m, 2H), 5.71-5.86 (m, 1H), 7.44 (m, 2H), 7.57-7.63 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.9, 72.5, 119.5, 124.1 (q, *J* = 272.0 Hz), 125.3 (q, *J* = 3.8 Hz), 126.0, 129.6 (q, *J* = 32.3 Hz), 133.6, 147.7. IR(neat, cm^{-1}): br 3380, 3079, 2910, 1928, 1643, 1621, 1416, 1327, 1168, 1124, 1070. MS *m/z*: 216. Anal. Calcd for $C_{11}H_{11}F_3O$: C, 61.11; H, 5.13. Found: C, 60.92; H, 5.14.

Methyl 4-(1-hydroxybut-3-enyl)benzoate

R_f = 0.33 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.39-2.53 (m, 2H), 2.89 (bs, 1H), 3.86 (s, 3H), 4.74 (dd, 1H, *J* = 5.5, 7.5 Hz), 5.06-5.14 (m, 2H), 5.66-5.82 (m, 1H), 7.34-7.39 (m, 2H), 7.92-7.97 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.6, 52.0, 72.9, 118.6, 125.6, 128.9, 129.5, 133.8, 149.0, 166.9. IR(neat, cm^{-1}): br 3475, 3075, 2951, 1938, 1721, 1641, 1611, 1436, 1286, 1110. MS (ESP+) for $C_{22}H_{26}O_3$ $[M+Na]^+$: 229.1. Found: 229.1. Anal. Calcd for $C_{12}H_{14}O_3$: C, 69.88; H, 6.84. Found: C, 69.69; H, 6.95.

1-(4-Chlorophenyl)but-3-en-1-ol

R_f = 0.43 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.35-2.53 (m, 2H), 2.40 (s, 1H), 4.66 (dd, 1H, *J* = 5.5, 7.4 Hz), 5.09-5.18 (m, 2H), 5.75 (tdd, 1H, *J* = 7.1, 9.7, 17.2 Hz), 7.22-7.33 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.7, 72.5, 118.7, 127.1, 128.4, 133.0, 133.9, 142.2. IR(neat, cm^{-1}): br 3373, 3078, 2907, 1901, 1641, 1597, 1493, 1411, 1091, 1014. MS *m/z*: 182. Anal. Calcd for $C_{10}H_{11}ClO$: C, 65.76; H, 6.07; Cl, 19.41. Found: C, 65.71; H, 6.17; Cl, 19.27.

1-Phenylbut-3-en-1-ol

R_f = 0.47 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.10 (s, 1H), 2.49-2.60 (m, 2H), 4.74 (dd, 1H, *J* = 5.5, 7.4 Hz), 5.12-5.21 (m, 2H), 5.82 (tdd, 1H, *J* = 7.1, 10.2, 17.1 Hz), 7.25-7.43 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.7, 73.2, 118.2, 125.7, 127.4, 128.3, 134.4, 143.8. IR (neat, cm^{-1}): br

3383, 3029, 2906, 1950, 1641, 1493, 1455, 1314, 1198, 1046, 916. MS *m/z*: 148. Anal. Calcd for $C_{10}H_{12}O$: C, 81.04; H, 8.16. Found: C, 80.85; H, 8.29.

1-*p*-Tolylbut-3-en-1-ol

R_f = 0.47 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.08 (s, 1H), 2.36 (s, 3H), 2.48-2.56 (m, 2H), 4.70 (t, 1H, *J* = 6.5 Hz), 5.12-5.21 (m, 2H), 5.82 (tdd, 1H, *J* = 7.1, 10.2, 17.2 Hz), 7.15-7.21 (m, 2H), 7.23-7.30 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 21.1, 43.7, 73.1, 118.1, 125.7, 129.0, 135.6, 137.1, 140.9. IR(neat, cm^{-1}): br 3383, 3077, 2922, 1904, 1640, 1514, 1435, 1307, 1198, 1044, 915, 816. MS *m/z*: 162. Anal. Calcd for $C_{11}H_{14}O$: C, 81.44; H, 8.70. Found: C, 81.52; H, 8.91.

1-(4-*tert*-Butylphenyl)but-3-en-1-ol

R_f = 0.43 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 1.33 (s, 9H), 2.13(s, 1H), 2.46-2.57 (m, 2H), 4.66-4.73 (m, 1H), 5.13-5.22 (m, 2H), 5.83 (tdd, 1H, *J* = 5.1, 10.1, 17.3 Hz), 7.26-7.42 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 31.3, 34.5, 43.6, 73.1, 118.1, 125.3, 125.5, 134.7, 140.8, 150.4. IR(neat, cm^{-1}): br 3362, 3076, 2964, 1641, 1509, 1410, 1363, 1269, 1109, 1051, 914, 835. MS *m/z*: 204. Anal. Calcd for $C_{14}H_{20}O$: C, 82.30; H, 9.87. Found: C, 82.20; H, 9.85.

1-(4-Methoxyphenyl)but-3-en-1-ol

R_f = 0.33 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.24 (s, 1H), 2.46-2.52 (m, 2H), 3.80 (s, 3H), 4.66 (t, 1H, *J* = 6.6 Hz), 5.09-5.18 (m, 2H), 5.79 (tdd, 1H, *J* = 7.1, 10.2, 17.2 Hz), 6.85-6.91 (m, 2H), 7.24-7.31 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.6, 55.2, 72.9, 113.6, 118.1, 127.0, 134.6, 136.0, 158.9. IR(neat, cm^{-1}): br 3404, 3075, 2934, 2836, 1612, 1514, 1464, 1302, 1250, 1177, 1038. MS *m/z*: 178. Anal. Calcd for $C_{11}H_{14}O_2$: C, 74.13; H, 7.92. Found: C, 73.98; H, 8.02.

1-(4-Butoxyphenyl)but-3-en-1-ol

R_f = 0.38 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 0.98 (t, 3H, *J* = 7.4 Hz), 1.43-1.56 (m, 2H), 1.71-1.82 (m, 2H), 2.11 (bs, 1H), 2.46-2.52 (m, 2H), 3.95 (t, 2H, *J* = 6.5 Hz), 4.66 (t, 1H, *J* = 6.5 Hz), 5.09-5.19 (m, 2H), 5.79 (tdd, 1H, *J* = 7.1, 10.1, 17.2 Hz), 6.84-6.91 (m, 2H), 7.23-7.29 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 13.8, 19.2, 31.3, 43.7, 67.6, 73.0, 114.3, 118.1, 127.0, 134.6, 135.8, 158.5. IR(neat, cm^{-1}): br 3385, 3075, 2961, 1707, 1617, 1507, 1246, 1173, 1035, 917, 833. MS *m/z*: 220. Anal. Calcd for $C_{14}H_{20}O_2$: C, 76.33; H, 9.15. Found: C, 76.07; H, 9.14.

Di-[1-(4-methoxyphenyl)but-3-en-1-yl] ether (obtained as a byproduct in the reaction with zinc)

R_f = 0.47 (EtOAc:Heptane 3:7). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.26-2.42 (m, 2H), 2.47-2.65 (m, 2H), 3.83 (s, 6H), 4.03-4.09 (m, 2H), 4.89-5.00 (m, 4H), 5.59-5.75 (m, 2H), 6.86 (m, 4H), 7.14 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 43.1, 55.5, 77.7, 113.9, 116.8, 128.6, 134.3, 135.4, 159.3. IR(neat, cm^{-1}): 3072, 2933, 2834, 1610, 1513, 1302, 1249, 1170, 1073. HRMS (ESP+) for $C_{22}H_{26}O_3$ $[M+Na]^+$: 361.1780. Found: 361.1777.

Table S1 Data for the competition experiments with Zinc.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
t-Bu	0.68	0.997	0.167491	-0.2	0.13	-0.26	-0.13
OMe	0.39	0.997	0.408935	-0.27	0.24	-0.78	-0.26
Me	0.74	0.998	0.130768	-0.17	0.11	-0.31	-0.17
Cl	1.45	0.998	-0.16137	0.23	0.12	0.11	0.19
COOMe	2.29	0.997	-0.35984	0.45	0.35	0.49	0.75
CF3	2.16	0.999	-0.33445	0.54	0.08	0.61	0.65
CN	2.98	0.997	-0.47422	0.66	0.46	0.66	1

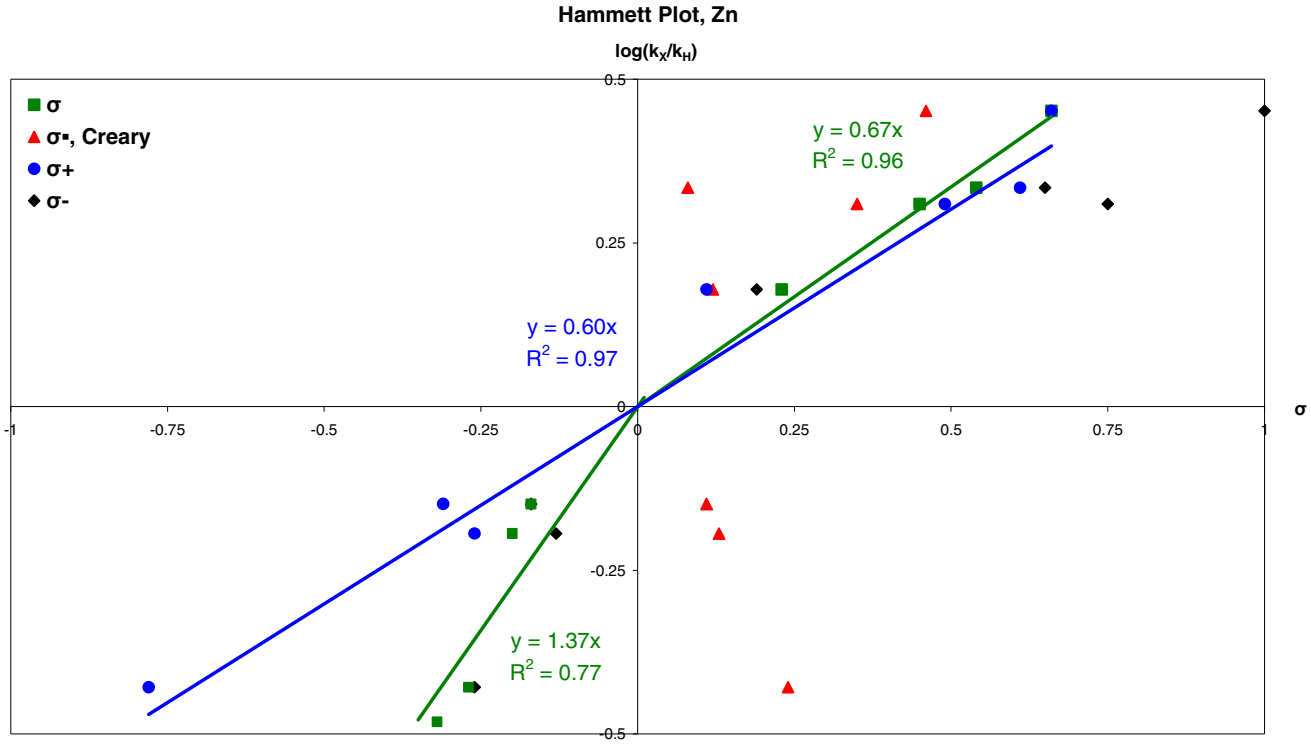

Figure S1 Hammett plot for the allylation with Zinc.

Table S2 Data for the competition experiments with Indium.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
Me	0.62	0.999	-0.20761	-0.17	0.11	-0.31	-0.17
Cl	1.62	0.997	0.209515	0.23	0.12	0.11	0.19
COOMe	2.31	0.991	0.363612	0.45	0.35	0.49	0.75
CN	3.18	0.988	0.502427	0.66	0.46	0.66	1
t-Bu	0.58	0.999	-0.23657	-0.2	0.13	-0.26	-0.13
CF3	2.12	0.995	0.326336	0.54	0.08	0.61	0.65

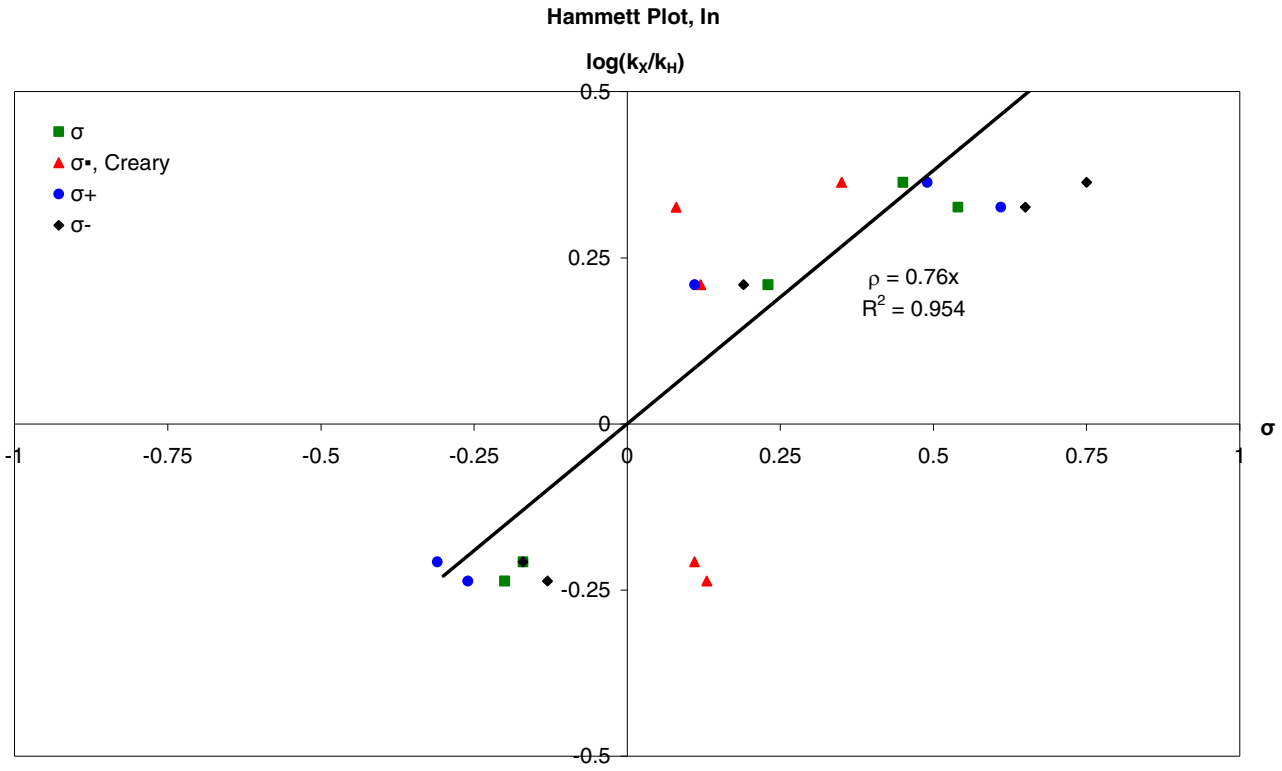

Figure S2 Hammett plot for the allylation with Indium.

Table S3 Data for the competition experiments with Tin.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
OMe	0.267	0.997	-0.57349	-0.27	0.24	-0.78	-0.26
Me	0.614	0.999	-0.21183	-0.17	0.11	-0.31	-0.17
Cl	1.32	0.998	0.120574	0.23	0.12	0.11	0.19
COOMe	2.76	0.995	0.440909	0.45	0.35	0.49	0.75
CF3	3.04	0.997	0.482874	0.54	0.08	0.61	0.65
CN	4.42	0.999	0.645422	0.66	0.46	0.66	1

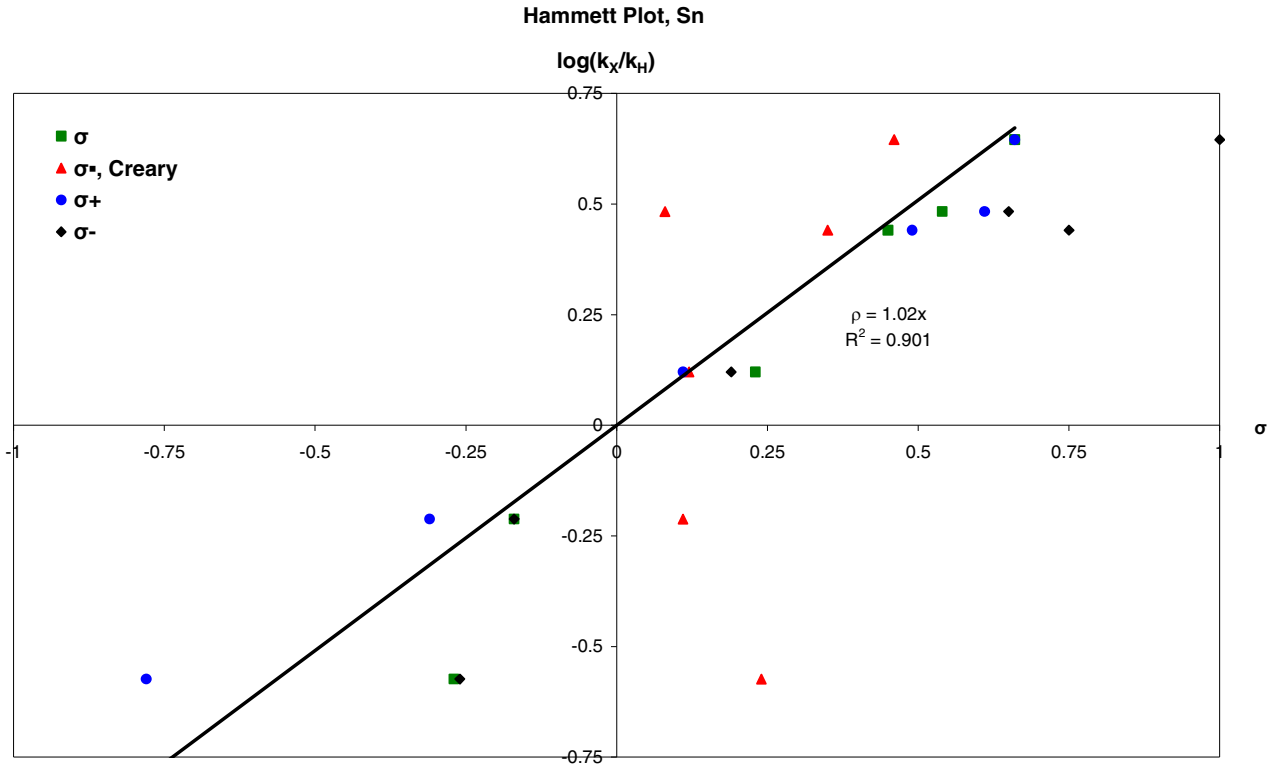

Figure S3 Hammett plot for the allylation with Tin.

Table S4 Data for the competition experiments with Antimony.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
OMe	0.32	0.987	-0.49485	-0.27	0.24	-0.78	-0.26
Me	0.72	0.999	-0.14267	-0.17	0.11	-0.31	-0.17
Cl	1.45	0.997	0.161368	0.23	0.12	0.11	0.19
COOMe	2.56	0.991	0.40824	0.45	0.35	0.49	0.75
CN	5.3	0.988	0.724276	0.66	0.46	0.66	1
CF3	3.25	0.995	0.511883	0.54	0.08	0.61	0.65

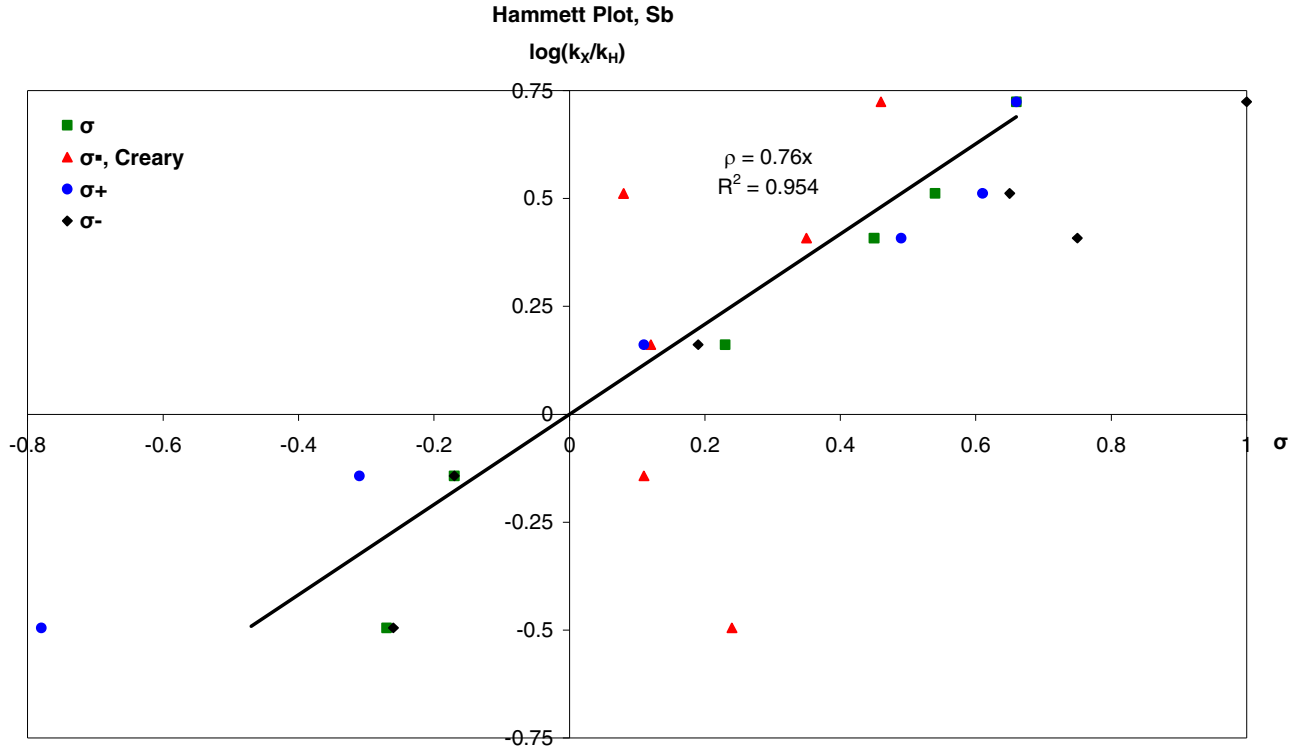

Figure S4 Hammett plot for the allylation with Antimony.

Table S5 Data for the competition experiments with Bismuth.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
OMe	0.383	0.997	-0.4168	-0.27	0.24	-0.78	-0.26
Me	0.682	0.999	-0.16622	-0.17	0.11	-0.31	-0.17
Cl	1.54	0.995	0.187521	0.23	0.12	0.11	0.19
COOMe	2.59	0.998	0.4133	0.45	0.35	0.49	0.75
CF3	3.5	0.993	0.544068	0.54	0.08	0.61	0.65
CN	5.07	0.996	0.705008	0.66	0.46	0.66	1
t-Bu	0.723	0.999	-0.14086	-0.2	0.13	-0.26	-0.13

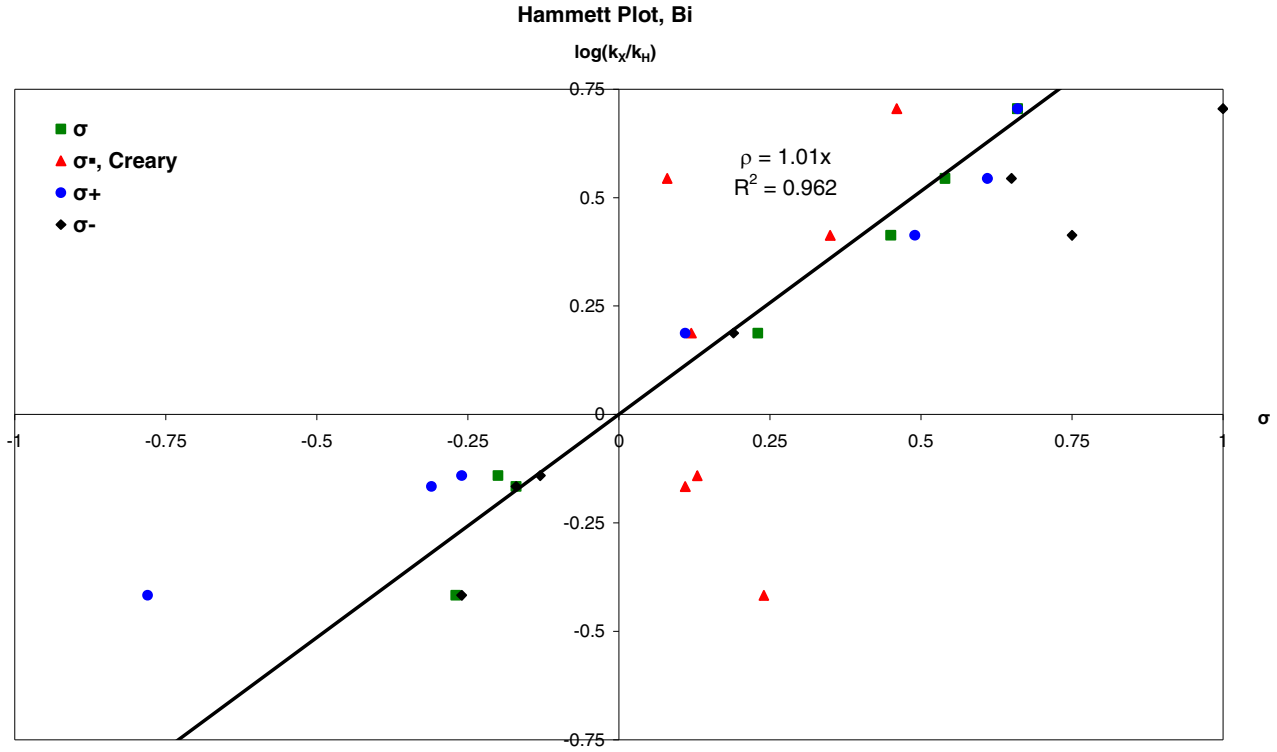

Figure S5 Hammett plot for the allylation with Bismuth.

Table S6 Data for the competition experiments with Magnesium.

X	kX/kH	R^2	log(kX/kH)	σ	σ▪, Creary	σ+	σ-
Me	0.256	0.999	-0.59176	-0.17	0.11	-0.31	-0.17
Cl	4.09	0.995	0.611723	0.23	0.12	0.11	0.19
COOMe	45.6	0.998	1.658965	0.45	0.35	0.49	0.75
CF3	32.6	0.993	1.513218	0.54	0.08	0.61	0.65

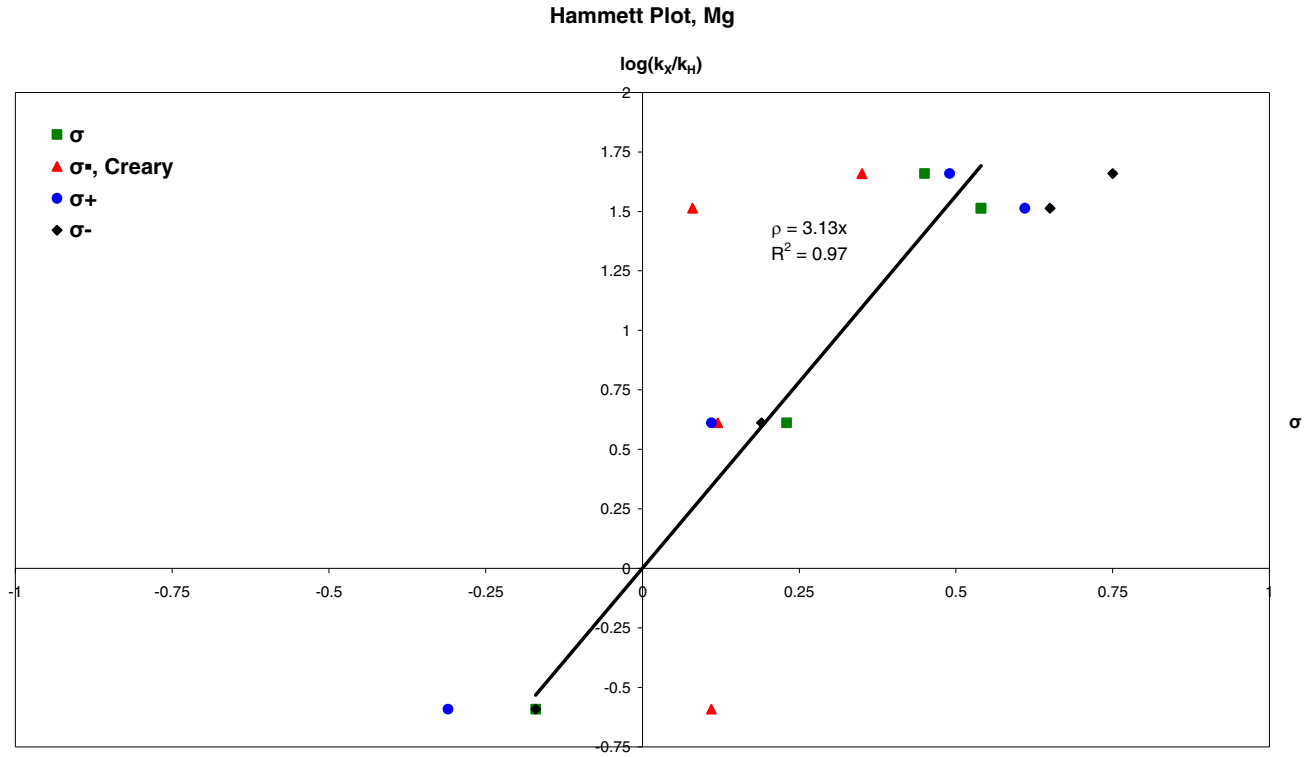

Figure S6 Hammett plot for the allylation with Magnesium.

References

1. Ren, P.-D.; Jin, Q.-H.; Yao, Z.-P. *Synth. Commun.* **1997**, *27*, 2761-2767.
2. Khurana, J.M.; Sehgal, A. *J. Chem. Soc., Chem. Commun.* **1994**, 571-572.

PhCHO_vac_min_freq.out
E_scf = -345.56622929035 a.u.
E_Gibbs = -345.486322 a.u.
ZPE = 69.282 kcal/mol

C	-1.08674	0.82233	0.00000
C	-0.37979	-0.38689	0.00000
C	1.02335	-0.37678	0.00000
C	1.70783	0.83371	0.00000
C	0.99676	2.03953	0.00000
C	-0.39971	2.03526	0.00000
H	-2.17505	0.80744	0.00000
H	1.54983	-1.32670	0.00000
H	2.79450	0.84479	0.00000
H	1.53427	2.98436	0.00000
H	-0.94790	2.97336	0.00000
C	-1.11585	-1.67142	0.00000
O	-0.59304	-2.76955	0.00000
H	-2.22443	-1.57021	0.00000

PhCHO_THF_min_freq.out
E_solv = -345.57467162825 a.u.

C	-1.08854	0.82082	0.00000
C	-0.37757	-0.38804	0.00000
C	1.02860	-0.37848	0.00000
C	1.71242	0.83327	0.00000
C	0.99747	2.03927	0.00000
C	-0.40128	2.03425	0.00000
H	-2.17739	0.80425	0.00000
H	1.56299	-1.32490	0.00000
H	2.79978	0.84525	0.00000
H	1.53378	2.98527	0.00000
H	-0.95099	2.97188	0.00000
C	-1.11865	-1.66410	0.00000
O	-0.59878	-2.77091	0.00000
H	-2.22441	-1.56204	0.00000

HomoAllyl_vac_min_freq.out
E_scf = -462.85955668038 a.u.
E_Gibbs = -462.717558 a.u.
ZPE = 112.334 kcal/mol

C	0.15535	-0.46022	2.51502
C	1.37592	-0.30333	1.99180
C	2.15432	0.96639	1.88610
C	2.56184	1.26701	0.36145
O	1.53494	1.38651	-0.44049
H	-0.39902	0.38190	2.92665
H	-0.35032	-1.42517	2.52493
H	1.87629	-1.18326	1.57554
H	3.05779	0.89002	2.51673
H	1.55680	1.81313	2.25056
H	3.29437	0.41031	0.13723
C	5.04336	4.88776	0.36634
C	3.78651	4.85164	-0.24653
C	3.03032	3.67876	-0.22913
C	3.49838	2.52443	0.40581
C	4.76192	2.56871	1.00870
C	5.53111	3.73588	0.99233
H	5.64094	5.79900	0.35016
H	3.40369	5.74394	-0.74392
H	2.05741	3.57299	-0.70734
H	5.15613	1.67206	1.48984
H	6.51417	3.75011	1.46462

HomoAllyl_THF_min_freq.out
E_solv = -462.94663857743 a.u.

C	0.15027	-0.49680	2.49125
C	1.37280	-0.30839	1.98436

```
  C        2.11562        0.98950        1.88927
  C        2.57145        1.28274        0.40192
  O        1.55425        1.35588       -0.45109
  H       -0.43692        0.32760        2.89475
  H       -0.32006       -1.47901        2.50992
  H        1.90904       -1.17548        1.58742
  H        2.99608        0.95371        2.55197
  H        1.48122        1.81951        2.22808
  H        3.30803        0.43593        0.20217
  C        5.06385        4.88205        0.34708
  C        3.79312        4.86826       -0.23616
  C        3.01923        3.70571       -0.19857
  C        3.48294        2.54314        0.42351
  C        4.76103        2.56712        0.99998
  C        5.54691        3.72243        0.96467
  H        5.67619        5.78108        0.31239
  H        3.41226        5.76210       -0.72888
  H        2.04021        3.64157       -0.66642
  H        5.15485        1.66441        1.46828
  H        6.54068        3.71835        1.41003

Zn_h1allyl_vac_min_freq.out
E_scf = -196.10785574274 a.u.
E_Gibbs = -196.071989 a.u.
ZPE = 44.209 kcal/mol
 Zn       -0.84567        1.73592       -0.64213
 Br       -0.61546        2.90110       -2.72449
  C       -1.10058        1.87677        2.23836
  C       -1.08003        0.83646        1.17057
  C       -2.18984        2.35401        2.85430
  H       -0.24869        0.13359        1.28945
  H       -2.11907        3.12382        3.61694
  H       -2.01566        0.26874        1.12608
  H       -3.18824        1.98937        2.61901
  H       -0.12700        2.28157        2.52205

Zn_h1allyl_THF_min_freq.out
E_solv = -196.14188581571 a.u.
 Zn       -1.00675        1.13668       -1.14345
 Br       -0.39733        3.34574       -2.27977
  C       -1.22002        1.98150        1.78190
  C       -1.13505        0.77652        0.91325
  C       -2.27658        2.36299        2.51885
  H       -0.20777        0.22151        1.10468
  H       -2.24133        3.24649        3.15325
  H       -1.98787        0.10724        1.06789
  H       -3.21287        1.80476        2.51838
  H       -0.31717        2.59312        1.84964

Zn_allyl_PhCHO_chair_eqPh_vac_Reac_min_freq.out
E_scf = -541.69980780465 a.u.
E_Gibbs = -541.564389 a.u.
ZPE = 114.445 kcal/mol
 Zn       -0.17021       -0.06293        0.14346
  C       -0.17940        0.04487        2.21319
  C        1.21517       -0.05938        2.68304
  C        2.05290        0.95558        2.97531
  C        2.48131        1.43394       -0.03724
  O        1.29231        1.39358       -0.38609
  H       -0.64652        0.99773        2.48479
  H       -0.80510       -0.77966        2.56805
  H        1.61144       -1.07580        2.75724
  H        3.07137        0.77430        3.30802
  H        1.72366        1.99271        2.95403
 Br       -0.91550       -1.19278       -1.87305
  H        3.02101        0.50389        0.19621
  C        4.80077        4.99032        0.12477
```

```
  C        3.44913        5.06382       -0.23244
  C        2.68023        3.90765       -0.28518
  C        3.26418        2.66685        0.02425
  C        4.62134        2.59887        0.37907
  C        5.38789        3.75933        0.42908
  H        5.39822        5.89735        0.16452
  H        3.00240        6.02490       -0.47060
  H        1.63204        3.94071       -0.56569
  H        5.06715        1.63561        0.61696
  H        6.43742        3.70852        0.70411

Zn_allyl_PhCHO_chair_eqPh_vac_Reac_min_solv2_freq.out
E_solv = -541.72332286478 a.u.
 Zn       -0.44003        0.24822        0.78010
  C        0.74174       -1.36260        1.40751
  C        2.17709       -1.11427        1.14741
  C        3.10837       -0.73516        2.04160
  C        2.03964        2.12419        0.60288
  O        1.10434        1.61191       -0.02711
  H        0.53928       -1.56118        2.46585
  H        0.36040       -2.19986        0.80693
  H        2.49570       -1.22306        0.10783
  H        4.14003       -0.55669        1.74804
  H        2.87013       -0.60644        3.09726
 Br       -2.05060        0.53025       -1.17347
  H        1.92832        2.31248        1.68208
  C        5.76212        3.50006       -0.91622
  C        4.92882        2.74448       -1.75457
  C        3.69907        2.28589       -1.29075
  C        3.30828        2.56953        0.03178
  C        4.15573        3.31729        0.87000
  C        5.37419        3.79226        0.39421
  H        6.71849        3.86066       -1.28717
  H        5.24877        2.51624       -2.76982
  H        3.04380        1.70660       -1.93573
  H        3.84635        3.52825        1.89139
  H        6.01970        4.38061        1.04131

Zn_allyl_PhCHO_chair_eqPh_vac_Prod_min_freq.out
E_scf = -541.71327377987 a.u.
E_Gibbs = -541.571575 a.u.
ZPE = 116.518 kcal/mol
 Zn        0.16895        0.08060       -0.24079
  C        0.07007       -0.31032        2.24464
  C        1.41352       -0.24605        2.10518
  C        2.20277        1.01028        1.95716
  C        2.68925        1.21345        0.46728
  O        1.62453        1.23245       -0.42635
  H       -0.52130        0.58991        2.41339
  H       -0.45456       -1.25874        2.32859
  H        1.96920       -1.18319        2.02011
  H        3.08383        0.97826        2.60916
  H        1.60187        1.88385        2.23636
 Br       -1.67091       -1.05659       -1.24326
  H        3.37855        0.37611        0.24629
  C        4.97143        4.89481        0.36040
  C        3.66228        4.86652       -0.12201
  C        2.92921        3.67868       -0.10265
  C        3.49758        2.50560        0.40108
  C        4.81471        2.53839        0.87487
  C        5.54836        3.72437        0.85764
  H        5.54201        5.81999        0.34239
  H        3.21063        5.77182       -0.52060
  H        1.91769        3.64235       -0.49354
  H        5.27604        1.62644        1.25193
  H        6.57152        3.73360        1.22543
```

Zn_allyl_PhCHO_chair_eqPh_vac_Prod_min_solv_freq.out
E_solv = -541.75034632945 a.u.

Zn	-0.25140	0.67693	0.25259
C	1.25346	-1.77101	0.75178
C	1.96106	-1.18602	-0.22826
C	2.93207	-0.05732	-0.07251
C	2.42731	1.21823	-0.81968
O	1.22470	1.70687	-0.29813
H	1.40456	-1.52232	1.79979
H	0.55660	-2.57922	0.54290
H	1.80479	-1.52847	-1.25435
H	3.90298	-0.34610	-0.49818
H	3.08948	0.18726	0.98574
Br	-2.22211	-0.46079	1.19100
H	2.30697	0.92272	-1.87970
C	5.52735	4.25744	-0.72226
C	5.46319	3.34865	-1.78186
C	4.45839	2.37800	-1.81195
C	3.50506	2.29954	-0.78834
C	3.57551	3.21798	0.26566
C	4.57903	4.18810	0.30219
H	6.30467	5.01795	-0.69867
H	6.18867	3.40224	-2.59092
H	4.40665	1.68201	-2.64856
H	2.82400	3.18050	1.04695
H	4.61695	4.89510	1.12852

Zn_allyl_PhCHO_chair_eqPh_vac_TS_freq.out
E_scf = -541.69447961459 a.u.
E_Gibbs = -541.554831 a.u.
ZPE = 114.995 kcal/mol

Zn	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.16300
C	1.39400	0.00000	2.42784
C	2.23079	1.10625	2.38441
C	2.63937	1.24650	0.24329
O	1.52132	1.19738	-0.38344
H	-0.54429	0.92080	2.38433
H	-0.55334	-0.90331	2.41942
H	1.86936	-0.97865	2.53329
H	3.25281	1.01534	2.73875
H	1.79827	2.10120	2.45450
Br	-1.34268	-1.10782	-1.66763
H	3.26218	0.34239	0.27418
C	4.84862	4.91591	0.30469
C	3.50009	4.91799	-0.06216
C	2.77548	3.72893	-0.07567
C	3.39523	2.52382	0.28362
C	4.75032	2.52653	0.64446
C	5.47387	3.71661	0.65486
H	5.41222	5.84514	0.31186
H	3.01557	5.84868	-0.34534
H	1.73284	3.71394	-0.37724
H	5.23805	1.59102	0.91246
H	6.52472	3.70990	0.93171

ZnBr_allyl_PhCHO_chair_eqPh_THF_QST_TS2_freq.out
E_solv = -541.72028934485 a.u.

Zn	-0.05734	-0.02952	0.07777
C	-0.04219	0.10171	2.25937
C	1.35032	0.08350	2.54592
C	2.20418	1.17204	2.49715
C	2.66557	1.14864	0.32857
O	1.56419	1.12607	-0.32315
H	-0.57463	1.03404	2.45721
H	-0.59910	-0.79262	2.54333

```
  H        1.80964       -0.89669        2.69300
  H        3.21983        1.07234        2.86874
  H        1.79519        2.18017        2.49781
 Br        0.56825       -2.32031       -0.86786
  H        3.22751        0.21503        0.45890
  C        5.05069        4.71456        0.16294
  C        3.74600        4.71357       -0.34001
  C        2.96956        3.55886       -0.26538
  C        3.48825        2.38951        0.30964
  C        4.80291        2.39302        0.80441
  C        5.57727        3.55115        0.73486
  H        5.65627        5.61605        0.10466
  H        3.33677        5.61062       -0.79898
  H        1.96127        3.54055       -0.66721
  H        5.21975        1.48789        1.24334
  H        6.59354        3.54883        1.12224

InBr2_allyl_vac_min_freq.out
E_scf = -145.62506275487 a.u.
E_Gibbs = -145.593816 a.u.
ZPE = 44.832 kcal/mol
 In       -0.79587        2.14564       -1.13342
 Br       -2.63521        2.97350       -2.67367
 Br        1.52999        2.93359       -1.77371
  C       -1.03311        1.93451        1.83058
  C       -1.20516        1.01715        0.66174
  C       -2.02463        2.55761        2.48020
  H       -0.50953        0.17304        0.68553
  H       -1.82296        3.21759        3.31857
  H       -2.22790        0.64030        0.56978
  H       -3.06878        2.42050        2.20571
  H       -0.00479        2.10836        2.14961

InBr2_allyl_THF_min_freq.out
E_solv = -145.64059435888 a.u.
 In       -0.87826        2.13834       -1.07739
 Br       -2.14196        2.21617       -3.30887
 Br        1.13352        3.72088       -1.28244
  C       -0.99698        1.86079        1.93652
  C       -1.42259        1.09689        0.72757
  C       -1.81022        2.58572        2.71553
  H       -0.92833        0.12313        0.64154
  H       -1.43123        3.11559        3.58600
  H       -2.50556        0.95494        0.66435
  H       -2.87750        2.67177        2.51456
  H        0.06485        1.81439        2.17918

InBr2_allyl_PhCHO_chair_eq_Reac_vac_min_freq.out
E_scf = -491.23053056704 a.u.
E_Gibbs = -491.099223 a.u.
ZPE = 115.247 kcal/mol
 In       -0.83397        0.20672        1.39935
  C       -0.27482       -1.57454        2.48443
  C        0.82307       -2.30296        1.78245
  C        2.11658       -2.29632        2.12812
  C        1.57284        1.73689        0.12579
  O        1.04220        1.32667        1.17432
  H        0.02048       -1.25386        3.48960
  H       -1.17848       -2.18721        2.57488
  H        0.52507       -2.86485        0.89572
  H        2.86021       -2.84231        1.55427
  H        2.47387       -1.75677        3.00360
 Br       -1.30504       -0.00999       -1.14539
  H        1.09686        1.50557       -0.83922
  C        5.13245        4.01977       -0.02211
  C        4.47706        3.66829       -1.20527
  C        3.30785        2.91699       -1.14557
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  C        2.79505        2.51572        0.10168
  C        3.46007        2.87383        1.29039
  C        4.62550        3.62438        1.22315
  H        6.04526        4.60787       -0.06784
  H        4.87714        3.98077       -2.16510
  H        2.78531        2.63763       -2.05741
  H        3.04656        2.55837        2.24300
  H        5.14425        3.90706        2.13430
 Br       -2.22317        2.06945        2.48890

InBr2_allyl_PhCHO_chair_eq_Reac_THF_min_freq.out
E_solv = -491.25078204117 a.u.
 In       -0.76186        0.18157        1.46091
  C       -0.52494       -1.55070        2.71094
  C        0.49142       -2.49276        2.15302
  C        1.73841       -2.65823        2.61363
  C        1.52573        1.84440        0.17247
  O        1.07494        1.25983        1.18617
  H       -0.25617       -1.18919        3.70902
  H       -1.52056       -2.00517        2.76579
  H        0.17161       -3.07514        1.28694
  H        2.42702       -3.35730        2.14461
  H        2.11135       -2.10453        3.47449
 Br       -1.26064       -0.19878       -1.08184
  H        1.00277        1.72851       -0.78702
  C        4.94932        4.31721        0.12698
  C        4.23199        4.08982       -1.05286
  C        3.10840        3.27053       -1.02659
  C        2.70304        2.67487        0.18641
  C        3.43258        2.90795        1.37247
  C        4.55125        3.72810        1.33731
  H        5.82611        4.96005        0.10669
  H        4.54954        4.55218       -1.98315
  H        2.53957        3.08740       -1.93551
  H        3.10682        2.44617        2.29911
  H        5.11775        3.91652        2.24494
 Br       -2.16393        2.24305        2.21244

InBr2_allyl_PhCHO_chair_eq_prod_vac_min_freq.out
E_scf = -491.23572920737 a.u.
E_Gibbs = -491.097486 a.u.
ZPE = 117.171 kcal/mol
 In       -0.28614        0.06889        1.21578
  C        1.32787       -2.00623        1.35299
  C        1.84034       -1.47942        0.21249
  C        2.81268       -0.35271        0.15225
  C        2.08958        1.00457       -0.21802
  O        1.10019        1.30848        0.72287
  H        1.73337       -1.74202        2.32878
  H        0.61273       -2.82581        1.32550
  H        1.44442       -1.83694       -0.74026
  H        3.57247       -0.55254       -0.61190
  H        3.31448       -0.21076        1.11541
 Br       -2.00861       -0.63112       -0.52074
  H        1.65526        0.87790       -1.22438
  C        5.11789        4.08677       -0.39650
  C        4.87392        3.27535       -1.50614
  C        3.88404        2.29430       -1.44821
  C        3.13132        2.11115       -0.28271
  C        3.37471        2.93098        0.82331
  C        4.36393        3.91356        0.76530
  H        5.88614        4.85445       -0.44031
  H        5.44819        3.41117       -2.41905
  H        3.68849        1.67359       -2.32137
  H        2.77283        2.80354        1.71720
  H        4.54241        4.54890        1.62919
 Br       -1.04195        0.13488        3.62780
```

InBr2_allyl_PhCHO_chair_eq_prod_THF_min_freq.out
E_solv = -491.25370059223 a.u.

In	-0.22026	-0.00666	1.19440
C	1.31354	-2.00114	1.41054
C	1.87917	-1.51969	0.26635
C	2.85274	-0.39625	0.21069
C	2.14478	0.94257	-0.24469
O	1.09412	1.27889	0.62601
H	1.70828	-1.72312	2.38914
H	0.62040	-2.84045	1.37965
H	1.53269	-1.92055	-0.68881
H	3.63804	-0.62453	-0.51900
H	3.31517	-0.22416	1.18847
Br	-2.08126	-0.64474	-0.44796
H	1.76659	0.77822	-1.26612
C	5.09588	4.10679	-0.37043
C	4.83200	3.34482	-1.51160
C	3.87231	2.33027	-1.46948
C	3.17038	2.06531	-0.28770
C	3.43736	2.83372	0.85204
C	4.39469	3.84901	0.81107
H	5.83792	4.90122	-0.40290
H	5.36498	3.54597	-2.43805
H	3.65978	1.74948	-2.36583
H	2.87636	2.64611	1.76269
H	4.58877	4.44376	1.70099
Br	-1.09388	0.30183	3.56867

InBr2_allyl_PhCHO_chair_eq_vac_TS_freq.out
E_scf = -491.22026019911 a.u.
E_Gibbs = -491.083129 a.u.
ZPE = 115.917 kcal/mol
Imaginary Eigenfrequency: -309.00 cm-1

In	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.28281
C	1.39740	0.00000	2.55060
C	2.22135	1.12104	2.52772
C	2.58418	1.34850	0.47089
O	1.42888	1.43082	-0.11689
H	-0.54736	0.91482	2.51711
H	-0.54344	-0.90911	2.54230
H	1.88114	-0.97626	2.61711
H	3.24350	1.02460	2.88079
H	1.77546	2.10405	2.65765
Br	1.01668	-2.17136	-0.90339
H	3.13940	0.40796	0.37666
C	5.05903	4.83914	0.60166
C	5.61151	3.57813	0.83925
C	4.80002	2.44671	0.80494
C	3.42934	2.56718	0.53196
C	2.88038	3.83420	0.28839
C	3.69466	4.96350	0.32482
H	5.69163	5.72246	0.62649
H	6.67347	3.47747	1.04584
H	5.23093	1.46309	0.98186
H	1.82316	3.91696	0.05712
H	3.26700	5.94330	0.13042
Br	-2.15074	0.82740	-1.06137

InBr2_allyl_PhCHO_chair_eq_THF_QST_TS_freq.out
E_solv = -491.23927823806 a.u.

In	-0.03043	-0.01972	0.03551
C	-0.00921	-0.00228	2.28071
C	1.39605	0.00877	2.54601
C	2.21654	1.12928	2.46497
C	2.64913	1.18838	0.42636

O	1.51584	1.23659	-0.22000
H	-0.55630	0.91595	2.50871
H	-0.54485	-0.90627	2.57394
H	1.87892	-0.96141	2.67668
H	3.23174	1.05322	2.84319
H	1.76454	2.11773	2.52129
Br	0.58775	-2.29488	-1.02425
H	3.19709	0.24028	0.42392
C	5.15330	4.65706	0.26353
C	5.69182	3.41811	0.62585
C	4.86920	2.29491	0.69686
C	3.50238	2.40226	0.39578
C	2.96792	3.64551	0.02365
C	3.79230	4.76694	-0.04172
H	5.79432	5.53369	0.21048
H	6.75150	3.32791	0.85068
H	5.28855	1.32918	0.97302
H	1.91456	3.71851	-0.22912
H	3.37567	5.72687	-0.33679
Br	-2.05400	1.00401	-1.16965

SnII_h3allyl_Br_vac_min_freq.out
E_scf = -133.89146982322 a.u.
E_Gibbs = -133.855276
ZPE = 44.238 kcal/mol
E_Gibbs, 60C = -133.860472

Sn	-0.45826	0.90888	-0.40515
C	2.01486	1.00682	-0.08100
C	1.62489	2.22602	-0.67072
C	1.71263	-0.27408	-0.58539
H	1.80041	3.15112	-0.13151
H	1.95106	-1.14592	0.01496
H	1.55232	2.31565	-1.75270
H	1.64926	-0.44174	-1.65870
H	2.27622	1.05217	0.97894
Br	-0.76961	0.80948	-3.09874

SnII_h3allyl_Br_THF_min.out
E_solv = -133.90373033159 a.u.

Sn	-0.46043	0.91014	-0.36275
C	2.00067	1.00540	-0.10743
C	1.60248	2.22351	-0.69801
C	1.68958	-0.27592	-0.61034
H	1.78005	3.15105	-0.16338
H	1.93039	-1.14871	-0.01199
H	1.51961	2.31069	-1.78053
H	1.61614	-0.44509	-1.68365
H	2.27154	1.05206	0.95008
Br	-0.75581	0.80858	-3.14941

Sn_allyl_PhCHO_chair_eqPh_Reac_vac_min_freq.out
E_scf = -479.48420248865 a.u.
E_Gibbs = -479.346154 a.u.
ZPE = 114.862 kcal/mol
E_Gibbs, 60C, H = -479.353414
E_Gibbs, 60C, D = -479.356877

Sn	-0.05213	0.06015	-0.02149
C	-0.06913	0.04003	2.25960
C	1.27403	0.07484	2.85250
C	1.99106	-0.98950	3.27315
C	2.57859	-1.54905	0.52949
O	1.37870	-1.60498	0.16752
H	-0.66510	0.92116	2.52347
H	-0.63244	-0.86283	2.52349
H	1.75104	1.05441	2.88029
H	2.98891	-0.87194	3.68684

```
  H        1.56955       -1.99225        3.29525
  H        3.07595       -0.57560        0.59918
  C        4.99210       -4.99592        1.10095
  C        3.64129       -5.15001        0.76649
  C        2.83838       -4.03115        0.58126
  C        3.38693       -2.74479        0.73186
  C        4.74515       -2.59642        1.06229
  C        5.54426       -3.72037        1.24762
  H        5.61579       -5.87410        1.24594
  H        3.22135       -6.14513        0.65043
  H        1.78993       -4.12925        0.31786
  H        5.16400       -1.59912        1.17430
  H        6.59344       -3.60619        1.50446
 Br        1.97295        1.88977       -0.25054

Sn_allyl_PhCHO_chair_eqPh_Reac_THF_min_freq.out
E_solv = -479.49781071798 a.u.
 Sn       -0.10209       -0.06645        0.06298
  C        0.02080        0.13595        2.30363
  C        1.38763        0.20070        2.85033
  C        2.09383       -0.83129        3.35399
  C        2.67373       -1.52598        0.53085
  O        1.46600       -1.58802        0.19568
  H       -0.55156        1.04762        2.50905
  H       -0.54976       -0.71954        2.68234
  H        1.87464        1.17442        2.78262
  H        3.10747       -0.70191        3.72591
  H        1.66039       -1.82494        3.45605
  H        3.16149       -0.54986        0.62575
  C        5.07302       -4.97986        1.07440
  C        3.75545       -5.12025        0.61702
  C        2.95972       -3.99514        0.44075
  C        3.48585       -2.71670        0.71127
  C        4.81430       -2.58030        1.15685
  C        5.60185       -3.71274        1.34520
  H        5.68993       -5.86364        1.21788
  H        3.35637       -6.10750        0.40038
  H        1.93706       -4.08178        0.08669
  H        5.21769       -1.59104        1.36157
  H        6.62383       -3.61279        1.70045
 Br        1.81752        1.92308       -0.40052

Sn_allyl_PhCHO_chair_eqPh_Prod_vac_min_freq.out
E_scf = -479.50788449590 a.u.
E_Gibbs = -479.366021 a.u.
ZPE = 116.700 kcal/mol
E_Gibbs, 60C, H = -479.373054
E_Gibbs, 60C, D = -479.376664
 Sn       -0.47468        0.40579        1.33399
  C        1.24982       -1.94200        1.50737
  C        1.78572       -1.47289        0.35920
  C        2.80468       -0.38643        0.27763
  C        2.13540        0.99923       -0.06418
  O        1.20653        1.30556        0.94659
  H        1.64387       -1.64678        2.47835
  H        0.50306       -2.73256        1.50327
  H        1.38686       -1.84008       -0.58597
  H        3.53860       -0.61037       -0.50554
  H        3.33834       -0.26894        1.22704
 Br       -1.29470       -0.09723       -1.20626
  H        1.62931        0.89666       -1.03525
  C        5.22925        4.00295       -0.38890
  C        4.89984        3.20863       -1.48880
  C        3.88887        2.25332       -1.38199
  C        3.19997        2.07627       -0.17631
  C        3.53212        2.87780        0.92048
  C        4.54041        3.83652        0.81378
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  H        6.01288        4.75180       -0.47127
  H        5.42339        3.33869       -2.43259
  H        3.62613        1.64694       -2.24726
  H        2.98177        2.75521        1.84793
  H        4.78559        4.45847        1.67126

Sn_allyl_PhCHO_chair_eqPh_Prod_THF_min_freq.out
E_solv = -479.51806407753 a.u.
 Sn       -0.44743        0.05837       -0.66412
  C        1.02822       -1.97011        0.99248
  C        1.99098       -1.64018        0.10545
  C        2.90537       -0.46426        0.23996
  C        2.47958        0.70914       -0.70788
  O        1.16692        1.12439       -0.38247
  H        0.91713       -1.43477        1.93436
  H        0.39059       -2.84010        0.84855
  H        2.09056       -2.23589       -0.80475
  H        3.92993       -0.75596       -0.02314
  H        2.90923       -0.09547        1.27114
 Br       -1.61775        1.03630        1.64901
  H        2.52974        0.33548       -1.74317
  C        5.22414        4.04498       -0.37828
  C        5.09528        3.35693       -1.58610
  C        4.20559        2.28306       -1.68675
  C        3.43461        1.88591       -0.58904
  C        3.56079        2.59198        0.61710
  C        4.45201        3.66023        0.72350
  H        5.91767        4.87870       -0.29423
  H        5.68093        3.65618       -2.45241
  H        4.10288        1.75380       -2.63217
  H        2.94886        2.31177        1.47087
  H        4.54518        4.19563        1.66577

Sn_allyl_PhCHO_chair_eqPh_vac_TS_freq.out
E_scf = -479.48291681528 a.u.
E_Gibbs = -479.342271 a.u.
ZPE = 115.191 kcal/mol
E_Gibbs, 60C, H = -479.349136
E_Gibbs, 60C, D = -479.352663
Imaginary Eigenfrequency: -239.50 cm-1
 Sn        0.00000        0.00000        0.00000
  C        0.00000        0.00000        2.38734
  C        1.37058        0.00000        2.78532
  C        2.16761       -1.11807        2.92831
  C        2.58565       -1.45792        0.71625
  O        1.39396       -1.53336        0.23234
  H       -0.55659        0.91453        2.59764
  H       -0.57351       -0.90166        2.61176
  H        1.85915        0.97263        2.83281
  H        3.18681       -1.01790        3.28868
  H        1.72162       -2.10410        3.02483
  H        3.11789       -0.50607        0.64829
  C        5.00700       -4.96366        0.98881
  C        3.63887       -5.08396        0.72626
  C        2.83980       -3.94760        0.64319
  C        3.40574       -2.67527        0.82447
  C        4.78074       -2.56077        1.08502
  C        5.57676       -3.70019        1.16741
  H        5.62860       -5.85310        1.04963
  H        3.19789       -6.06670        0.58221
  H        1.77917       -4.02616        0.42611
  H        5.22210       -1.57522        1.21691
  H        6.64081       -3.60507        1.36566
 Br        1.89540        1.96119       -0.22631

Sn_allyl_PhCHO_chair_eqPh_THF_QST_TS_freq.out
E_solv = -479.49187158961 a.u.
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 Sn       -0.00377        0.02075        0.01677
  C        0.02217       -0.03422        2.38812
  C        1.39978       -0.01605        2.76856
  C        2.21156       -1.12713        2.87057
  C        2.58892       -1.44166        0.65674
  O        1.39700       -1.52554        0.17695
  H       -0.55383        0.85901        2.63512
  H       -0.52573       -0.95505        2.59381
  H        1.87434        0.96510        2.84529
  H        3.23605       -1.02633        3.21738
  H        1.77272       -2.11753        2.96061
  H        3.12785       -0.49238        0.59402
  C        5.09112       -4.89724        0.84488
  C        3.70641       -5.05356        0.70745
  C        2.87687       -3.93572        0.65331
  C        3.43122       -2.64689        0.74011
  C        4.82102       -2.49599        0.87804
  C        5.64759       -3.61679        0.92741
  H        5.73513       -5.77249        0.88515
  H        3.27663       -6.05006        0.64040
  H        1.80256       -4.04689        0.53846
  H        5.24989       -1.49758        0.93655
  H        6.72308       -3.49289        1.02568
 Br       -2.05135       -1.85171       -0.09703

SnBr3_h1allyl_vac_min_freq.out
E_scf = -160.30426510358 a.u.
E_Gibbs = -160.275028
ZPE = 45.639 kcal/mol
E_Gibbs, 60C = -160.281675
 Sn       -0.83379        1.94699       -0.75681
 Br       -0.99612        0.29654       -2.72462
 Br        1.60977        2.72962       -0.59049
  C       -1.15615        1.88155        2.27720
  C       -1.47760        1.02704        1.09846
  C       -2.05206        2.61821        2.94341
  H       -0.96475        0.05960        1.11323
  H       -1.76132        3.22129        3.79828
  H       -2.55193        0.85970        0.97287
  H       -3.10308        2.63985        2.66404
  H       -0.11224        1.89772        2.58734
 Br       -2.27668        3.99392       -1.32669

SnBr3_h1allyl_THF_min.out
E_solv = -160.31608262926 a.u.
 Sn       -0.83254        1.81616       -0.72494
 Br       -0.71370        0.41504       -2.89728
 Br        1.47095        2.97895       -0.52194
  C       -1.11149        1.79296        2.26416
  C       -1.52855        0.92332        1.13067
  C       -1.91221        2.69565        2.84879
  H       -1.09308       -0.07902        1.14254
  H       -1.55917        3.30472        3.67716
  H       -2.61172        0.86240        0.99216
  H       -2.94122        2.84937        2.52852
  H       -0.08485        1.67634        2.60759
 Br       -2.38792        3.81858       -1.30424

SnBr3_allyl_PhCHO_eq_Reac_vac_min_freq.out
E_scf = -505.88557472616 a.u.
E_Gibbs = -505.756589
ZPE =   115.982 kcal/mol
E_Gibbs, 60C, H = -505.765720
E_Gibbs, 60C, D = -505.769119
  Sn        0.09834        0.29366        0.60069
  C       -0.01995       -0.09518        2.73101
  C       -0.73282       -1.37321        3.01080
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  C       -1.98474       -1.45807        3.47547
  C        2.51362       -1.96954        0.00404
  O        1.81247       -1.47852        0.89565
  H        1.02405       -0.11011        3.05701
  H       -0.53337        0.77625        3.14552
  H       -0.17647       -2.28500        2.79773
  H       -2.45564       -2.41977        3.65724
  H       -2.57949       -0.57311        3.69027
  H        2.36992       -1.65050       -1.04045
  C        5.54253       -4.87522        0.62023
  C        4.82053       -4.39285        1.71980
  C        3.82519       -3.44280        1.53275
  C        3.54825       -2.96991        0.23713
  C        4.27560       -3.45709       -0.86180
  C        5.27203       -4.40979       -0.66894
  H        6.32108       -5.61816        0.77210
  H        5.04093       -4.76180        2.71728
  H        3.25407       -3.05302        2.36955
  H        4.05555       -3.08533       -1.85986
  H        5.83645       -4.78833       -1.51590
 Br        2.15258        1.57776       -0.35974
 Br       -0.80477       -1.42588       -1.12921
 Br       -1.73922        2.14525        0.31835

SnBr3_allyl_PhCHO_eq_Reac_THF_min.out
E_sol: -505.90479783941
 Sn        0.17900        0.22266        0.62406
  C       -0.30675       -0.00481        2.72587
  C       -0.66958       -1.40348        3.07787
  C       -1.92842       -1.81836        3.27678
  C        2.18385       -2.18047       -0.04608
  O        1.61395       -1.50935        0.84411
  H        0.58218        0.36950        3.24547
  H       -1.12898        0.70090        2.86657
  H        0.15339       -2.10975        3.17043
  H       -2.14747       -2.84881        3.54529
  H       -2.77823       -1.14302        3.18975
  H        1.88659       -2.04562       -1.09698
  C        5.27498       -4.98320        0.62593
  C        4.74225       -4.28071        1.71871
  C        3.72198       -3.36079        1.52077
  C        3.23011       -3.13798        0.21646
  C        3.77070       -3.84600       -0.87758
  C        4.79089       -4.76859       -0.66944
  H        6.07470       -5.70150        0.78836
  H        5.13091       -4.45600        2.71783
  H        3.30145       -2.80475        2.35300
  H        3.38641       -3.66721       -1.87921
  H        5.21057       -5.31718       -1.50791
 Br        2.29012        1.38705       -0.41277
 Br       -1.04072       -1.28110       -1.14311
 Br       -1.39462        2.37212        0.19104

SnBr3_allyl_PhCHO_eq_Prod_vac_min.out
E_scf: -505.88698160631
E_Gibbs = -505.753281
ZPE =   117.504 kcal/mol
E_Gibbs, 60C, H = -505.761997
E_Gibbs, 60C, D = -505.765614
 Sn        0.09738        0.29235        0.60095
  C       -0.01871       -0.09455        2.73191
  C       -0.74045       -1.36721        3.01413
  C       -1.99194       -1.44214        3.48113
  C        2.51385       -1.96934        0.00223
  O        1.81086       -1.48086        0.89375
  H        1.02600       -0.11686        3.05589
  H       -0.52496        0.78079        3.14566
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  H       -0.19113       -2.28308        2.80013
  H       -2.46982       -2.40013        3.66458
  H       -2.57959       -0.55246        3.69642
  H        2.37116       -1.64855       -1.04205
  C        5.54897       -4.86878        0.61837
  C        4.82272       -4.39129        1.71743
  C        3.82533       -3.44351        1.53016
  C        3.55030       -2.96809        0.23508
  C        4.28144       -3.45064       -0.86333
  C        5.28018       -4.40093       -0.67041
  H        6.32939       -5.60979        0.77045
  H        5.04143       -4.76235        2.71451
  H        3.25102       -3.05756        2.36642
  H        4.06267       -3.07724       -1.86104
  H        5.84784       -4.77573       -1.51688
 Br        2.15223        1.57417       -0.35994
 Br       -0.80466       -1.42789       -1.12957
 Br       -1.73902        2.14529        0.31943

SnBr3_allyl_PhCHO_eq_Prod_THF_min_freq2.out
E_solv = -505.89637368219 a.u.
 Sn       -0.49624        0.51329        1.08946
  C        1.19644       -1.91301        1.50456
  C        1.70822       -1.39969        0.36482
  C        2.75524       -0.33463        0.31560
  C        2.17044        0.98471       -0.25547
  O        1.06377        1.44892        0.53036
  H        1.59872       -1.64188        2.47805
  H        0.43150       -2.68619        1.48751
  H        1.31998       -1.74892       -0.59334
  H        3.57451       -0.64458       -0.34520
  H        3.17219       -0.14459        1.31096
 Br       -1.86466       -1.06533       -0.44975
  H        1.82385        0.80011       -1.27992
  C        5.20403        4.06261       -0.33017
  C        4.84812        3.39420       -1.50397
  C        3.85153        2.41508       -1.47720
  C        3.21221        2.08808       -0.27592
  C        3.57172        2.76239        0.89867
  C        4.56058        3.74648        0.87044
  H        5.97504        4.82921       -0.35050
  H        5.33909        3.63864       -2.44300
  H        3.56884        1.90546       -2.39635
  H        3.06596        2.52851        1.83118
  H        4.82746        4.26855        1.78640
 Br       -2.07093        2.58104        1.00279
 Br       -0.74167        0.03072        3.62741

SnBr3_allyl_PhCHO_eq_vac_QST_TS
E_scf: -505.86397381697
E_Gibbs = -505.728186
ZPE =  116.971 kcal/mol
E_Gibbs, 60C, H = -505.736452
E_Gibbs, 60C, D = -505.740021
  Sn       -2.67003        1.86155        0.21789
  C       -1.20360        2.62069       -1.42039
  C        0.07854        2.43621       -0.84363
  C        0.76388        1.21616       -0.85340
  C       -0.16122        0.21303        0.54241
  O       -1.44621        0.21777        0.27000
  H       -1.46377        1.97369       -2.26043
  H       -1.55472        3.64454       -1.52934
  H        0.45753        3.23487       -0.20499
  H        1.79036        1.20397       -0.49722
  H        0.56105        0.53055       -1.67246
 Br       -1.89640        2.55571        2.61430
  H        0.15493        0.80013        1.41179
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```
  C        1.85545       -3.55931        0.21572
  C        2.41911       -2.52289        0.96322
  C        1.76279       -1.29743        1.05817
  C        0.53650       -1.10197        0.40812
  C       -0.02969       -2.14507       -0.33655
  C        0.63104       -3.36811       -0.43033
  H        2.36552       -4.51609        0.14272
  H        3.36531       -2.67097        1.47631
  H        2.19637       -0.49364        1.65002
  H       -0.99215       -1.99479       -0.81519
  H        0.18603       -4.17794       -1.00194
 Br       -4.57082        0.14354       -0.12879
 Br       -4.20050        3.99771       -0.22931

SnBr3_allyl_PhCHO_eq_THF_QST_TS.out
E_sol: -505.88513030405
 Sn        0.00799        0.00348       -0.00614
  C       -0.01979       -0.05853        2.27225
  C        1.35757       -0.03311        2.63391
  C        2.13038        1.13680        2.65301
  C        2.56809        1.35253        0.80328
  O        1.44813        1.41588        0.09560
  H       -0.60368        0.83683        2.50139
  H       -0.55428       -0.98693        2.46759
  H        1.86743       -0.99210        2.73515
  H        3.11741        1.07264        3.10373
  H        1.61186        2.08045        2.81335
 Br        1.67568       -1.67921       -1.12324
  H        3.18298        0.45768        0.65230
  C        4.90223        4.95739        0.84060
  C        5.48950        3.73458        1.17895
  C        4.72247        2.57028        1.17996
  C        3.36174        2.62222        0.84316
  C        2.77423        3.84967        0.50744
  C        3.54534        5.01160        0.50505
  H        5.50122        5.86475        0.83466
  H        6.54522        3.68651        1.43376
  H        5.18423        1.61798        1.43095
  H        1.72595        3.88279        0.22810
  H        3.08896        5.95991        0.23250
 Br       -1.20865        1.65737       -1.60644
 Br       -2.06596       -1.72791       -0.07865

Sb_Br2_h1allyl_vac_min.out
E_scf: -149.10282616555
E_Gibbs = -149.070214
ZPE =  45.129 kcal/mol
E_Gibbs, 60C = -149.076101
 SB       -0.95373        2.17822       -0.78929
 Br       -1.22790        0.10382       -2.44375
 Br        1.69652        2.27010       -0.49673
  C       -1.07423        1.86340        2.23065
  C       -1.28102        0.99323        1.03384
  C       -2.05377        2.44829        2.92995
  H       -0.59279        0.14454        0.99126
  H       -1.83820        3.08596        3.78219
  H       -2.30871        0.62061        0.95892
  H       -3.10417        2.29623        2.68839
  H       -0.03754        2.04479        2.51226

Sb_Br2_h1allyl_THF_min.out
E_sol: -149.11365031000
 SB       -1.07326        2.09924       -0.71132
 Br       -1.01861        0.10013       -2.52627
 Br        1.59179        2.44841       -0.51053
  C       -0.92793        1.71565        2.21814
  C       -1.16005        0.80627        1.05074
```

C	-1.87567	2.46819	2.79639
H	-0.41706	0.01116	0.95838
H	-1.63967	3.14118	3.61652
H	-2.16183	0.36285	1.04288
H	-2.91825	2.42617	2.48292
H	0.10362	1.79961	2.55845

SbBr2_allyl_PhCHO_chair_eqPh_vac_reac_min_freq.out
E_scf = -494.67567923222 a.u.
E_Gibbs = -494.540734 a.u.
ZPE = 115.942 kcal/mol

SB	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.23185
C	1.35004	0.00000	2.85075
C	1.97841	1.09347	3.31129
C	2.85274	1.21851	0.29485
O	1.66021	1.39024	-0.06486
H	-0.58805	0.88290	2.49114
H	-0.56252	-0.90481	2.48861
H	1.85440	-0.96294	2.89725
H	2.96159	1.02778	3.76977
H	1.51447	2.07718	3.28384
Br	-1.38115	2.44771	0.04037
H	3.19648	0.21195	0.55646
C	5.67981	4.35865	0.28017
C	6.08035	3.05823	0.60103
C	5.14161	2.03281	0.61015
C	3.79856	2.31089	0.29276
C	3.39973	3.62357	-0.03074
C	4.34374	4.64105	-0.03362
H	6.41365	5.16029	0.27421
H	7.11863	2.84983	0.84097
H	5.43701	1.01559	0.85553
H	2.35810	3.81723	-0.26864
H	4.04688	5.65616	-0.27971
Br	2.01398	-2.07410	0.00698

SbBr2_allyl_PhCHO_eq_Reac_THF_min_freq2.out
E_solv = -494.69897241270 a.u.

SB	0.34690	0.34078	1.39340
C	-0.15903	-1.01008	-0.27803
C	0.44543	-2.36288	-0.08896
C	-0.23166	-3.44968	0.30281
C	1.72129	2.41489	-0.99376
O	1.90585	1.46147	-0.22275
H	-1.25080	-1.04492	-0.31538
H	0.21635	-0.50608	-1.17371
H	1.51661	-2.44143	-0.27948
H	0.26269	-4.41002	0.43130
H	-1.30000	-3.41795	0.50765
Br	-1.44864	2.22369	0.61676
H	0.69285	2.71850	-1.24642
C	4.80023	4.75832	-2.72715
C	5.14156	3.71945	-1.84918
C	4.14445	2.93607	-1.28171
C	2.79495	3.19428	-1.59079
C	2.45768	4.23836	-2.47095
C	3.46174	5.01820	-3.03947
H	5.58450	5.36988	-3.16689
H	6.18487	3.53065	-1.61110
H	4.38649	2.13067	-0.59462
H	1.41253	4.43373	-2.70162
H	3.20575	5.82667	-3.71864
Br	-1.52486	-0.93464	3.00430

SbBr2_allyl_PhCHO_eq_Prod_vac_min_freq.out

E_scf = -494.69107681264 a.u.
E_Gibbs = -494.554408 a.u.
ZPE = 117.020 kcal/mol

SB	-0.68035	-0.18911	0.12680
C	1.36766	-2.73566	0.89361
C	1.99763	-2.13316	-0.12607
C	2.87907	-0.92628	0.00227
C	2.21632	0.35534	-0.57526
O	1.04768	0.67629	0.18702
H	1.50802	-2.40949	1.92270
H	0.73344	-3.60512	0.73997
H	1.83972	-2.50996	-1.13741
H	3.81823	-1.08845	-0.54243
H	3.13285	-0.73429	1.05118
Br	-2.00596	2.13761	0.30066
H	1.92914	0.16669	-1.61825
C	5.02172	3.63777	-0.45686
C	4.93861	2.81965	-1.58432
C	4.01373	1.77600	-1.62245
C	3.16945	1.53423	-0.53311
C	3.25467	2.35958	0.59316
C	4.17505	3.40701	0.62878
H	5.73655	4.45605	-0.42774
H	5.58565	2.99945	-2.43897
H	3.94245	1.15048	-2.51040
H	2.58280	2.19201	1.42903
H	4.22695	4.04802	1.50512
Br	-0.79614	-0.70720	-2.52059

SbBr2_allyl_PhCHO_eq_Prod_THF_min_freq.out
E_solv = -494.70792742817 a.u.

SB	-0.52181	-0.28610	0.25564
C	1.35431	-2.67819	0.45246
C	1.95512	-2.04517	-0.57578
C	2.89574	-0.88920	-0.42878
C	2.21656	0.44664	-0.84580
O	1.10939	0.71548	0.01798
H	1.59746	-2.44260	1.48825
H	0.66616	-3.50493	0.28816
H	1.71130	-2.34689	-1.59499
H	3.77284	-1.04223	-1.06875
H	3.24387	-0.78957	0.60557
Br	-1.87536	2.07140	0.68457
H	1.84333	0.34797	-1.87520
C	5.05590	3.71602	-0.68827
C	5.20271	2.68810	-1.62454
C	4.27456	1.64739	-1.67437
C	3.19076	1.61515	-0.78429
C	3.04440	2.65058	0.14445
C	3.97220	3.69549	0.19112
H	5.77825	4.52815	-0.64931
H	6.03918	2.69744	-2.31956
H	4.39509	0.86058	-2.41709
H	2.19638	2.64153	0.82056
H	3.84321	4.49600	0.91621
Br	-1.11844	-0.59323	-2.38663

SbBr2_allyl_PhCHO_chair_eqPh_vac_QST_TS2_freq.out
E_scf = -494.66639369386 a.u.
E_Gibbs = -494.527353 a.u.
ZPE = 116.535 kcal/mol
Imaginary Eigenfrequency: -326.92 cm-1

Sb	-0.00278	-0.00233	-0.00119
C	0.00570	-0.00066	2.33213
C	1.38827	0.00470	2.70078
C	2.19219	1.14126	2.68683
C	2.63048	1.26736	0.70650

```
  O        1.45646        1.39901        0.12259
  H       -0.55540        0.91511        2.51871
  H       -0.54543       -0.90608        2.58994
  H        1.87182       -0.96157        2.82580
  H        3.19437        1.07126        3.10023
  H        1.72456        2.11979        2.75987
 Br       -1.72297        2.21528        0.03672
  H        3.11893        0.29273        0.63326
  C        5.22420        4.65692        0.56793
  C        5.74521        3.38264        0.80516
  C        4.89255        2.28274        0.85524
  C        3.51263        2.45298        0.66488
  C        2.99249        3.73446        0.42422
  C        3.85000        4.82965        0.37551
  H        5.88941        5.51538        0.52800
  H        6.81391        3.24668        0.94499
  H        5.29530        1.28726        1.02954
  H        1.92519        3.85472        0.26435
  H        3.44836        5.82061        0.18341
 Br        2.04194       -2.07052        0.02549

SbBr2_allyl_PhCHO_chair_eqPh_THF_QST_TS2_freq.out
E_solv = -494.69242386894 a.u.
 Sb       -0.00977        0.00155       -0.00325
  C        0.02323       -0.00356        2.30672
  C        1.40819        0.00965        2.69224
  C        2.20782        1.14444        2.67986
  C        2.67530        1.19696        0.67172
  O        1.50607        1.33684        0.07666
  H       -0.53866        0.90730        2.51761
  H       -0.52667       -0.90840        2.57138
  H        1.88766       -0.95371        2.85480
  H        3.20608        1.08191        3.10466
  H        1.74326        2.12736        2.70666
 Br       -1.64552        2.34487        0.05837
  H        3.14341        0.21223        0.63739
  C        5.37209        4.49841        0.43662
  C        5.85102        3.21646        0.72452
  C        4.96326        2.14580        0.80922
  C        3.58852        2.35402        0.60681
  C        3.11074        3.64429        0.32090
  C        4.00303        4.70960        0.23427
  H        6.06506        5.33349        0.36818
  H        6.91448        3.05109        0.87611
  H        5.33536        1.14589        1.02224
  H        2.04843        3.79829        0.15667
  H        3.63384        5.70610        0.00595
 Br        1.93540       -2.16695       -0.02648

Bi_Br2_h1allyl_vac_min.out
E_scf: -149.16092593982
E_Gibbs = -149.129808
ZPE =  44.858
E_Gibbs, 60C = -149.135842
 Bi       -0.88713        2.08850       -0.66466
 Br       -1.25797        0.07131       -2.43284
 Br        1.80922        2.20900       -0.45736
  C       -0.98432        1.73199        2.36193
  C       -1.16448        0.82214        1.19725
  C       -1.97453        2.36649        3.00561
  H       -0.43727        0.00872        1.15052
  H       -1.77215        3.04040        3.83268
  H       -2.17783        0.41390        1.12024
  H       -3.02084        2.21453        2.74595
  H        0.04588        1.91585        2.66611

Bi_Br2_h1allyl_THF_min.out
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E_sol: -149.17607071120

Bi	-0.99332	2.01489	-0.57218
Br	-1.00409	0.14945	-2.59933
Br	1.71977	2.38443	-0.47873
C	-0.76580	1.57673	2.28836
C	-0.97716	0.59723	1.18373
C	-1.71543	2.40025	2.76950
H	-0.19141	-0.15164	1.07955
H	-1.48721	3.13980	3.53235
H	-1.96097	0.11715	1.19312
H	-2.75325	2.33846	2.44259
H	0.25711	1.68231	2.64869

BiBr2_allyl_PhCHO_chair_eqPh_vac_reac_min_freq.out
E_scf = -494.73672377555 a.u.
E_Gibbs = -494.603322 a.u.
ZPE = 115.600 kcal/mol
E_Gibbs, 60C, H = -494.611572
E_Gibbs, 60C, D = -494.615027

Bi	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.30308
C	1.35417	0.00000	2.89733
C	1.98803	1.08951	3.36009
C	2.77424	1.49010	0.38337
O	1.57854	1.60648	0.02162
H	-0.59022	0.88484	2.55042
H	-0.56365	-0.90508	2.55354
H	1.87027	-0.95834	2.92276
H	2.98125	1.02112	3.79664
H	1.51722	2.06982	3.35758
Br	-1.72956	2.24114	0.00337
H	3.18292	0.49203	0.58398
C	5.40288	4.79411	0.64443
C	5.87607	3.50043	0.88642
C	5.00305	2.42139	0.80460
C	3.65282	2.63848	0.47672
C	3.18074	3.94413	0.23314
C	4.05892	5.01573	0.31936
H	6.08535	5.63762	0.70922
H	6.91993	3.33834	1.13637
H	5.35674	1.40938	0.98830
H	2.13486	4.09067	-0.01753
H	3.70450	6.02584	0.13435
Br	2.20491	-1.89786	-0.06874

BiBr2_allyl_PhCHO_chair_eqPh_THF_reac_min_freq2.out
E_solv = -494.76544726231 a.u.

Bi	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.29677
C	1.35261	0.00000	2.90056
C	1.98895	1.09101	3.36132
C	2.78183	1.48516	0.37839
O	1.57972	1.58293	0.01321
H	-0.58764	0.88518	2.54920
H	-0.57306	-0.90040	2.54202
H	1.85938	-0.96298	2.94099
H	2.98013	1.02302	3.80293
H	1.52500	2.07592	3.34881
Br	-1.76398	2.28037	0.05595
H	3.19861	0.49800	0.60367
C	5.44272	4.75867	0.64120
C	5.88670	3.46456	0.93499
C	5.00086	2.39648	0.84164
C	3.66404	2.62455	0.45416
C	3.22334	3.93170	0.15667
C	4.11528	4.99153	0.25121
H	6.13487	5.59398	0.71592

```
  H        6.91692        3.29453        1.23450
  H        5.33362        1.38554        1.06543
  H        2.19236        4.09426       -0.14207
  H        3.78609        6.00178        0.02461
 Br        2.15248       -1.97230       -0.05445

BiBr2_allyl_PhCHO_chair_eqPh_vac_prod_min_freq.out
E_scf = -494.75067972049 a.u.
E_Gibbs = -494.614615 a.u.
ZPE = 116.821 kcal/mol
 Bi        0.00000        0.00000        0.00000
  C        0.00000        0.00000        3.26480
  C        1.32032        0.00000        3.01860
  C        2.13855        1.22033        2.71095
  C        2.51296        1.31519        1.19588
  O        1.32825        1.46188        0.41930
  H       -0.55935        0.93067        3.33796
  H       -0.54595       -0.91451        3.48528
  H        1.84344       -0.95434        2.99069
  H        3.07152        1.19625        3.28888
  H        1.60491        2.13382        2.98243
 Br       -0.46320        0.92354       -2.51675
  H        3.03833        0.39736        0.90035
  C        5.13881        4.69869        0.60241
  C        5.65191        3.46787        1.01828
  C        4.79890        2.37768        1.18811
  C        3.42517        2.50471        0.94947
  C        2.91727        3.73796        0.52800
  C        3.77153        4.82848        0.35482
  H        5.80247        5.54830        0.46457
  H        6.71718        3.35346        1.20194
  H        5.20758        1.41720        1.49855
  H        1.85703        3.83161        0.31867
  H        3.36734        5.78092        0.02035
 Br        1.72799       -2.08518       -0.36229

BiBr2_allyl_PhCHO_chair_eqPh_THF_prod_min_freq2.out
E_solv = -494.76811082843 a.u.
 Bi        0.00000        0.00000        0.00000
  C        0.00000        0.00000        2.65469
  C        1.37099        0.00000        2.65254
  C        2.20312        1.20248        2.42792
  C        2.59371        1.32894        0.88819
  O        1.40337        1.44699        0.13718
  H       -0.55573        0.93500        2.72069
  H       -0.55336       -0.91332        2.86648
  H        1.88799       -0.95702        2.71887
  H        3.13964        1.12667        2.99090
  H        1.67902        2.11931        2.71273
 Br       -1.91447        2.13626       -0.08701
  H        3.14828        0.42397        0.61286
  C        5.09806        4.78871        0.23339
  C        5.66772        3.51829        0.35003
  C        4.85296        2.40230        0.55606
  C        3.46412        2.54673        0.65329
  C        2.89727        3.82310        0.53579
  C        3.71044        4.93746        0.32481
  H        5.73004        5.65744        0.06547
  H        6.74473        3.39233        0.27029
  H        5.30019        1.41269        0.63069
  H        1.81804        3.93589        0.58628
  H        3.26017        5.92254        0.22585
 Br        2.02182       -2.06636       -0.35168

BiBr2_allyl_PhCHO_chair_eqPh_vac_QST_TS_freq.out
E_scf = -494.72729203268 a.u.
E_Gibbs = -494.590003 a.u.
```

ZPE = 116.176 kcal/mol
E_Gibbs, 60C, H = -494.597710
E_Gibbs, 60C, D = -494.601283
Imaginary Eigenfrequency: -332.67 cm-1

Bi	-0.02442	0.02800	-0.00096
C	-0.00418	0.02433	2.41285
C	1.38022	0.03502	2.74862
C	2.17813	1.17736	2.75780
C	2.61165	1.38085	0.77062
O	1.44291	1.52886	0.19135
H	-0.57269	0.93644	2.59217
H	-0.54924	-0.88925	2.65371
H	1.87464	-0.93030	2.83830
H	3.18419	1.10083	3.16008
H	1.70546	2.15010	2.86675
Br	-1.90828	2.13890	0.01684
H	3.10769	0.41159	0.66966
C	5.20011	4.78189	0.79665
C	5.72028	3.50217	1.00539
C	4.87117	2.39809	1.00036
C	3.49512	2.56905	0.78573
C	2.97644	3.85579	0.57391
C	3.83000	4.95553	0.57882
H	5.86254	5.64345	0.79950
H	6.78604	3.36546	1.16586
H	5.27429	1.39911	1.15288
H	1.91252	3.97674	0.39443
H	3.42832	5.95061	0.40886
Br	2.05673	-2.01634	-0.02972

BiBr2_allyl_PhCHO_chair_eqPh_THF_QST_TS_freq.out
E_solv = -494.75637134682 a.u.

Bi	-0.01820	0.00836	-0.00405
C	0.02906	-0.02522	2.39245
C	1.41280	0.01299	2.75666
C	2.20089	1.15842	2.76731
C	2.67350	1.30379	0.74420
O	1.51025	1.44718	0.15427
H	-0.55687	0.87201	2.59511
H	-0.50077	-0.94850	2.63101
H	1.91022	-0.94490	2.90011
H	3.19525	1.09665	3.20155
H	1.72438	2.13454	2.82311
Br	-1.77509	2.28881	0.05758
H	3.16123	0.32887	0.68121
C	5.32113	4.66046	0.73045
C	5.81739	3.37289	0.95733
C	4.94763	2.28371	0.96618
C	3.57346	2.47745	0.74763
C	3.07828	3.77359	0.52708
C	3.95207	4.85815	0.51576
H	5.99999	5.50990	0.71999
H	6.88072	3.21835	1.12174
H	5.33443	1.28042	1.13287
H	2.01609	3.91782	0.35327
H	3.56802	5.85966	0.33897
Br	1.99276	-2.12215	-0.04553

PhCHO_vac_radanion
E_scf: -345.55881682899
E_Gibbs, H = -345.483636
E_Gibbs, D = -345.486786
ZPE = 66.718

C	2.46038	1.43407	-0.05341
O	1.23819	1.34662	-0.36257
H	3.02760	0.50190	0.20877
C	4.82623	5.02127	0.12731

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  C        3.46061        5.06147       -0.23486
  C        2.69185        3.91468       -0.29571
  C        3.24883        2.62304        0.00794
  C        4.63659        2.60379        0.37315
  C        5.39171        3.76056        0.42937
  H        3.00195        6.02415       -0.47272
  H        1.64185        3.95138       -0.57505
  H        5.09550        1.64221        0.61074
  H        6.44477        3.69917        0.71230
  H        5.42359        5.92977        0.17244

PhCHO_THF_radanion
E_solv = -345.64136050956 a.u.
  C        2.47287        1.43580       -0.04995
  O        1.23825        1.35098       -0.36476
  H        3.02879        0.50629        0.21044
  C        4.82079        5.01588        0.12671
  C        3.45855        5.06265       -0.23515
  C        2.68931        3.91287       -0.29579
  C        3.24991        2.62616        0.00823
  C        4.63544        2.60086        0.37346
  C        5.39049        3.75900        0.42921
  H        3.00041        6.02345       -0.47224
  H        1.64004        3.95664       -0.57559
  H        5.09165        1.63915        0.61043
  H        6.44156        3.69852        0.71121
  H        5.41798        5.92284        0.17212

Zn_allyl_PhCHO_2H2O_reac_solv_min.out
E_sol: -681.24505551464 a.u.
 Zn       -0.39826       -0.06163        0.61627
  C        0.82476       -1.47665        1.56517
  C        2.24585       -1.09345        1.46964
  C        2.98140       -0.44659        2.39339
  C        1.93957        2.00741        0.46474
  O        1.10911        1.44165       -0.25968
  H        0.46838       -1.52986        2.60155
  H        0.62051       -2.43350        1.06862
  H        2.73476       -1.33572        0.52207
  H        4.01991       -0.18300        2.20910
  H        2.56779       -0.17065        3.36352
  H        1.72031        2.14769        1.53315
  C        5.64089        3.66589       -0.80584
  C        4.83081        3.00697       -1.74191
  C        3.61656        2.45572       -1.34562
  C        3.20897        2.56155       -0.00252
  C        4.02476        3.22463        0.93114
  C        5.23914        3.77617        0.52951
  H        6.58917        4.09513       -1.12089
  H        5.15299        2.92826       -2.77722
  H        2.97880        1.94180       -2.05988
  H        3.69912        3.30365        1.96655
  H        5.87022        4.28887        1.25071
  O       -0.75804        1.61776        2.06205
  H       -0.42492        1.62453        2.97688
  H       -0.75203        2.54935        1.77973
  O       -1.71894        0.97351       -0.70150
  H       -2.51832        1.37570       -0.31297
  H       -1.28311        1.69557       -1.19161

Zn_allyl_PhCHO_2H2O_TS.out
E_sol: -681.23867761391 a.u.
 Zn       -0.02181       -0.00605        0.01211
  C       -0.00542        0.03389        2.20923
  C        1.37967        0.04048        2.55147
  C        2.23240        1.12547        2.55361
  C        2.66831        1.15515        0.27468
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  O        1.53249        1.29279       -0.28272
  H       -0.55904        0.95878        2.39613
  H       -0.56315       -0.85955        2.49893
  H        1.83913       -0.93631        2.72130
  H        3.25121        1.01384        2.91394
  H        1.84093        2.14064        2.52926
  H        3.10617        0.15483        0.35457
  C        5.51518        4.34479        0.11702
  C        4.15968        4.61123       -0.11036
  C        3.22169        3.58437       -0.02743
  C        3.63054        2.27866        0.28948
  C        4.99071        2.01774        0.52232
  C        5.92858        3.04633        0.43417
  H        6.24696        5.14559        0.03987
  H        3.83753        5.61883       -0.36321
  H        2.17081        3.77995       -0.22151
  H        5.31130        1.00377        0.75640
  H        6.98189        2.83548        0.60310
  O       -1.27843       -1.54642       -0.76021
  H       -1.64592       -1.36290       -1.64646
  H       -0.63357       -2.26960       -0.89969
  O        1.38667       -1.85608       -0.25879
  H        2.04502       -1.89900       -0.97597
  H        1.82524       -2.27091        0.50540

Zn_allyl_PhCHO_2H2O_prod_solv_min.out
E_sol: -681.26791794140 a.u.
 Zn       -0.30479        0.63623       -0.13740
  C        1.13419       -1.63790        1.14296
  C        1.93454       -1.21977        0.14940
  C        2.94267       -0.11516        0.26074
  C        2.60153        1.07247       -0.68232
  O        1.32160        1.59852       -0.46874
  H        1.19625       -1.20985        2.14343
  H        0.42399       -2.44967        1.00026
  H        1.84535       -1.69663       -0.83003
  H        3.93842       -0.49294       -0.01227
  H        2.99227        0.22881        1.30117
  H        2.67697        0.66744       -1.71174
  C        5.43942        4.37261       -0.55544
  C        4.83204        3.98973       -1.75467
  C        3.94356        2.91195       -1.77325
  C        3.62949        2.20549       -0.60224
  C        4.23999        2.60681        0.59528
  C        5.14166        3.67514        0.61849
  H        6.14016        5.20463       -0.53666
  H        5.05145        4.52805       -2.67448
  H        3.47667        2.61684       -2.71220
  H        4.02215        2.08505        1.52424
  H        5.61512        3.96052        1.55576
  O       -1.47663        2.44768       -0.25295
  H       -0.87427        3.16950       -0.51444
  H       -2.17112        2.45634       -0.93752
  O       -1.73536       -0.16935        1.16225
  H       -1.96222       -1.11179        1.05753
  H       -1.58521       -0.04339        2.11800
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