

Radical Allylations by Reaction of Azides with Allylindium Dichloride

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Electronic Supplementary Information

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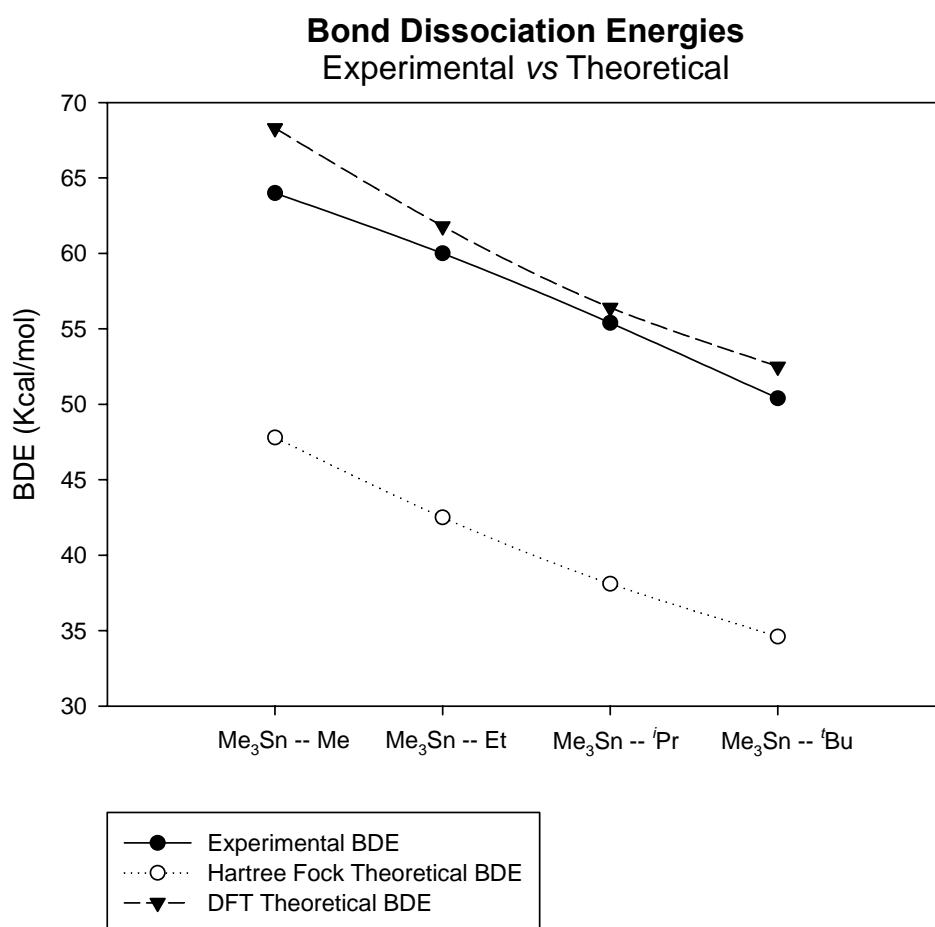
- Page 1: Calculation details, calculated values for the BDEs of tetraalkylstannanes, plot of calculated BDEs vs experimental values, calculated BDEs of allyltrimethylstannane and allylindium dichloride.
- Page 2: Reaction pathway and calculated energies for 1,5-H transfer of indium- or tin-substituted aminyl radicals.
- Page 3: Cartesian coordinates of all compounds, intermediates, and transition states.

All the structures were optimized both with DFT (B3LYP functional) and Hartree-Fock methods using the basis set LanL2DZ with Effective Core Potentials (ECP).¹

All the structures were fully optimized and gave no imaginary frequencies.

	Me ₃ Sn---Me	Me ₃ Sn---Et	Me ₃ Sn--- ⁱ Pr	Me ₃ Sn--- ^t Bu
Experimental	64.0	60.0	55.4	50.4
Theoretical DFT - [DEV (%)]	68.3 [6.7]	61.8 [3.0]	56.4 [1.8]	52.5 [4.2]
Theoretical HF - [DEV (%)]	47.8 [25.3]	42.5 [29.2]	38.1 [31.2]	34.6 [31.3]

All values are expressed in Kcal / mol; DEV = deviation from the experimental value.²



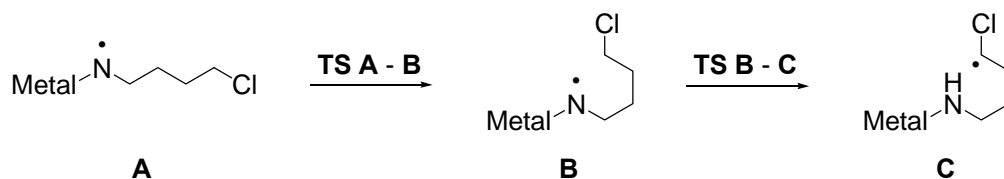
	DFT (B3LYP)	HF
BDE Me₃Sn---allyl	49.83	26.72
BDE Cl₂In---allyl	42.30	19.00
(BDE Me₃Sn---allyl) – (BDE Cl₂In---allyl)	7.53	7.72

All values are expressed in Kcal / mol

¹ (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270; (b) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 284; (c) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

² Y.-r. Luo, *Handbook of Bond Dissociation Energies in Organic Compounds*, CRC Press: Boca Raton, 2003, p. 297.

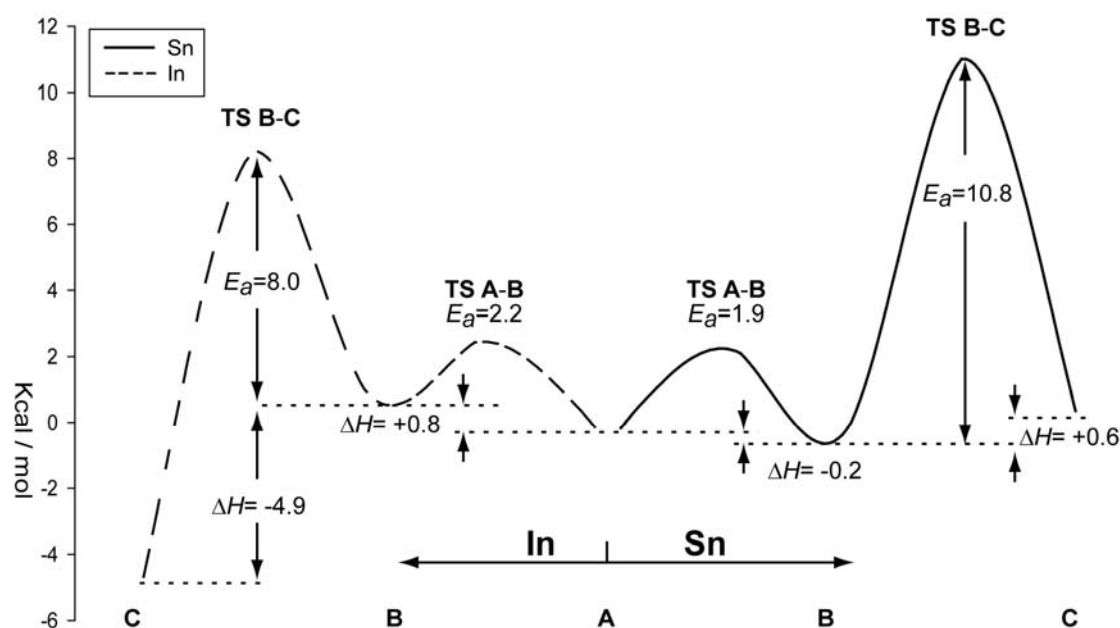
Reaction pathway for 1,5-H transfer of aminyl radicals and calculated energies for intermediates and transition states



Metal	Method	ΔH (A – B)	E_a (A – B)	ΔH (B – C)	E_a (B – C)
Sn	DFT (B3LYP)	-0.2	1.9	0.6	10.8
	HF	0.2	2.5	2.6	29.6
In	DFT (B3LYP)	0.8	2.2	-4.9	8.0
	HF	1.5	2.7	-2.6	26.0

All values are expressed in Kcal / mol

All the structures were optimized both with spin-unrestricted DFT (B3LYP functional) and Hartree-Fock methods using the basis set LanL2DZ with Effective Core Potentials (ECP). Energies were adjusted for zeropoint vibrational energies and for thermal corrections to 298 K. Computed $\langle S^2 \rangle$ values were in the range 0.7539-0.7599 before annihilation and 0.7500 after annihilation of higher multiplicity spin states. Minima were localized by full optimization of the starting structures, while the transition states were located by a full transition state search. The optimized calculations were confirmed to be either ground or transition states by performing harmonic vibration frequency analyses (no imaginary frequencies were found for intermediates, whereas all the transition states were characterized by a unique imaginary frequency corresponding to the desired process).



Reaction profiles for 1,5-H shift of tin- and indium-aminyls (DFT, UB3LYP, LanL2DZ ECP)

Cartesian coordinates of all compounds and intermediates involved in BDEs calculations

Density Functional Theory - B3LYP / LanL2DZ ECP

Tetramethylstannane – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -162.872147

Sn	0.00001200	0.00002700	-0.00005100
C	0.00992600	-1.73792600	1.26205700
H	0.02766800	-2.65549800	0.65935800
H	0.89267600	-1.74055800	1.91489600
H	-0.88519200	-1.76340700	1.89733300
C	-0.02701200	1.77042800	1.21580600
H	0.85541300	1.80890100	1.86795000
H	-0.02864500	2.67202300	0.58920400
H	-0.92252500	1.79363200	1.85060500
C	-1.74589300	-0.03494200	-1.25060900
H	-1.77372300	0.84559100	-1.90584800
H	-1.75432300	-0.93226800	-1.88321000
H	-2.65966200	-0.03716500	-0.64190700
C	1.76293700	0.00230800	-1.22700600
H	1.78049100	0.88296200	-1.88241700
H	1.79921900	-0.89488100	-1.85879600
H	2.66826100	0.02009100	-0.60609500

Ethyltrimethylstannane – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -202.142764

Sn	-0.27866500	-0.00000400	0.00445000
C	-0.42824900	1.75780800	-1.22323800
H	-0.36065000	2.66744700	-0.61206900
H	0.37725200	1.78510400	-1.96872200
H	-1.38750600	1.77562700	-1.75714100
C	-0.42709700	-1.74482700	-1.24175100

H	0.37822800	-1.76372100	-1.98768800
H	-0.35874200	-2.66082500	-0.64024100
H	-1.38646100	-1.75771300	-1.77561400
C	-1.88279700	-0.00823100	1.43490200
H	-1.83351500	-0.90140000	2.07155000
H	-1.83288200	0.87701800	2.08245900
H	-2.85576000	-0.00476100	0.92607300
C	1.61912600	-0.00465500	1.03223800
H	1.65432000	-0.88797900	1.68800200
H	1.65445900	0.87289700	1.69569800
C	2.84856100	-0.00057900	0.08617600
H	2.85747000	0.88840500	-0.55972600
H	3.79182000	-0.00250200	0.65156200
H	2.85795700	-0.88448800	-0.56662500

iso-Propyltrimethylstannane – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -241.416699

Sn	-0.45647500	0.00005100	-0.00457700
C	-0.64590700	-0.00194000	2.13773400
H	-0.17570700	-0.89297900	2.57376400
H	-0.17223300	0.88621400	2.57588300
H	-1.70513300	-0.00021100	2.42716100
C	-1.41484500	1.75556000	-0.79356800
H	-0.97516200	2.66672300	-0.36698800
H	-1.30891000	1.80233400	-1.88546100
H	-2.48666500	1.75078900	-0.55501000
C	-1.41563200	-1.75377300	-0.79637200
H	-1.30996700	-1.79885800	-1.88835900
H	-0.97625800	-2.66580200	-0.37132800
H	-2.48740100	-1.74892000	-0.55756400
C	1.64445000	0.00008500	-0.55000300

H	1.67864300	0.00034800	-1.65224200
C	2.36535400	1.27764800	-0.04666400
H	2.34781200	1.34149300	1.05121300
H	3.42317000	1.27978100	-0.35420500
H	1.90498700	2.19342200	-0.44310200
C	2.36514300	-1.27781300	-0.04723600
H	1.90455700	-2.19335400	-0.44396300
H	3.42292700	-1.28007000	-0.35488500
H	2.34769600	-1.34206500	1.05061500

***tert*-Butyltrimethylstannane – B3LYP / LanL2DZ ECP**

Sum of electronic and thermal Enthalpies = -280.692784

Sn	0.60574100	0.00043300	-0.00088700
C	1.33149400	-0.53600100	1.95086900
H	0.97691200	0.17183300	2.71150300
H	0.99489900	-1.54198100	2.23378700
H	2.42948200	-0.52826900	1.96518900
C	1.33593700	-1.42341500	-1.43683300
H	0.99286700	-2.43778800	-1.19446400
H	0.98969000	-1.17567200	-2.44874200
H	2.43402900	-1.42875800	-1.44473100
C	1.34073700	1.95707600	-0.50813700
H	0.99696200	2.26123300	-1.50548800
H	0.99598000	2.70538800	0.21739100
H	2.43887300	1.96578600	-0.50952500
C	-1.57878500	0.00125800	-0.00182100
C	-2.09875200	-1.41052000	0.38171800
H	-1.76550700	-1.71032500	1.38555800
H	-3.20204700	-1.42488200	0.38497200
H	-1.76540200	-2.17966800	-0.32958000
C	-2.10582600	1.03416300	1.02924100

H	-1.77295100	2.05605700	0.79542100
H	-3.20969300	1.04232700	1.03324500
H	-1.77763000	0.79593300	2.05165900
C	-2.10567000	0.37596600	-1.41221700
H	-1.77670300	-0.34224400	-2.17744200
H	-3.20955800	0.38071600	-1.41985000
H	-1.77207400	1.37748700	-1.72146900

Methyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -39.80344

C	0.00000000	0.00000000	0.00001300
H	0.00000000	1.08612500	-0.00002600
H	0.94061200	-0.54306200	-0.00002600
H	-0.94061200	-0.54306200	-0.00002600

Ethyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -79.084459

C	-0.80220500	0.00000000	-0.01212900
H	-1.36203600	-0.93199800	0.02805600
H	-1.36203600	0.93199800	0.02805600
C	0.70198400	0.00000000	-0.00211600
H	1.11029400	0.89014600	-0.49920200
H	1.10480800	0.00000000	1.02776700
H	1.11029400	-0.89014600	-0.49920300

iso-Propyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -118.366965

C	0.00000000	0.54308000	-0.01786900
H	-0.00001100	1.63004000	0.04252100
C	1.30933100	-0.20120600	0.00108500
H	2.16614700	0.47427100	-0.10835600

H	1.44767000	-0.76316800	0.94297000
H	1.35985900	-0.94811400	-0.80877200
C	-1.30933200	-0.20121500	0.00107900
H	-2.16610500	0.47419300	-0.10911000
H	-1.35953500	-0.94863200	-0.80831300
H	-1.44802000	-0.76254400	0.94328600

tert-Butyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -157.649383

C	0.00165400	-0.00011200	-0.13508700
C	-0.81452400	-1.26293400	0.01422600
H	-0.31530900	-2.12409700	-0.45142500
H	-0.98002200	-1.52920400	1.07696800
H	-1.80906200	-1.15646000	-0.44123000
C	-0.68860200	1.33535900	0.01437900
H	-0.06688600	2.15735500	-0.36596300
H	-1.64776800	1.35579600	-0.52283700
H	-0.91600300	1.57055000	1.07275900
C	1.50309400	-0.07253300	0.01439900
H	1.99995900	0.76850000	-0.48986500
H	1.81939800	-0.03480800	1.07554900
H	1.90596100	-1.00631000	-0.40145800

Trimethylstannyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -122.959794

Sn	0.00000000	0.00000000	0.29063200
C	0.00000000	2.02317500	-0.49054100
H	0.00000000	1.99057600	-1.58914700
H	-0.89014800	2.56944200	-0.15573400
H	0.89014800	2.56944200	-0.15573400
C	1.75212100	-1.01158800	-0.49054100

H	2.67027600	-0.51383000	-0.15573400
H	1.78012800	-2.05561200	-0.15573400
H	1.72388900	-0.99528800	-1.58914700
C	-1.75212100	-1.01158800	-0.49054100
H	-1.78012800	-2.05561200	-0.15573400
H	-2.67027600	-0.51383000	-0.15573400
H	-1.72388900	-0.99528800	-1.58914700

Allyltrimethylstannane – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -240.213954

Sn	-0.51728900	0.01460600	-0.01184200
C	-2.19264000	0.15222900	1.32650800
H	-3.12103200	0.32874700	0.76761200
H	-2.31043200	-0.77577300	1.90105700
H	-2.05761700	0.97990600	2.03494000
C	-0.31914800	1.82367200	-1.14454900
H	-0.35595700	2.70209300	-0.48733600
H	0.63955000	1.83236800	-1.67808000
H	-1.12700900	1.91328400	-1.88230200
C	-0.77125900	-1.66061700	-1.32964400
H	0.06799700	-1.73111600	-2.03321700
H	-0.82730100	-2.59970400	-0.76383300
H	-1.69684200	-1.55681200	-1.91084400
C	1.29494900	-0.26899200	1.15945500
H	1.45135200	0.63924200	1.75753900
H	1.10811700	-1.10008800	1.85492000
C	2.48623900	-0.55655600	0.28567800
H	2.53702000	-1.56663600	-0.13017500
C	3.46709900	0.31663300	-0.04359500
H	3.48198100	1.33509600	0.34205300
H	4.28317000	0.03085300	-0.70334700

Allylindium dichloride – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -149.096535

C	1.73974200	-0.18794100	0.99642700
H	2.01181100	0.77838000	1.43414800
H	1.72225500	-0.95245300	1.78073900
C	2.63691300	-0.57420300	-0.15342000
H	2.64140700	-1.63217000	-0.42209800
C	3.41550300	0.27897800	-0.85926400
H	3.45949200	1.34338900	-0.63397400
H	4.04003800	-0.07552900	-1.67512800
In	-0.25072500	-0.00253600	0.22492400
Cl	-1.26720200	2.08393500	-0.27796800
Cl	-1.57647100	-1.87442600	-0.39305600

Allyl radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -117.174750

C	0.00000000	1.24313300	-0.19833200
H	0.00000000	2.17389800	0.36291600
H	0.00000000	1.31276500	-1.28474800
C	0.00000000	0.00000000	0.44738500
H	0.00000000	0.00000000	1.53934200
C	0.00000000	-1.24313300	-0.19833200
H	0.00000000	-1.31276500	-1.28474800
H	0.00000000	-2.17389800	0.36291600

Dichloroindium radical – B3LYP / LanL2DZ ECP

Sum of electronic and thermal Enthalpies = -31.854381

In	0.00000000	0.00000000	0.49848800
Cl	0.00000000	2.08300200	-0.71840900
Cl	0.00000000	-2.08300200	-0.71840900

Cartesian coordinates of all compounds and intermediates involved in BDEs calculations

Hartree-Fock - HF / LanL2DZ ECP

Tetramethylstannane – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -161.502607 (Hartree/Particle)

Sn	0.00000600	0.00001000	-0.00001600
C	0.01567300	-1.73533100	1.25287200
H	0.03383000	-2.64192400	0.65512600
H	0.88997200	-1.73814900	1.89715400
H	-0.86831200	-1.76412800	1.88314800
C	-0.03036300	1.76032700	1.21724700
H	0.84345600	1.79934200	1.86100600
H	-0.03606100	2.65473100	0.60117300
H	-0.91490000	1.77858900	1.84714300
C	-1.74060000	-0.03564200	-1.24516000
H	-1.77092000	0.83696500	-1.89102600
H	-1.74729400	-0.92132300	-1.87367400
H	-2.64466900	-0.04185100	-0.64336200
C	1.75526600	0.01060100	-1.22488900
H	1.76971600	0.88355000	-1.87084200
H	1.79288900	-0.87473700	-1.85279500
H	2.65215800	0.02870500	-0.61268300

Ethyltrimethylstannane – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -200.486345 (Hartree/Particle)

Sn	0.27790600	0.00355400	-0.00000200
C	0.43806300	-1.22715500	1.74567900
H	0.33060900	-0.63272500	2.64828400
H	-0.33025900	-1.99459300	1.75180800
H	1.40578200	-1.71926300	1.77880300
C	0.43799300	-1.22816800	-1.74497400

H	-0.33022200	-1.99571800	-1.75053400
H	0.33032700	-0.63429200	-2.64791800
H	1.40577700	-1.72016000	-1.77794200
C	1.86037600	1.44575000	-0.00044700
H	1.80398100	2.08024100	-0.88013700
H	1.80386600	2.08091300	0.87875000
H	2.82901900	0.95443500	-0.00019600
C	-1.61602800	1.01844000	-0.00026100
H	-1.65126500	1.67006400	-0.87074100
H	-1.65126200	1.67051200	0.86988400
C	-2.84593600	0.08053300	-0.00001600
H	-2.85800200	-0.56005900	0.87677300
H	-3.77246300	0.64706400	-0.00015900
H	-2.85800800	-0.56050900	-0.87647700

***iso*-Propyltrimethylstannane – HF / LanL2DZ**

Sum of electronic and thermal Enthalpies = -239.473026 (Hartree/Particle)

Sn	-0.45534800	0.00000100	-0.00316700
C	-0.65816600	-0.00028800	2.12997900
H	-0.19415800	-0.88035700	2.56525800
H	-0.19352800	0.87929700	2.56556400
H	-1.70766900	0.00004000	2.41030200
C	-1.40812900	1.74542900	-0.79924800
H	-0.99057600	2.64937700	-0.36586500
H	-1.28308100	1.79708400	-1.87698600
H	-2.47277900	1.73001600	-0.58416400
C	-1.40822300	-1.74515500	-0.79973400
H	-1.28335200	-1.79640200	-1.87751200
H	-0.99057100	-2.64925400	-0.36676000
H	-2.47283700	-1.72985400	-0.58446600
C	1.63635400	0.00000500	-0.54019600

H	1.66778600	0.00000000	-1.62911000
C	2.36429100	1.27145300	-0.04464700
H	2.35605000	1.33597100	1.04027100
H	3.40555500	1.26643500	-0.35932500
H	1.91125500	2.17816600	-0.43447700
C	2.36428500	-1.27144300	-0.04463600
H	1.91124400	-2.17815800	-0.43445700
H	3.40554800	-1.26643500	-0.35931700
H	2.35604400	-1.33595000	1.04028200

***tert*-Butyltrimethylstannane – HF / LanL2DZ**

Sum of electronic and thermal Enthalpies = -278.461693 (Hartree/Particle)

Sn	-0.60311900	-0.00000100	-0.00001300
C	-1.33570400	-1.35832200	-1.48620100
H	-0.99510100	-1.07433100	-2.47748300
H	-0.99985400	-2.37202100	-1.28890900
H	-2.42209200	-1.35972100	-1.49209000
C	-1.33548800	-0.60793600	1.91950300
H	-0.99698400	-1.60944200	2.16791700
H	-0.99738300	0.06822300	2.69911600
H	-2.42187900	-0.60982000	1.92462300
C	-1.33535600	1.96638600	-0.43318200
H	-0.99564200	2.68250900	0.30915500
H	-0.99849200	2.30293300	-1.40917200
H	-2.42175000	1.97207000	-0.43262800
C	1.57034500	-0.00006500	-0.00001800
C	2.10033800	-1.42064700	0.31168900
H	1.77482600	-2.14633800	-0.42830100
H	3.18972900	-1.42404000	0.31243000
H	1.77484300	-1.76985400	1.28753900
C	2.10025500	0.44033400	-1.38616100

H	1.77476000	1.44404500	-1.64458800
H	3.18964600	0.44135800	-1.38953900
H	1.77469000	-0.23015300	-2.17649300
C	2.10021800	0.98022900	1.07441700
H	1.77464600	0.70221900	2.07285400
H	3.18960900	0.98260000	1.07706000
H	1.77470600	1.99992600	0.88886700

Methyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -39.517258 (Hartree/Particle)

C	0.00000000	0.00000000	0.00001200
H	0.00000000	1.07410800	-0.00002300
H	0.93020500	-0.53705400	-0.00002300
H	-0.93020500	-0.53705400	-0.00002300

Ethyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -78.509378 (Hartree/Particle)

C	-0.00937600	0.80348200	0.00000000
H	0.06409900	1.35478300	0.92075300
H	0.06409900	1.35478300	-0.92075300
C	-0.00937600	-0.70468900	0.00000000
H	-0.50990400	-1.09890900	-0.87769300
H	1.00412200	-1.10450500	0.00000000
H	-0.50990400	-1.09890900	0.87769300

iso-Propyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -117.50317 (Hartree/Particle)

C	0.00000000	0.54414700	-0.05724800
H	0.00000400	1.60517700	0.12828400
C	1.31015600	-0.20356400	0.00564700
H	2.14883000	0.44227700	-0.22833500

H	1.48586100	-0.62210400	0.99740400
H	1.32002200	-1.03382200	-0.69534900
C	-1.31015700	-0.20356200	0.00564800
H	-2.14885100	0.44233100	-0.22811500
H	-1.32010900	-1.03368400	-0.69551000
H	-1.48575200	-0.62229800	0.99734100

tert-Butyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -156.497342 (Hartree/Particle)

C	0.00000500	-0.00000300	-0.18943000
C	1.47712500	-0.25335100	0.02198800
H	2.08020900	0.53398900	-0.41864000
H	1.72706200	-0.29618600	1.08415800
H	1.78336800	-1.19668600	-0.41858400
C	-0.95797300	-1.15254600	0.02198800
H	-1.92803300	-0.94609300	-0.41861400
H	-0.57765500	-2.06851500	-0.41861100
H	-1.12006500	-1.34755500	1.08415800
C	-0.51915400	1.40589900	0.02198800
H	-1.50255700	1.53450600	-0.41863200
H	-0.60701600	1.64376700	1.08415800
H	0.14467000	2.14278000	-0.41859300

Trimethylstannyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -121.909186 (Hartree/Particle)

Sn	0.00000000	0.00000000	0.28531900
C	0.00000000	2.01357200	-0.48183700
H	0.00000000	1.99231300	-1.56814100
H	-0.87930100	2.55487600	-0.14807800
H	0.87930100	2.55487600	-0.14807800
C	1.74380400	-1.00678600	-0.48183700

H	2.65223800	-0.51594100	-0.14807800
H	1.77293700	-2.03893500	-0.14807800
H	1.72539400	-0.99615600	-1.56814100
C	-1.74380400	-1.00678600	-0.48183700
H	-1.77293700	-2.03893500	-0.14807800
H	-2.65223800	-0.51594100	-0.14807800
H	-1.72539400	-0.99615600	-1.56814100

Allyltrimethylstannane – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -238.317223 (Hartree/Particle)

Sn	-0.51536600	0.01400700	-0.01039700
C	-2.16897200	0.10079500	1.34576500
H	-3.09844700	0.26383900	0.80815900
H	-2.25979400	-0.82646000	1.90367200
H	-2.04342000	0.91262200	2.05606400
C	-0.37273100	1.84113300	-1.10945800
H	-0.32231700	2.69252600	-0.43740000
H	0.51810700	1.84426800	-1.72915300
H	-1.23699300	1.97029700	-1.75420200
C	-0.76762300	-1.63252900	-1.35322500
H	0.05059800	-1.67831200	-2.06522600
H	-0.80075600	-2.57292300	-0.81109400
H	-1.69433500	-1.53202000	-1.91043200
C	1.29919300	-0.26783700	1.13006400
H	1.45537300	0.62320000	1.73093000
H	1.13066700	-1.09450200	1.81556300
C	2.49630300	-0.54646800	0.26138800
H	2.54821600	-1.53830400	-0.15883800
C	3.47191800	0.31758200	-0.04032600
H	3.48696800	1.31973900	0.35029900
H	4.28591300	0.03964100	-0.68372500

Allylindium dichloride – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -147.696511 (Hartree/Particle)

C	1.72762100	-0.16243900	0.97419900
H	1.99022500	0.79326000	1.40891000
H	1.72178800	-0.91156600	1.75610700
C	2.66565100	-0.55050600	-0.14351800
H	2.67773100	-1.59496400	-0.40489500
C	3.46044500	0.28925000	-0.81474600
H	3.50088800	1.34113400	-0.59491200
H	4.10388000	-0.06375900	-1.59786400
In	-0.25005000	-0.00185000	0.20336900
Cl	-1.30638800	2.04626800	-0.26145800
Cl	-1.56798700	-1.86575600	-0.36372100

Allyl radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -116.365462 (Hartree/Particle)

C	0.00000000	1.24274300	-0.20017500
H	0.00000000	2.16289700	0.35349000
H	0.00000000	1.31071900	-1.27342900
C	0.00000000	0.00000000	0.45222900
H	0.00000000	0.00000000	1.52859700
C	0.00000000	-1.24274300	-0.20017500
H	0.00000000	-1.31071900	-1.27342900
H	0.00000000	-2.16289700	0.35349000

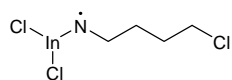
Dichloroindium radical – HF / LanL2DZ

Sum of electronic and thermal Enthalpies = -31.300777 (Hartree/Particle)

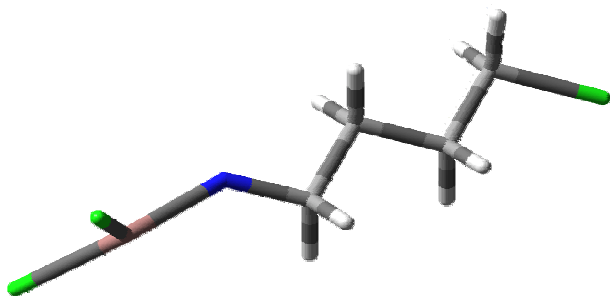
In	0.00000000	0.00000000	0.51168200
Cl	0.00000000	2.02385700	-0.73742300
Cl	0.00000000	-2.02385700	-0.73742300

*Cartesian coordinates and optimized geometries of all intermediates and transition states
involved in 1,5-H shift of metal-aminyll radicals*

Density Functional Theory - B3LYP / LanL2DZ ECP

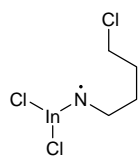


A In B3LYP / LanL2DZ ECP

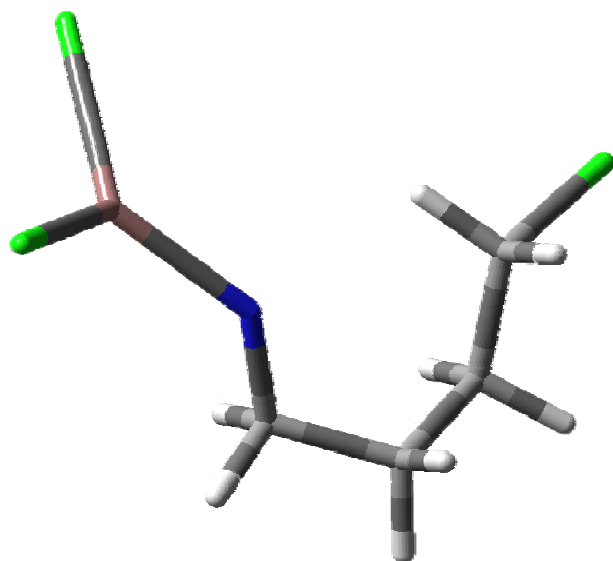


Sum of electronic and thermal Enthalpies = -258.608546 (Hartree/Particle)

C	4.93460500	0.00020500	0.69515900
H	4.98023300	0.89706400	1.31629000
H	4.98046300	-0.89612800	1.31703300
C	3.73574800	-0.00034500	-0.25215100
H	3.78846900	0.88301400	-0.90330500
H	3.78862000	-0.88431500	-0.90246300
C	2.40339600	-0.00008400	0.53609100
H	2.34159900	-0.88248400	1.18755000
H	2.34150700	0.88289500	1.18676000
C	1.18288400	-0.00058100	-0.40998600
H	1.22811300	0.87698000	-1.08342900
H	1.22825400	-0.87877400	-1.08263200
N	-0.07222200	-0.00051700	0.31829300
In	-2.01344700	-0.00004300	-0.04819400
Cl	-3.24980500	-2.01050100	0.01572600
Cl	-3.24853900	2.01121700	0.01561800
Cl	6.55407300	0.00000800	-0.28528700

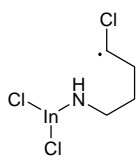


B In B3LYP / LanL2DZ ECP

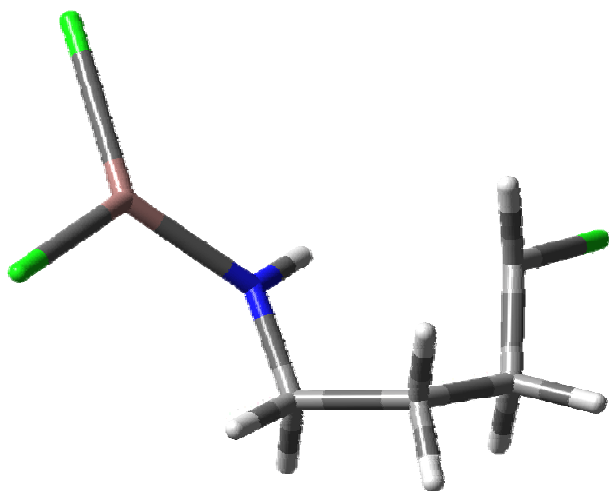


Sum of electronic and thermal Enthalpies = -258,60734 (Hartree/Particle)

C	-3.18206800	0.04820800	-0.59839100
H	-2.27784700	0.62141500	-0.39825200
H	-3.17510400	-0.31749800	-1.62682500
C	-3.43979600	-1.06445400	0.41917000
H	-4.42296200	-1.50616300	0.21158600
H	-3.49348500	-0.63254800	1.42839800
C	-2.37122500	-2.18639400	0.38304000
H	-2.74223200	-3.02986100	0.98453200
H	-2.24284800	-2.55629300	-0.64368100
C	-0.98789900	-1.78759900	0.94270700
H	-0.37955000	-2.70166700	1.08747500
H	-1.10068600	-1.35526300	1.95512000
N	-0.25395100	-0.87612600	0.07642300
In	1.50466200	0.03988600	0.09089200
Cl	1.66762500	2.34318400	0.57536800
Cl	3.38473300	-0.97460200	-0.91552900
Cl	-4.59530600	1.31363900	-0.53432000

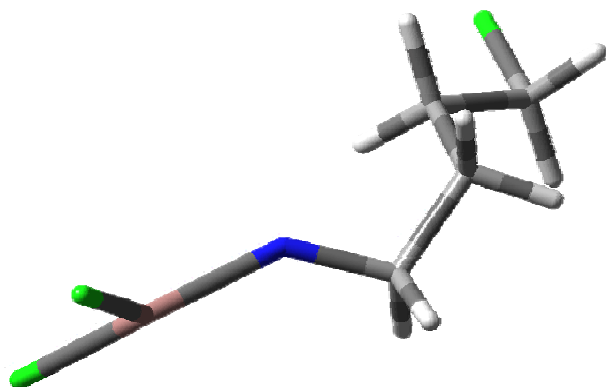
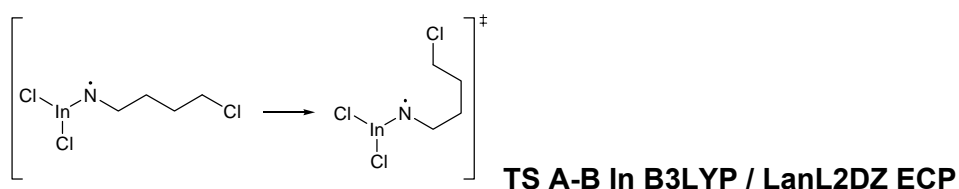


C In B3LYP / LanL2DZ ECP



Sum of electronic and thermal Enthalpies = -258,615101 (Hartree/Particle)

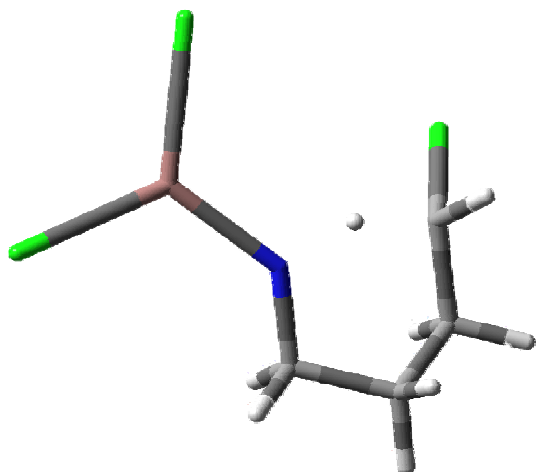
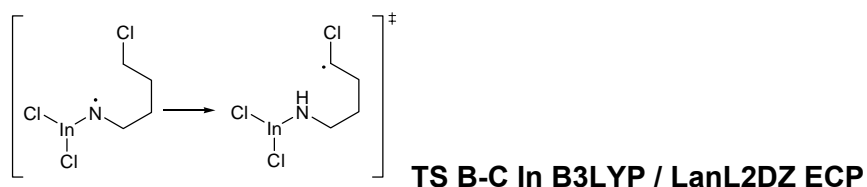
C	-3.31152900	0.18096200	-0.48441500
H	-2.82858400	0.55358500	-1.38427800
C	-3.39191000	-1.27711900	-0.13596300
H	-4.18083300	-1.75567000	-0.74588000
H	-3.71178000	-1.39003600	0.91029000
C	-2.05951500	-2.03942800	-0.36271700
H	-2.27055500	-3.11576000	-0.27845800
H	-1.68982000	-1.86327800	-1.38319800
C	-0.94344400	-1.68931000	0.65010100
H	-0.12499500	-2.41102300	0.53129800
H	-1.33592200	-1.82293600	1.67142400
N	-0.39751900	-0.31983600	0.49682400
In	1.43008200	0.15181000	0.08829900
Cl	2.15414000	2.38448900	-0.11538700
Cl	3.01396200	-1.56370100	-0.26919400
Cl	-4.68631900	1.24690300	0.04517900
H	-1.10081800	0.40388400	0.64219900



Sum of electronic and thermal Enthalpies = -258,604968 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -87.8750 cm^{-1}

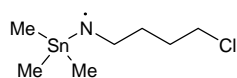
C	-4.53987800	-0.41260500	0.29659600
H	-5.15011700	-1.30692800	0.15306900
H	-4.54093900	-0.11777200	1.34866700
C	-3.12911300	-0.56300400	-0.27486000
H	-3.19556700	-0.78838000	-1.34455600
H	-2.59583200	0.39191300	-0.19670800
C	-2.33647100	-1.67927000	0.47027500
H	-2.95636900	-2.13746500	1.25727800
H	-2.07504600	-2.48308900	-0.22834500
C	-1.03779500	-1.16891900	1.13725400
H	-1.28728500	-0.38354000	1.87850700
H	-0.56789400	-1.98086900	1.72129300
N	-0.10955500	-0.60129500	0.17700500
Cl	-5.47897400	0.96646700	-0.59776500
In	1.74927700	0.04855200	0.07175200
Cl	2.24281600	2.34837600	0.26385300
Cl	3.45268300	-1.33961100	-0.79077500



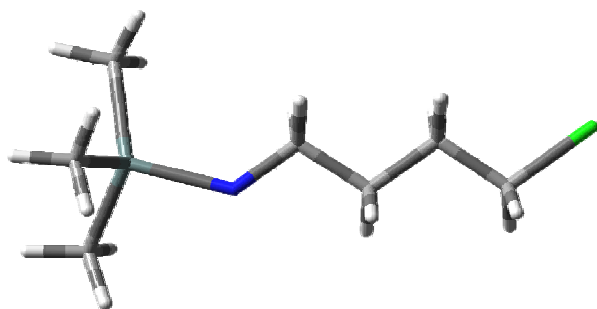
Sum of electronic and thermal Enthalpies = -258,594588 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -1397.3997 cm⁻¹

C	2.81612800	0.26684700	0.44708300
H	2.99457900	0.59927800	1.47209300
C	3.44272100	-1.06002000	0.04095700
H	4.46013500	-1.14804100	0.44873700
H	3.52092900	-1.11173900	-1.05228600
C	2.55388400	-2.22635900	0.54917600
H	2.99147100	-3.18644900	0.24701800
H	2.49619300	-2.21286100	1.64583100
C	1.12264900	-2.10519000	-0.03735000
H	0.49952800	-2.91302200	0.37847900
H	1.16912500	-2.25154500	-1.12926400
N	0.53178300	-0.81064000	0.34691000
Cl	3.21115800	1.68314400	-0.68213900
H	1.57767300	0.02041300	0.39322400
In	-1.19385100	0.03831700	0.02199600
Cl	-3.11058700	-1.25525200	-0.49371600
Cl	-1.54443600	2.32206300	0.47531400



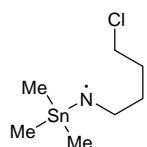
A Sn B3LYP / LanL2DZ ECP



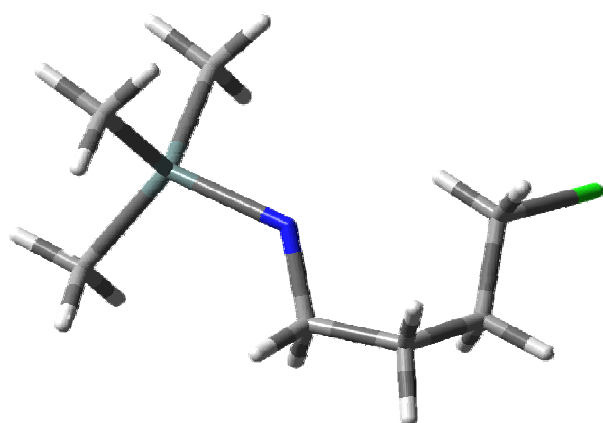
Sum of electronic and thermal Enthalpies = -349,729404 (Hartree/Particle)

C	4.67325800	-0.70150000	-0.04610500
H	4.80046400	-1.38208100	0.79826100
H	4.69599900	-1.25425800	-0.98760800
C	3.43547600	0.18206200	0.08910600
H	3.50762700	0.77007000	1.01452300
H	3.40685100	0.89641000	-0.74534100
C	2.14176500	-0.66848000	0.10355400
H	2.06734500	-1.26684600	-0.81577100
H	2.15156500	-1.37676100	0.94324400
C	0.87103500	0.20344400	0.22460200
H	0.93177400	0.79464200	1.16175000
H	0.85550200	0.95461700	-0.59002700
N	-0.34164800	-0.61391900	0.28399700
Cl	6.25320100	0.35046600	-0.06327700
Sn	-2.27593600	0.02604000	-0.02012000
C	-3.03059300	-1.29529500	-1.52072000
H	-2.75876200	-2.32782200	-1.27124800
H	-4.12378200	-1.22671100	-1.58872900
H	-2.60678200	-1.05388300	-2.50319900
C	-2.41233100	2.07843200	-0.64771500
H	-1.94536200	2.74532600	0.08838900
H	-1.91493700	2.22853400	-1.61449900
H	-3.46528700	2.37153500	-0.75580300

C	-3.25204600	-0.27295800	1.85912400
H	-4.33570100	-0.12971500	1.76055200
H	-3.06515100	-1.29220900	2.21751800
H	-2.87679500	0.43243900	2.61064300



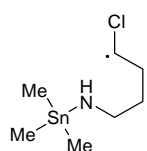
B Sn B3LYP / LanL2DZ ECP



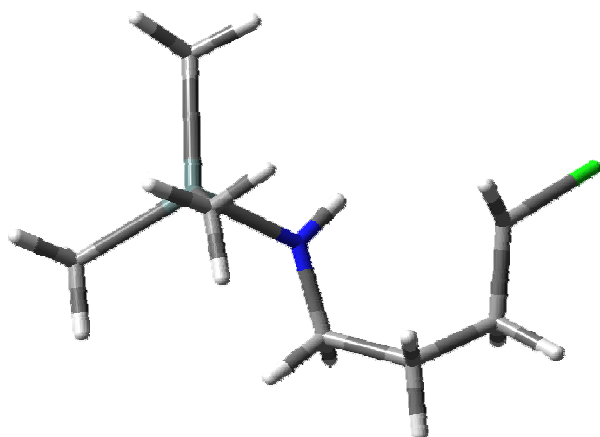
Sum of electronic and thermal Enthalpies = -258,60734 (Hartree/Particle)

C	-3.13976200	-0.14999200	0.51909800
H	-2.20296900	-0.69086900	0.40425600
H	-3.37501900	-0.02288400	1.57763500
C	-3.17201200	1.17023400	-0.25136300
H	-4.16788900	1.61941700	-0.14023900
H	-3.02944500	0.97317500	-1.32331700
C	-2.09738100	2.17498700	0.24116500
H	-2.35782700	3.17268000	-0.14568000
H	-2.11710100	2.24001700	1.33856900
C	-0.65687000	1.84427800	-0.20959000
H	0.00080900	2.69705700	0.05582200
H	-0.62199800	1.79350800	-1.31683500
N	-0.12170400	0.61747100	0.39038900
Cl	-4.49603900	-1.31686700	-0.14009400
Sn	1.73099000	-0.20418900	-0.00543500

C	1.33910400	-2.28773700	-0.25853000
H	0.77580000	-2.47102700	-1.18160000
H	2.27579000	-2.85761000	-0.30691800
H	0.74707500	-2.66121200	0.58546700
C	2.67707700	0.63383300	-1.74435600
H	2.81264300	1.71746000	-1.63491400
H	3.66546500	0.17845100	-1.89247200
H	2.07755700	0.44955700	-2.64488600
C	2.88185700	0.18012900	1.75718900
H	2.32341800	-0.13736000	2.64574900
H	3.83076800	-0.37054800	1.72579500
H	3.10591400	1.24970600	1.85250800



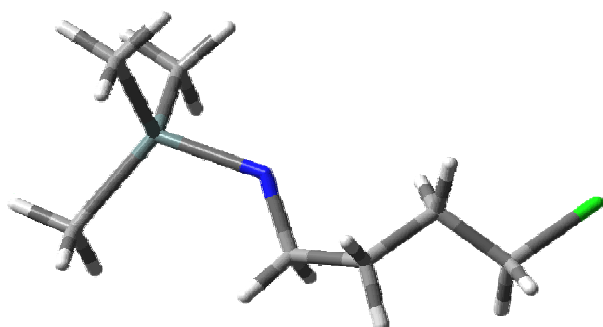
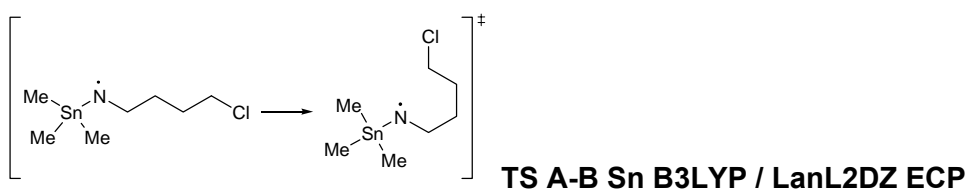
C Sn B3LYP / LanL2DZ ECP



Sum of electronic and thermal Enthalpies = -349,728784 (Hartree/Particle)

C	-3.09483600	-0.21295000	0.34073000
H	-2.55761500	-0.63715200	1.18401000
C	-3.17269800	1.25887600	0.06106100
H	-3.96912700	1.70844800	0.68394400
H	-3.48221800	1.42063400	-0.98271900
C	-1.84213400	2.00715000	0.33594300
H	-2.05194000	3.08780800	0.29539700

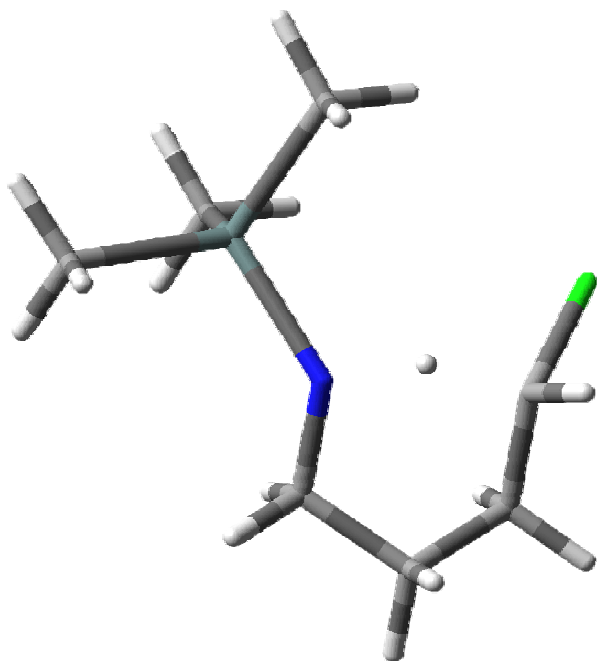
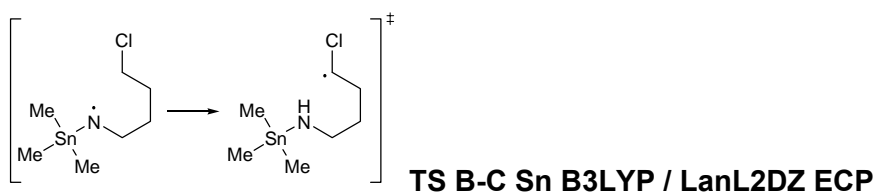
H	-1.48839900	1.78274800	1.35271500
C	-0.70896000	1.68579900	-0.67362900
H	0.10746100	2.40412600	-0.50450000
H	-1.08551300	1.89028800	-1.69179900
N	-0.16172800	0.32203400	-0.58379900
Cl	-4.53782700	-1.22898500	-0.13146000
Sn	1.67606300	-0.20660300	0.01109000
C	1.80224700	-2.30904000	-0.35567300
H	1.73441100	-2.52004600	-1.43020100
H	2.75444300	-2.71133900	0.01317600
H	0.98815100	-2.84162000	0.15236900
C	3.12072100	0.90816400	-1.11471500
H	2.97512600	1.98766900	-0.97752100
H	4.14144200	0.65941500	-0.79560000
H	3.02502300	0.68292300	-2.18412000
C	1.93694300	0.24159000	2.09449400
H	1.25665700	-0.36408600	2.70673000
H	2.96737600	0.03406300	2.41248100
H	1.72615900	1.30093700	2.29264700
H	-0.81712400	-0.39369100	-0.88937500



Sum of electronic and thermal Enthalpies = -349,726329 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -88.8750 cm⁻¹

C	4.36857200	-0.57588900	-0.17803500
H	4.92669900	-1.35112800	0.35174200
H	4.31912500	-0.80578700	-1.24506900
C	2.99414800	-0.31033000	0.43389500
H	3.11321500	-0.01822300	1.48276100
H	2.51573300	0.53978000	-0.06494200
C	2.08103300	-1.56791800	0.31541500
H	2.60568100	-2.38231700	-0.21166100
H	1.83999500	-1.94906000	1.31564200
C	0.75455200	-1.28676400	-0.43329700
H	0.99335400	-0.94355200	-1.46123600
H	0.19726400	-2.23493600	-0.56318200
N	-0.02493800	-0.23120000	0.21296300
Cl	5.46983000	0.96739100	-0.06825200
Sn	-2.03505200	0.15596000	-0.00062500
C	-2.12502800	2.12766100	-0.82151100
H	-3.14968000	2.51842300	-0.77877600
H	-1.47128100	2.79744600	-0.25043800
H	-1.79607800	2.13241500	-1.86786700
C	-2.78808200	0.09550100	1.99877500
H	-3.81894300	0.46984000	2.04013400
H	-2.77616100	-0.92956600	2.38897200
H	-2.16233600	0.71944200	2.64787100
C	-3.05976400	-1.25826100	-1.25532200
H	-2.98109300	-2.27499700	-0.84951200
H	-4.12498600	-0.99892900	-1.32249900
H	-2.64304700	-1.25807800	-2.27066700



Sum of electronic and thermal Enthalpies = -349,712468 (Hartree/Particle)

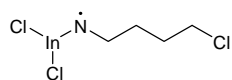
1 imaginary frequencies (negative Signs): -1640.0300 cm^{-1}

C	2.56922000	-0.20111500	-0.61990500
H	2.92038900	-0.30033800	-1.65002900
C	3.15846700	0.93406800	0.20431600
H	4.23445200	1.05567200	0.00794500
H	3.04369700	0.71237700	1.27312800
C	2.39171400	2.24388100	-0.13021200
H	2.81216600	3.07982900	0.44485100
H	2.50138300	2.48299900	-1.19720600
C	0.88619900	2.08070100	0.19917900
H	0.35468500	2.99757300	-0.10555200
H	0.77640100	1.99039700	1.29721700
N	0.31403300	0.93947600	-0.55635700
Cl	2.70763300	-1.88739300	0.17611000
Sn	-1.36083200	-0.10434900	-0.00377000

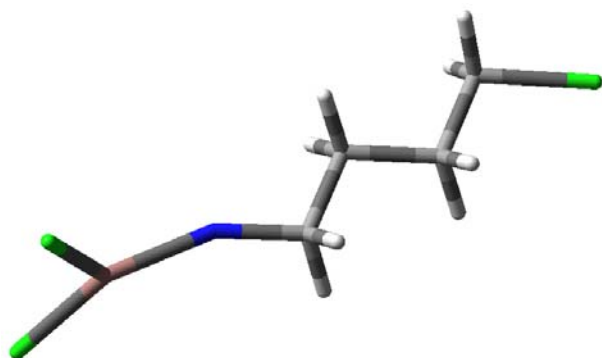
H	1.28269400	0.17273700	-0.74084100
C	-1.30840500	-0.68612000	2.06311200
H	-2.19950800	-1.27499100	2.31879400
H	-0.42042800	-1.29917200	2.26130100
H	-1.27948300	0.19245400	2.72050300
C	-1.39028200	-1.79802100	-1.29997600
H	-0.51988700	-2.43809400	-1.11065000
H	-2.29865100	-2.39478100	-1.14788100
H	-1.36039500	-1.47299000	-2.34714900
C	-2.99944500	1.22939900	-0.35967800
H	-2.95311700	1.61579300	-1.38499000
H	-3.95785600	0.71112400	-0.22485500
H	-2.96776800	2.07947000	0.33355300

*Cartesian coordinates and optimized geometries of all intermediates and transition states
involved in 1,5-H shift of metal-aminyll radicals*

Hartree-Fock - UF / LanL2DZ ECP

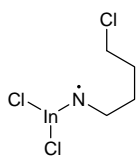


A In HF / LanL2DZ ECP

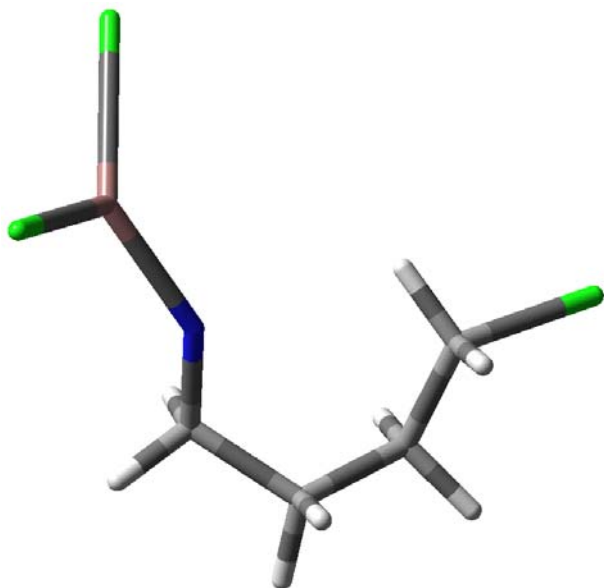


Sum of electronic and thermal Enthalpies = -256.368613 (Hartree/Particle)

C	-4.86158700	0.00016100	0.72255200
H	-4.86548200	-0.88383500	1.33567000
H	-4.86545200	0.88446000	1.33523200
C	-3.73940900	-0.00011300	-0.30708700
H	-3.83985100	-0.87209000	-0.94305800
H	-3.83981200	0.87156100	-0.94348000
C	-2.35853200	0.00002100	0.37476300
H	-2.25137000	0.87165300	1.01165500
H	-2.25140400	-0.87130700	1.01207500
C	-1.21879800	-0.00025300	-0.65321100
H	-1.30027800	-0.87128900	-1.30036700
H	-1.30026300	0.87044400	-1.30082000
N	0.08968700	-0.00014100	-0.03079300
In	2.01292200	-0.00000600	-0.03641600
Cl	3.21674100	1.99274400	0.09525400
Cl	3.21705600	-1.99255700	0.09536000
Cl	-6.53245100	-0.00002100	-0.13349900

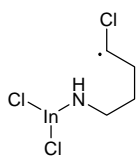


B In HF / LanL2DZ ECP

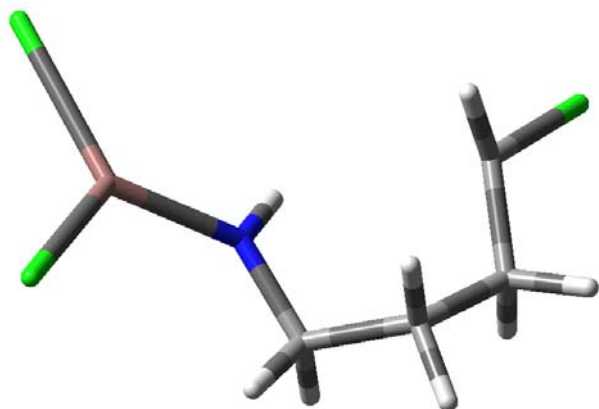


Sum of electronic and thermal Enthalpies = -256.366197 (Hartree/Particle)

C	3.13098000	0.11392700	0.56389900
H	2.30320900	0.73548700	0.28641500
H	3.00022000	-0.26504000	1.56174300
C	3.44600800	-0.98280900	-0.44777000
H	4.39098500	-1.43640700	-0.17564000
H	3.58339400	-0.53962000	-1.42790500
C	2.37533700	-2.09103200	-0.51657000
H	2.78721200	-2.90777000	-1.10270000
H	2.18241100	-2.48429600	0.47616000
C	1.03897300	-1.68967600	-1.15739500
H	0.46957500	-2.58735900	-1.38631200
H	1.21441500	-1.18891300	-2.10808500
N	0.23010500	-0.81216100	-0.31958400
In	-1.50260300	0.03221500	-0.07226700
Cl	-1.86886400	2.24504200	-0.70760500
Cl	-3.18767600	-1.03046000	1.14003200
Cl	4.59404700	1.29589300	0.68530900

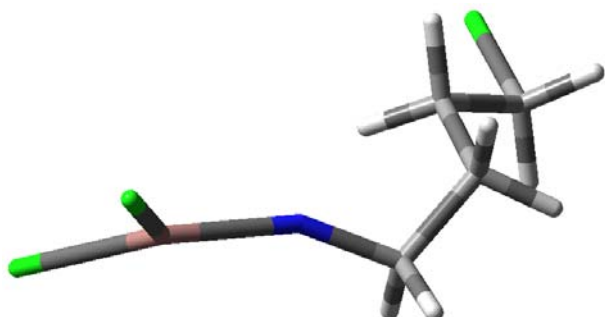
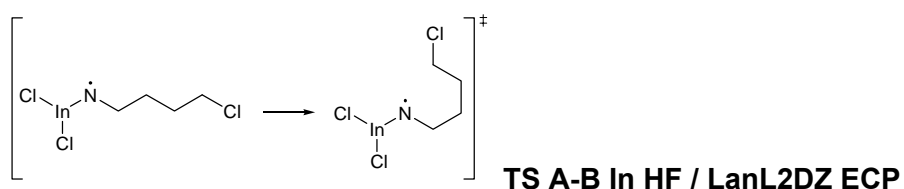


C In HF / LanL2DZ ECP



Sum of electronic and thermal Enthalpies = -256.370367 (Hartree/Particle)

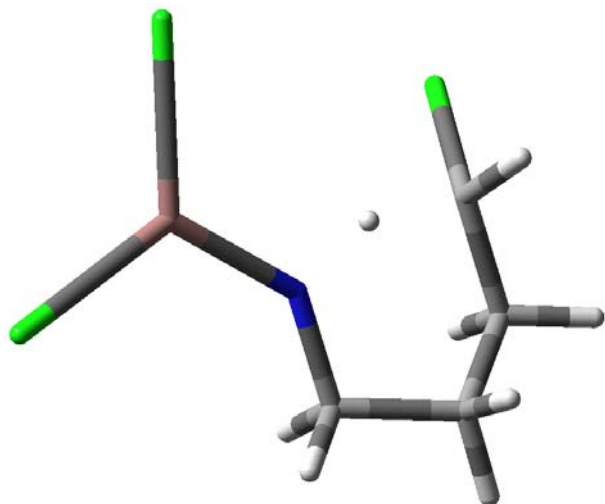
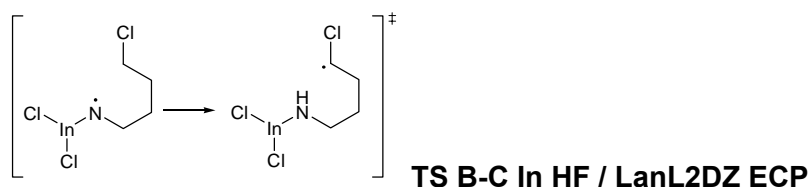
C	-3.29246500	0.19744000	-0.48165300
H	-2.79599800	0.52999900	-1.37187600
C	-3.35482800	-1.24571500	-0.06363200
H	-4.12066500	-1.74663900	-0.65267400
H	-3.67942400	-1.30740200	0.96962300
C	-2.01882500	-1.99738400	-0.23963500
H	-2.22649300	-3.05922600	-0.14660100
H	-1.63055300	-1.84063200	-1.24152100
C	-0.92890200	-1.64241100	0.78771800
H	-0.13139300	-2.36995300	0.69832200
H	-1.33452600	-1.75037300	1.78977700
N	-0.35442100	-0.29167900	0.63185100
In	1.43458500	0.14631800	0.10102900
Cl	2.19958400	2.34488500	-0.05014200
Cl	2.93752800	-1.55496500	-0.45815700
Cl	-4.74504600	1.21629100	-0.09865000
H	-0.98963400	0.43921100	0.88292100



Sum of electronic and thermal Enthalpies = -256.364329 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -97.4661 cm^{-1}

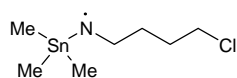
C	-4.46322300	-0.41255000	0.22153300
H	-5.06219000	-1.27508400	-0.01286700
H	-4.53706800	-0.17662500	1.26918500
C	-3.02125700	-0.54673700	-0.25596500
H	-3.01817300	-0.70920600	-1.32479400
H	-2.50038700	0.38636400	-0.08832100
C	-2.29224100	-1.70586200	0.47162100
H	-2.96836200	-2.21591800	1.15425200
H	-1.96982200	-2.44689200	-0.24923600
C	-1.06722100	-1.24831200	1.27867200
H	-1.36313600	-0.50577000	2.01806300
H	-0.65638500	-2.08812800	1.83329600
N	-0.03983600	-0.65108500	0.44873700
Cl	-5.31280700	1.01435700	-0.65361100
In	1.70668900	0.05053000	0.06146900
Cl	2.19504500	2.31328600	0.33490900
Cl	3.34071900	-1.29272400	-0.91941000



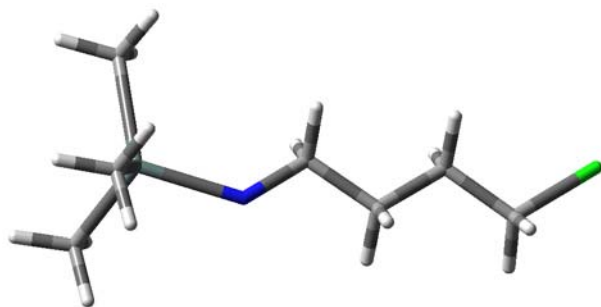
Sum of electronic and thermal Enthalpies = -256.324689 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -2667.4752 cm^{-1}

C	2.76582100	0.26388300	0.45392700
H	2.82664300	0.62368700	1.46526800
C	3.42280300	-1.07451200	0.15935600
H	4.37907200	-1.14746800	0.66540900
H	3.61110700	-1.15929700	-0.90296800
C	2.47930400	-2.21068000	0.60610700
H	2.93439400	-3.16970500	0.38787900
H	2.31609700	-2.16199600	1.67744300
C	1.12415500	-2.10993900	-0.12047700
H	0.45188600	-2.87193300	0.25843100
H	1.27099000	-2.29793700	-1.18024400
N	0.52235600	-0.78632600	0.10249500
Cl	3.27846500	1.63062300	-0.66576000
H	1.51967100	0.00738700	0.23721700
In	-1.20174600	0.04682400	0.01545600
Cl	-3.11254300	-1.22413000	-0.43301600
Cl	-1.50906000	2.30966500	0.47073300



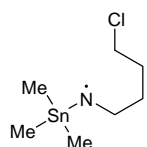
A Sn HF / LanL2DZ ECP



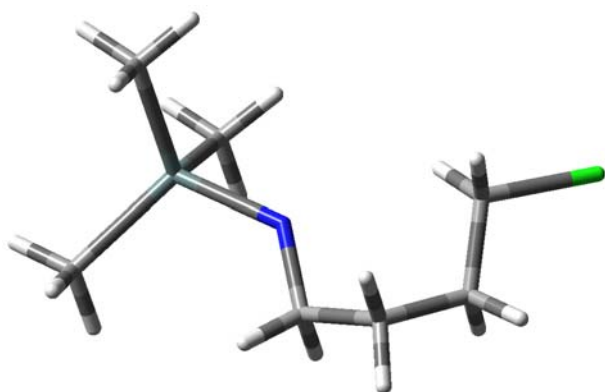
Sum of electronic and thermal Enthalpies = -346.993297 (Hartree/Particle)

C	4.67733000	-0.70271300	-0.00001800
H	4.74870000	-1.31114300	0.88433200
H	4.74860900	-1.31110300	-0.88440200
C	3.45087100	0.19940100	0.00006500
H	3.48153300	0.84296900	0.87199900
H	3.48142600	0.84298400	-0.87186200
C	2.15238400	-0.62932200	0.00014200
H	2.11510700	-1.27579300	-0.87040700
H	2.11518700	-1.27576100	0.87071400
C	0.89852900	0.25510800	0.00020300
H	0.91303600	0.91219300	0.87079500
H	0.91297300	0.91221600	-0.87036700
N	-0.32349200	-0.54549000	0.00030400
Cl	6.25293300	0.32641300	-0.00007800
Sn	-2.28541800	0.01628500	-0.00001900
C	-3.09735800	-0.84154100	-1.76940200
H	-2.88642900	-1.90501400	-1.79517700
H	-4.17311400	-0.70244800	-1.81081400
H	-2.66151600	-0.38684200	-2.65303800
C	-2.51254100	2.14438900	-0.00148300
H	-2.05207200	2.58465400	0.87762000
H	-2.05347700	2.58329400	-0.88199900
H	-3.56489900	2.41336500	-0.00084500

C	-3.09731800	-0.83910400	1.77056800
H	-4.17322100	-0.70093500	1.81124300
H	-2.88542700	-1.90233700	1.79831800
H	-2.66230500	-0.38243100	2.65359400



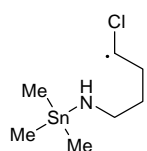
B Sn HF / LanL2DZ ECP



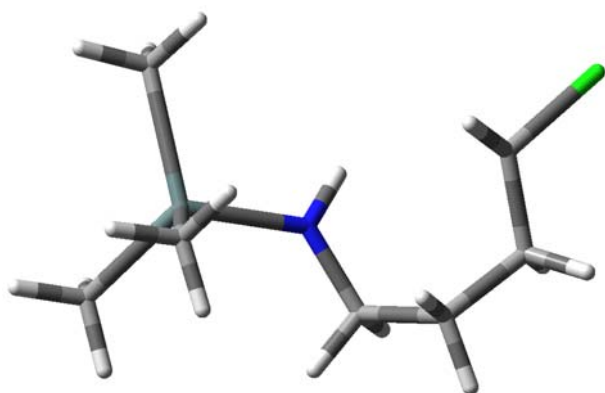
Sum of electronic and thermal Enthalpies = -346.992939 (Hartree/Particle)

C	-3.15497100	-0.22521900	0.44117900
H	-2.30492200	-0.80495300	0.14842500
H	-3.24351600	-0.19393300	1.51264200
C	-3.20225200	1.15875900	-0.19567300
H	-4.15795300	1.61229000	0.03902400
H	-3.15825300	1.06087600	-1.27475200
C	-2.07531000	2.09381900	0.29281200
H	-2.34587300	3.11086000	0.01980400
H	-2.01649100	2.06701300	1.37686400
C	-0.68295200	1.80357300	-0.28777000
H	-0.01362000	2.62211800	-0.02319500
H	-0.73872000	1.80188500	-1.37739600
N	-0.13822300	0.51384600	0.14035700
Cl	-4.65841600	-1.23053900	-0.12506100
Sn	1.77116300	-0.20518800	0.00114400

C	1.65996300	-1.81009600	-1.39207000
H	1.40230600	-1.44583900	-2.38114100
H	2.61080500	-2.32938800	-1.45870400
H	0.90227200	-2.52226200	-1.08398200
C	3.13061400	1.30653900	-0.66340400
H	3.14168600	2.14824100	0.02210000
H	4.13933100	0.90841100	-0.72340900
H	2.85391700	1.67229500	-1.64735900
C	2.24825400	-0.85962500	1.96739100
H	1.49838400	-1.56018700	2.31818300
H	3.21557100	-1.35157700	1.98948600
H	2.27751900	-0.02072600	2.65497100



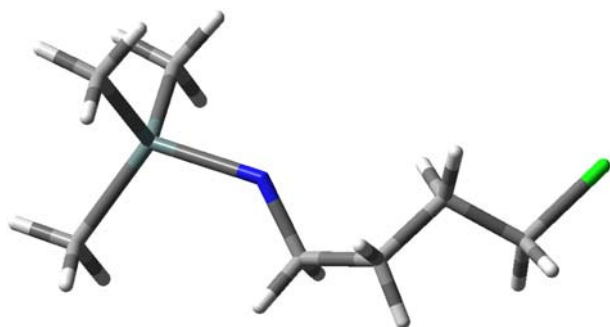
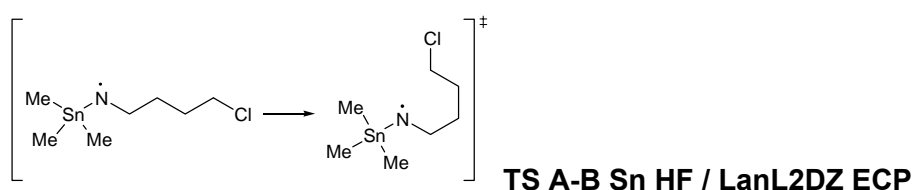
C Sn HF / LanL2DZ ECP



Sum of electronic and thermal Enthalpies = -346.988841 (Hartree/Particle)

C	3.10121800	0.23903100	0.30097600
H	2.57756800	0.67533600	1.12762900
C	3.14831600	-1.23944700	0.03348000
H	3.93640900	-1.67934200	0.64220400
H	3.43411100	-1.40825900	-0.99990700
C	1.81914300	-1.96206700	0.33644700
H	2.02110000	-3.03035500	0.33155000

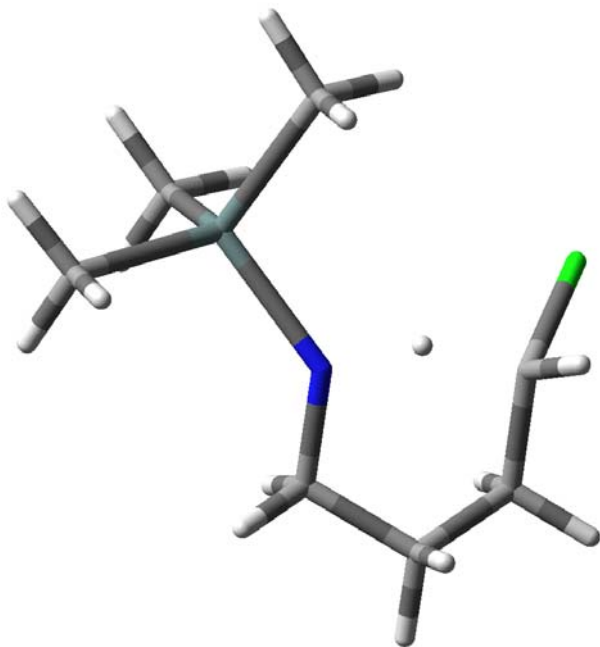
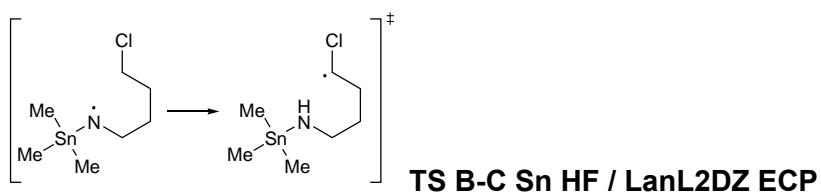
H	1.47943000	-1.70843800	1.33604800
C	0.68128100	-1.68344500	-0.66561400
H	-0.11791700	-2.39018500	-0.46150500
H	1.03361700	-1.91355900	-1.66968500
N	0.12997700	-0.32565900	-0.61489100
Cl	4.60091200	1.18366000	-0.12074400
Sn	-1.68023700	0.20621700	0.01207600
C	-1.78993100	2.31617300	-0.26109300
H	-1.67166900	2.57438700	-1.30877200
H	-2.74866200	2.69951800	0.07446500
H	-1.00984500	2.81780400	0.30291100
C	-3.17079700	-0.81356100	-1.12923300
H	-3.08706900	-1.88916300	-1.00460700
H	-4.16778400	-0.51619000	-0.81726200
H	-3.06017300	-0.58567900	-2.18463100
C	-1.89747700	-0.33441000	2.06791000
H	-1.15488200	0.17339500	2.67549000
H	-2.88272500	-0.06573900	2.43750700
H	-1.77015200	-1.40492200	2.20112200
H	0.72462900	0.36430000	-1.02670600



Sum of electronic and thermal Enthalpies = -346.989314 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -99.1879 cm⁻¹

C	4.32461500	-0.55519800	-0.20214000
H	4.91038400	-1.32133100	0.27518000
H	4.25678400	-0.73722400	-1.26097200
C	2.96395200	-0.35183100	0.45384600
H	3.10580200	-0.10168200	1.49591400
H	2.46561600	0.49594300	0.00562900
C	2.08249300	-1.62026500	0.31478300
H	2.62232700	-2.40699000	-0.21011800
H	1.84803100	-2.01106900	1.29738600
C	0.76297600	-1.35991600	-0.42884500
H	0.97605500	-0.98887700	-1.43262100
H	0.22995300	-2.30128200	-0.56183100
N	-0.06039900	-0.36821200	0.25921000
Cl	5.37158700	1.00240000	-0.05456400
Sn	-2.01258000	0.16615400	0.00366400
C	-1.94789200	2.15009000	-0.76357900
H	-2.94443500	2.57711500	-0.81658800
H	-1.33937300	2.77703200	-0.12115200
H	-1.51838400	2.16545100	-1.75994200
C	-2.86165400	0.06812000	1.95064800
H	-3.88102400	0.44118000	1.95075800
H	-2.87324100	-0.95435700	2.31378100
H	-2.27552700	0.66634300	2.63956200
C	-3.02651800	-1.15021600	-1.34516500
H	-3.00841400	-2.17181700	-0.97808200
H	-4.06472600	-0.85140300	-1.45753700
H	-2.56286700	-1.13278100	-2.32673700



Sum of electronic and thermal Enthalpies = -346.945744 (Hartree/Particle)

1 imaginary frequencies (negative Signs): -2897.8662 cm^{-1}

C	2.57379400	-0.19995900	-0.60617000
H	2.80689400	-0.30487900	-1.65064000
C	3.20510900	0.96570200	0.13487700
H	4.23883800	1.10040700	-0.16621400
H	3.20187500	0.76382800	1.19852300
C	2.38013500	2.24059300	-0.14705700
H	2.81925800	3.08201200	0.37775500
H	2.39824200	2.46949000	-1.20722300
C	0.91876000	2.05073700	0.30122100
H	0.34307100	2.93061500	0.03045200
H	0.89466700	1.96673200	1.38835200
N	0.32464400	0.88425200	-0.37242700
Cl	2.83899200	-1.85063500	0.19260300
Sn	-1.39230500	-0.11098300	-0.01000800

H	1.27669200	0.11335200	-0.56854000
C	-1.50361900	-0.75695400	2.02462800
H	-2.42252800	-1.30790300	2.20324600
H	-0.66649500	-1.40569300	2.26164700
H	-1.48182200	0.09073800	2.70295200
C	-1.37289800	-1.75983500	-1.35066100
H	-0.54310100	-2.42224200	-1.12781200
H	-2.29312700	-2.33121000	-1.27841100
H	-1.26645700	-1.41004500	-2.37206800
C	-2.95509900	1.27721500	-0.42995300
H	-2.85020000	1.66345000	-1.43827300
H	-3.92785300	0.80248400	-0.34293000
H	-2.92516000	2.11406300	0.26102100