Supporting Information

Mechanistic Insights Into the Insertion and Addition Reactions of Group 13 Analogues of the Six-membered N-heterocyclic Carbenes: Interplay of Electrophilicity, Basicity, and Aromaticity Govern the Reactivity

Zheng-Feng Zhang[1] and Ming-Der Su[1,2,a)]*

[1]Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan
[2]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan

[a)] E-mail: midesu@mail.ncyu.edu.tw

Contents:

Figure S8. The optimized **G13-6-C_2H_4-TS** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

Figure S9. The optimized **G13-6-C_2H_4-Prod** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

Figure S10. The Gibbs free activation energy ($\Delta G_{ACT,C2H4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{ACT,C2H4} = 1.167\Delta E_{st} + 22.35$ (the correlation coefficient r = 0.9081). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

Figure S11. The Gibbs free reaction enthalpy energy ($\Delta G_{REA,C2H4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{REA,C2H4} = 1.471\Delta E_{st} - 46.56$ (the correlation coefficient r = 0.9081). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

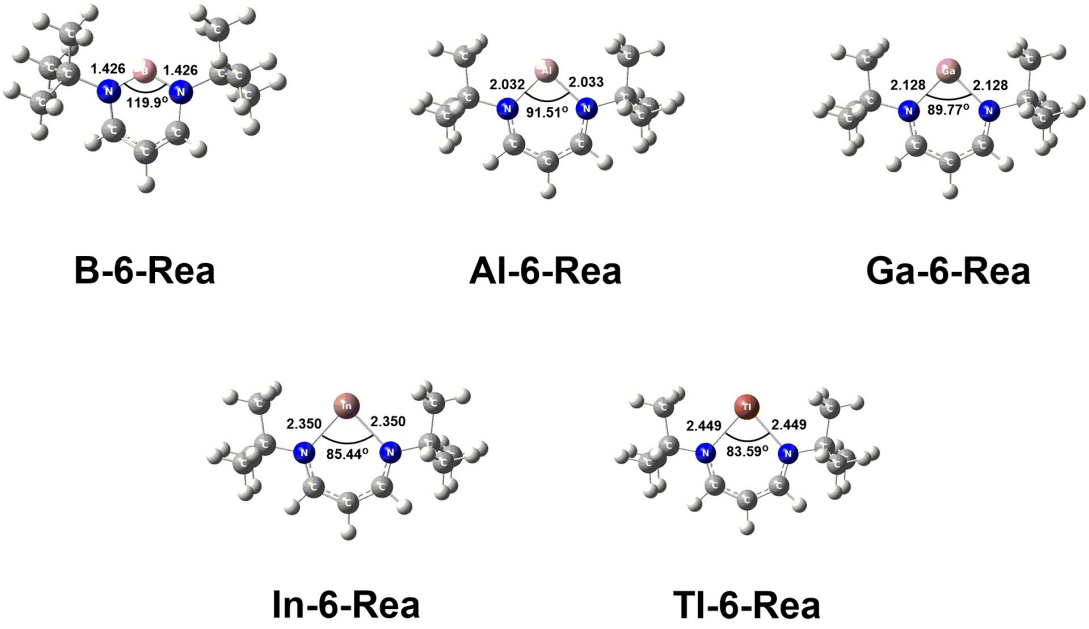

Figure S1. The optimized **G13-6-Rea** (G13 = B, Al, Ga, In, and Tl) structures at the BP86-D3(BJ)/def2-TZVP level of theory. Bond length (Å) and bond angle (°). The hydrogen is omitted for clarity.

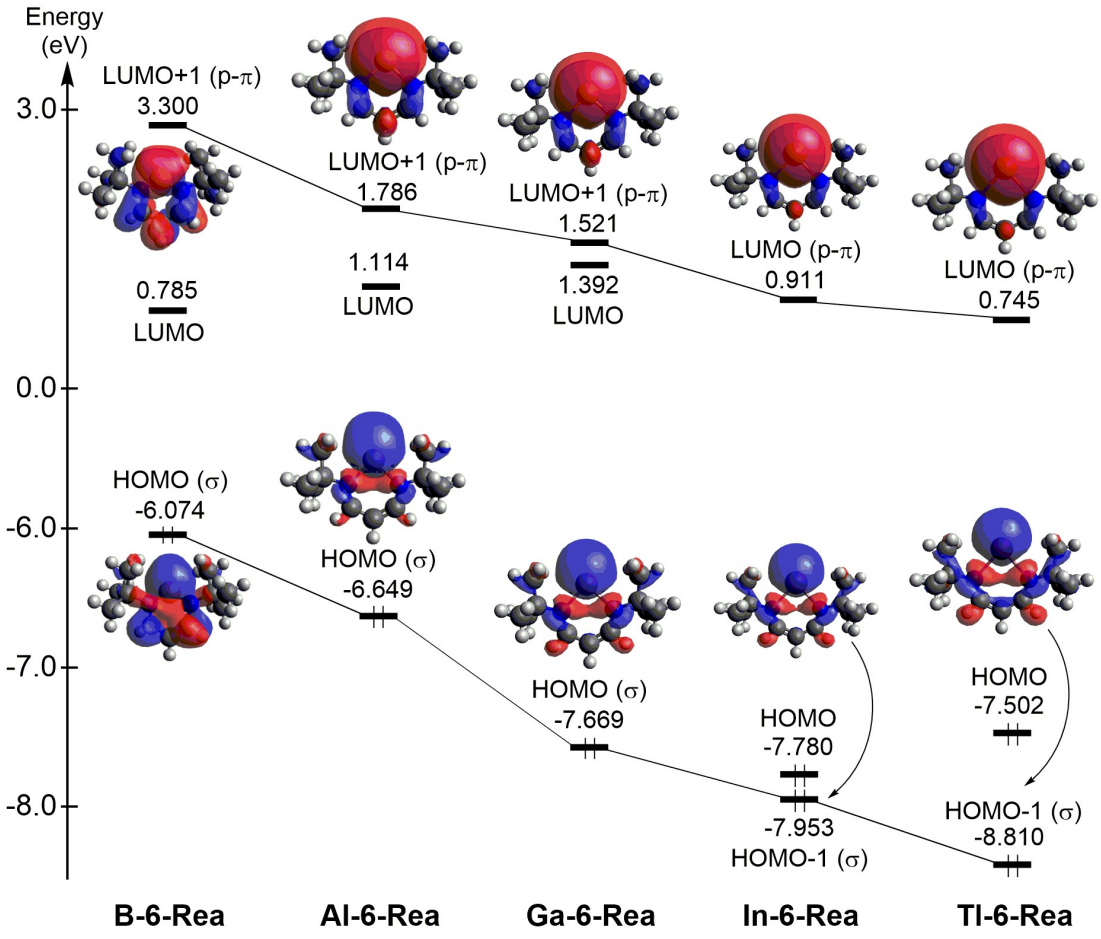

Figure S2. Calculated frontier molecular orbitals of the **G13-6-Rea** (G13 = B, Al, Ga, In, and Tl) molecules at the LC-BLYP/def2-TZVP level of theory. For more information see the text.

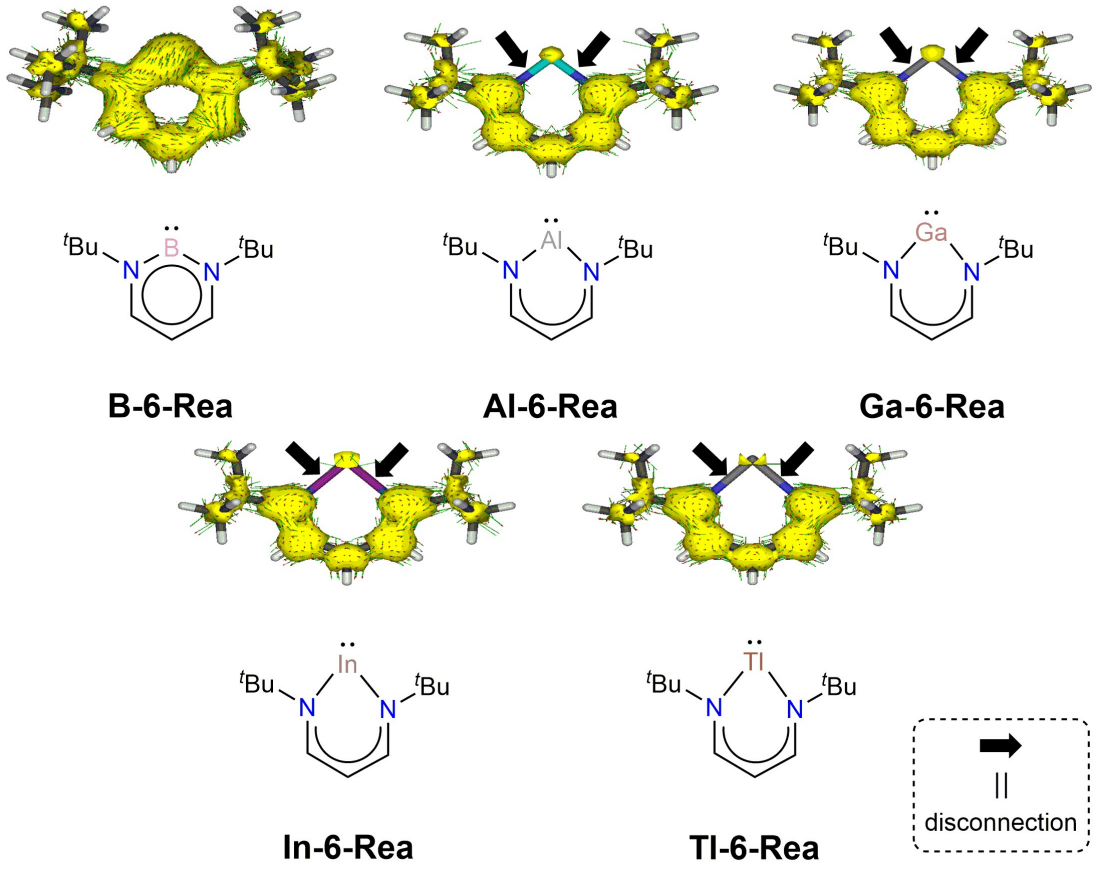

Figure S3. ACID plots for the six-membered **G13-6-Rea** (G13 = B, Al, Ga, In, and Tl) species. The current density vectors (green arrows with red tips) are plotted onto an isosurface of contour value 0.05. See the text.

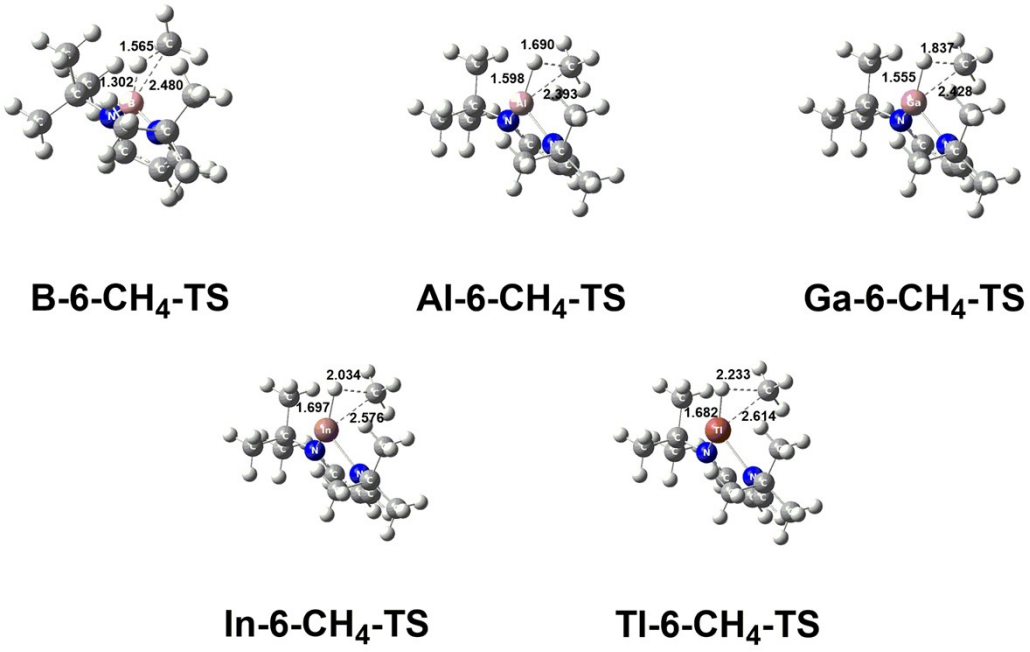

Figure S4. The optimized **G13-6-CH_4-TS** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

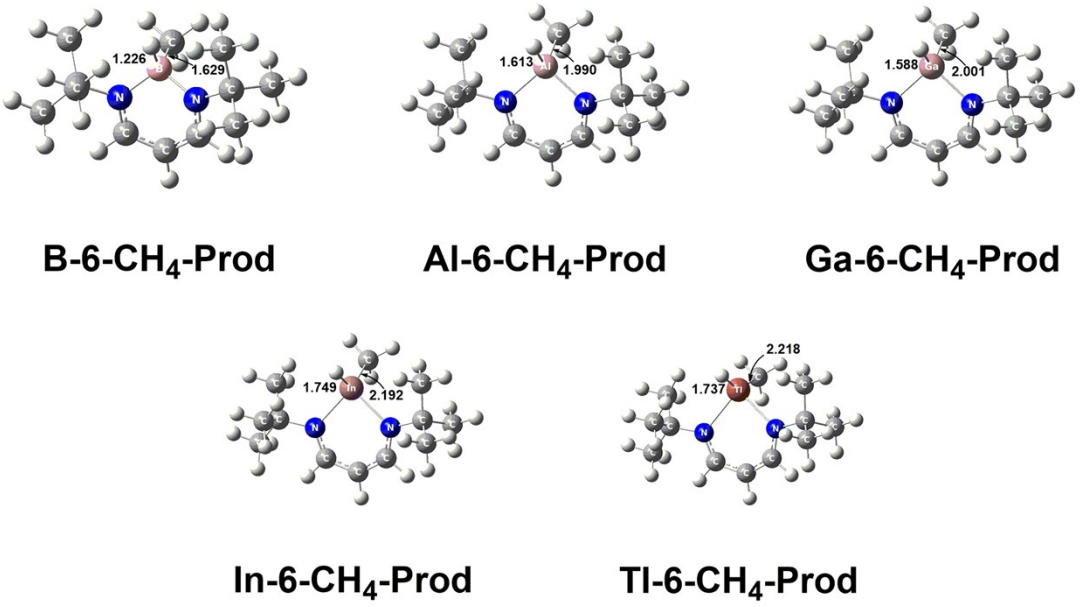

Figure S5. The optimized **G13-6-CH_4-Prod** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

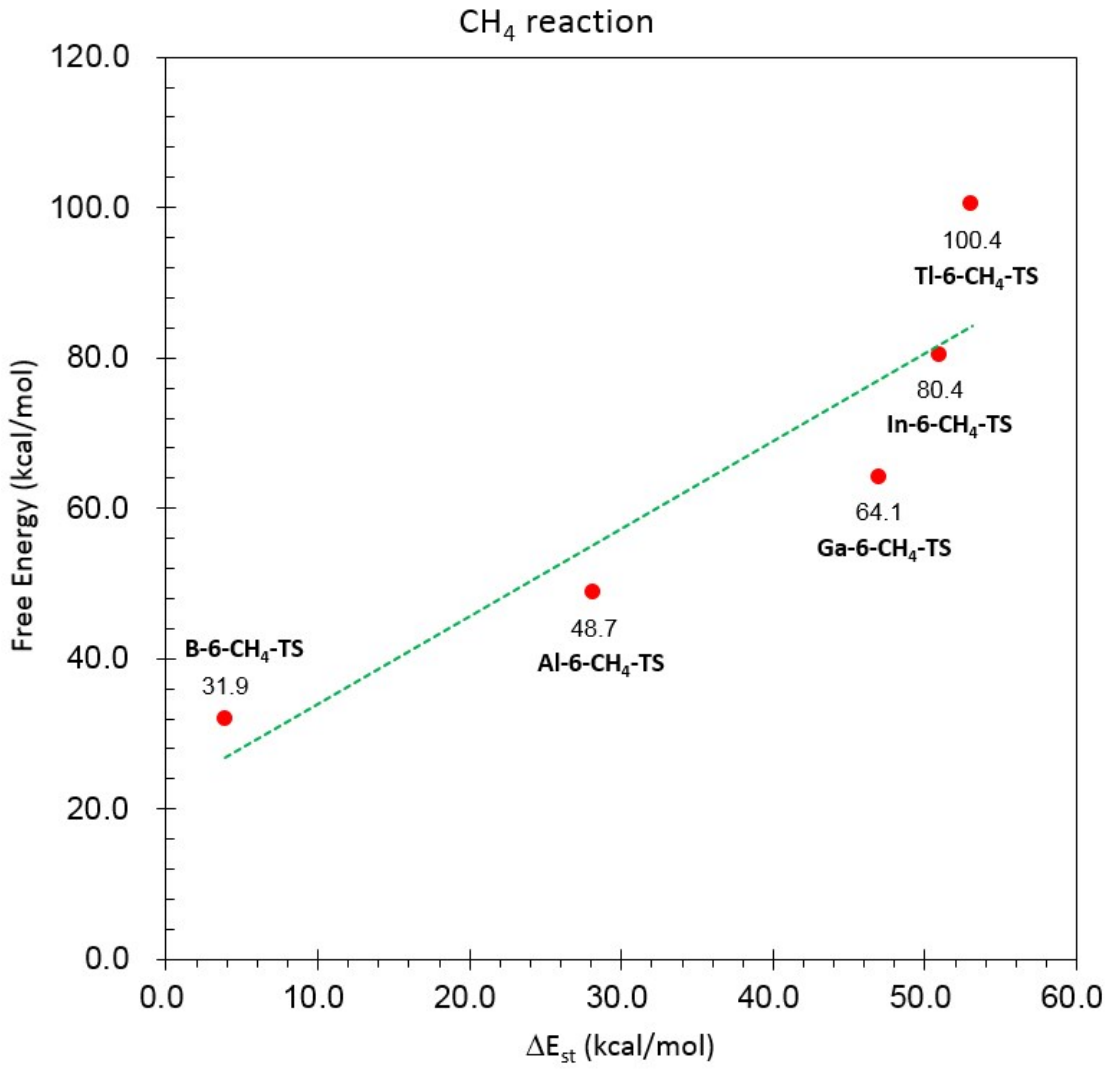

Figure S6. The Gibbs free activation energy ($\Delta G_{ACT,CH4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{ACT,CH4} = 1.167\Delta E_{st} + 22.35$ (the correlation coefficient r = 0.9081). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

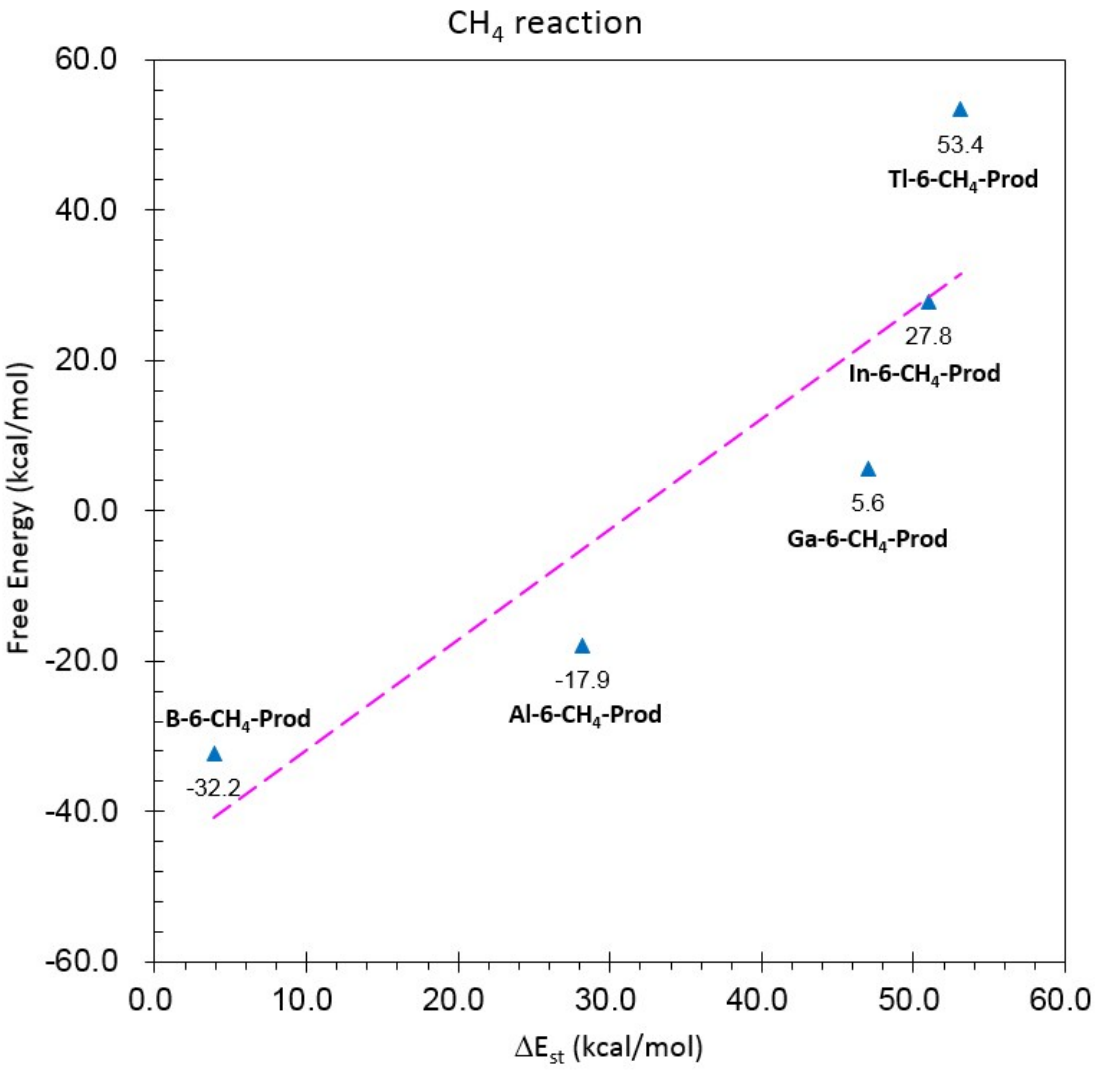

Figure S7. The Gibbs free reaction enthalpy energy ($\Delta G_{REA,CH4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{REA,CH4} = 1.471 \Delta E_{st} - 46.56$ (the correlation coefficient r = 0.8892). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

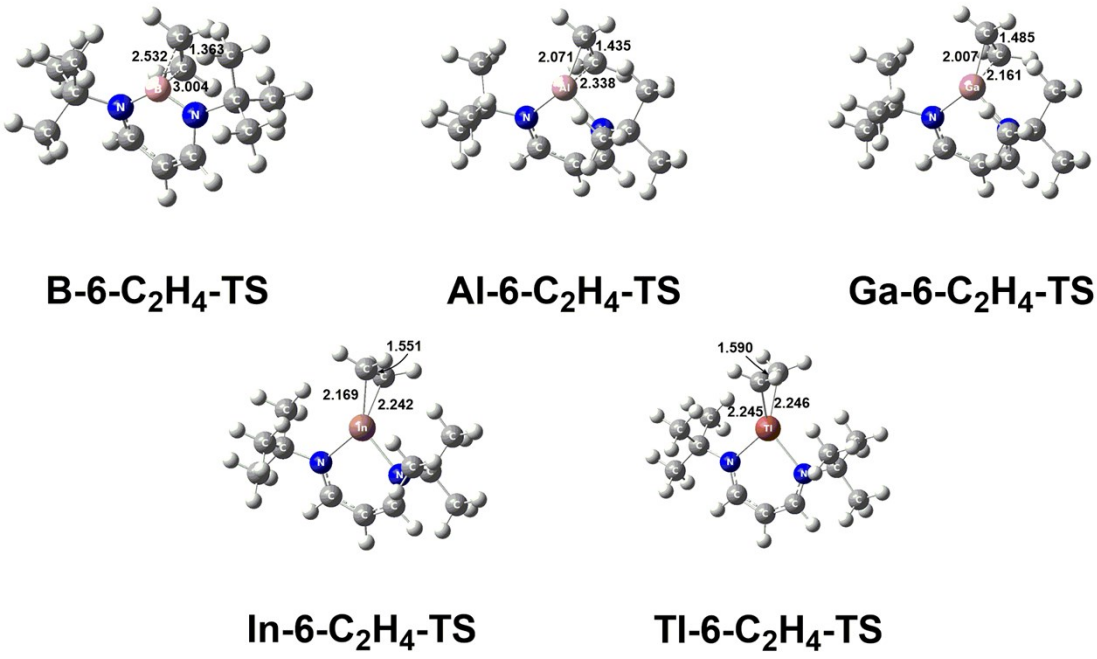

Figure S8. The optimized **G13-6-C_2H_4-TS** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

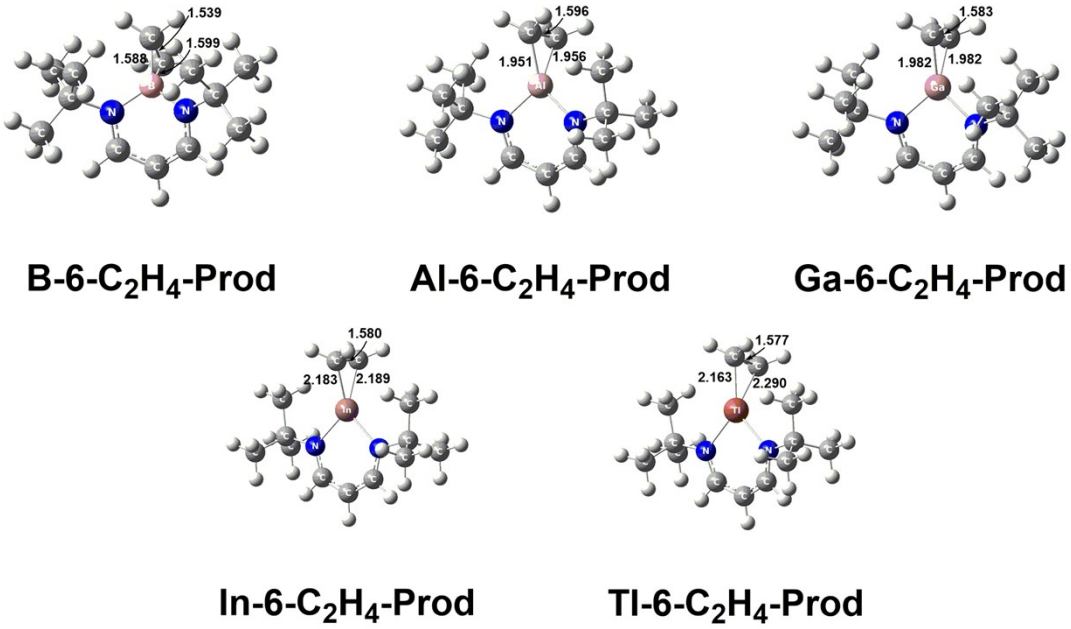

Figure S9. The optimized **G13-6-C_2H_4-Prod** (G13 = B, Al, Ga, In, and Tl) structures (Å) at the BP86-D3(BJ)/def2-TZVP level of theory. The hydrogen is omitted for clarity.

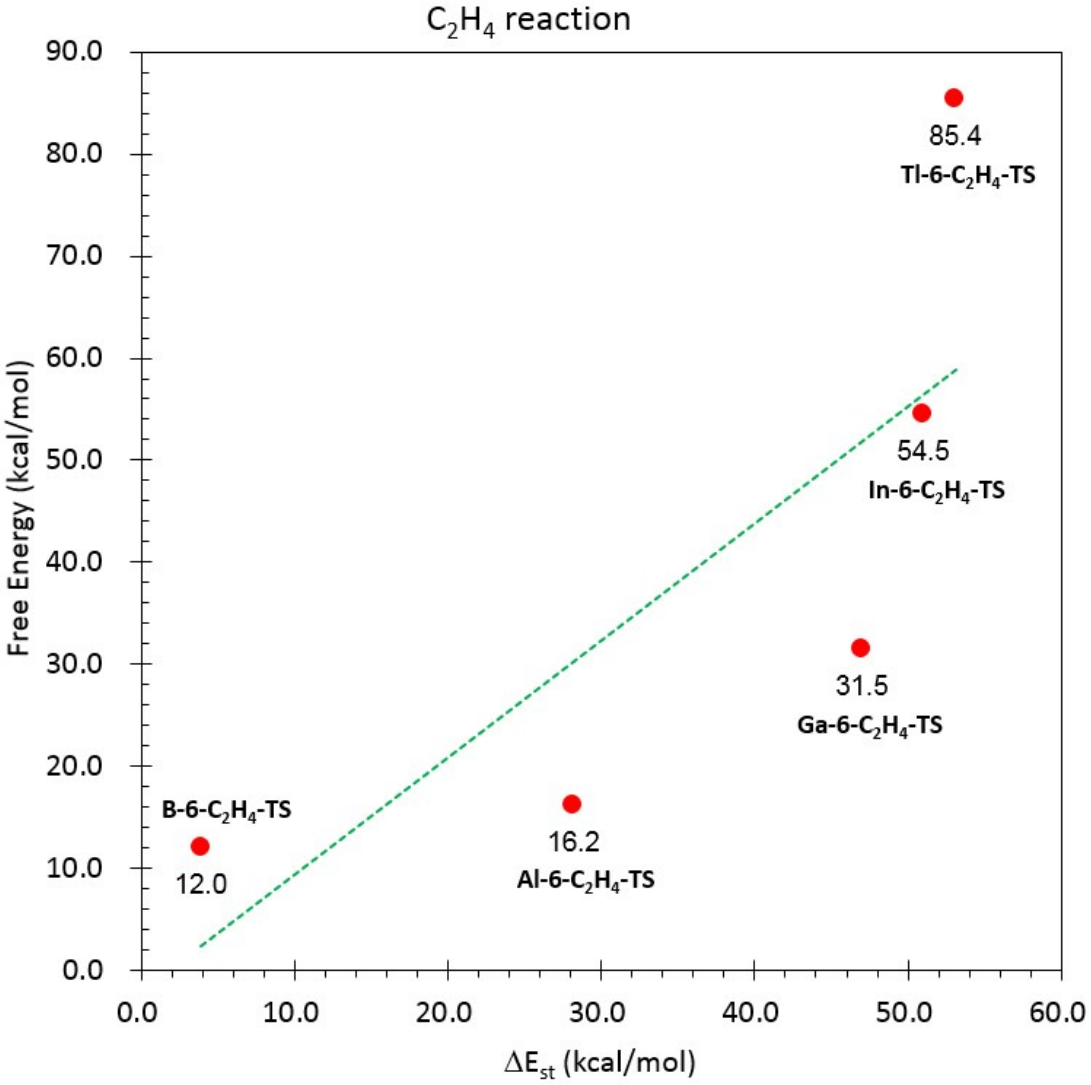

Figure S10. The Gibbs free activation energy ($\Delta G_{ACT,C2H4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{ACT,C2H4} = 1.149\Delta E_{st} - 2.180$ (the correlation coefficient r = 0.8357). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

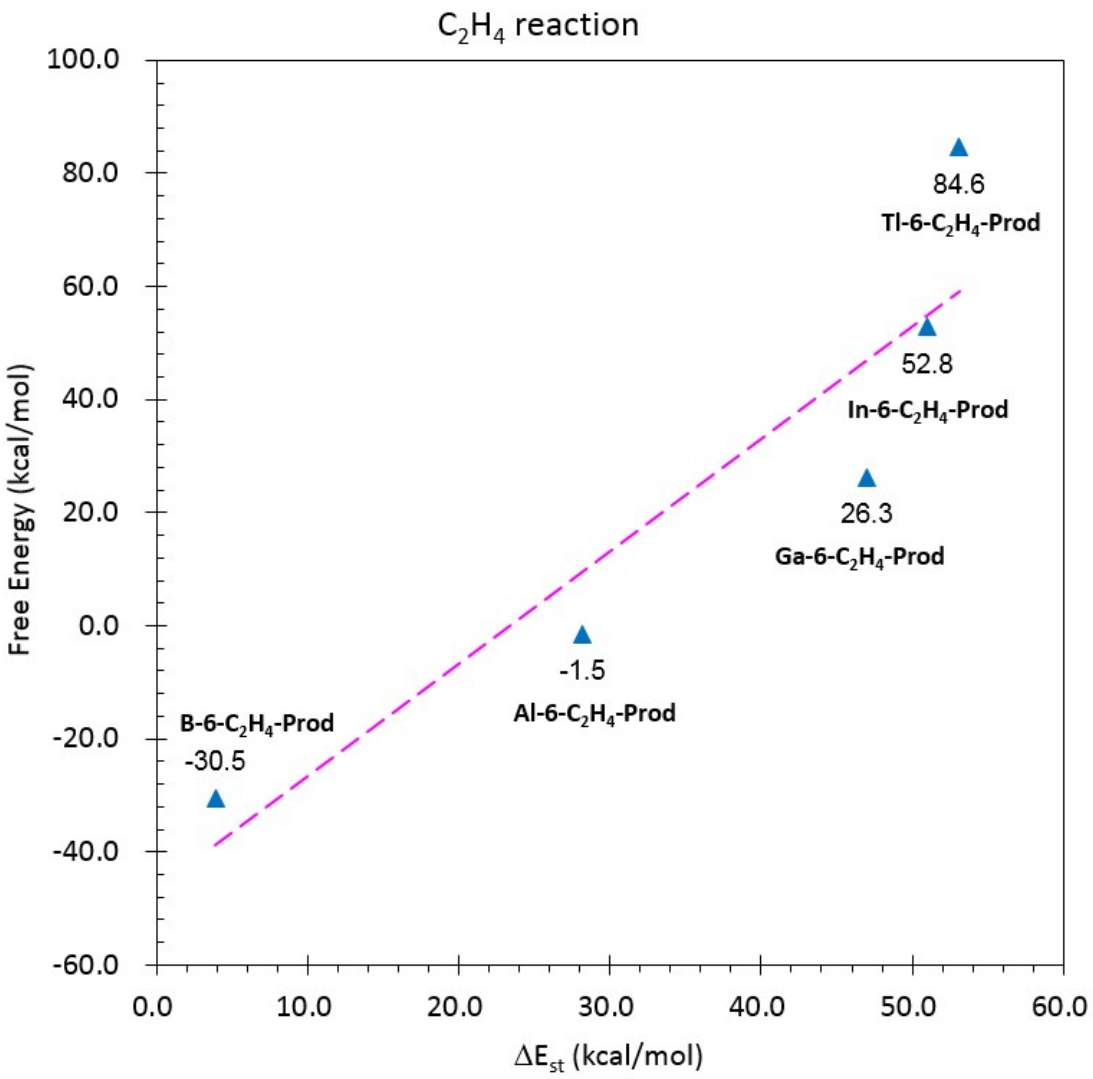

Figure S11. The Gibbs free reaction enthalpy energy ($\Delta G_{REA,C2H4}$) vs. the ΔE_{st}. The linear regression equation is $\Delta G_{REA,C2H4} = 1.988\Delta E_{st} - 46.50$ (the correlation coefficient r = 0.9181). All were calculated at the BP86-D3(BJ)/def2-TZVP level of theory.

Table S1. E_{HOMO} and E_{LUMO} (in eV) represent the energies of the highest occupied molecular orbital and the lowest unoccupied molecular orbital, respectively. μ, η and ω represent the electronic chemical potential, the chemical hardness, and electrophilicity index of **G13-6-Rea**, whose definitions can be obtained from eq.(3), eq.(4), and eq.(5) in the text, respectively. The calculations were performed at the BP86-D3(BJ)/def2-TZVP level of theory.

Table S2. Values of the Fukui function at the carbenic atom (G13) for **G13-6-Rea** calculated through eqs. (a), (b), and (c). The calculations were performed at the BP86-D3(BJ)/def2-TZVP level of theory.

Table S3-S34. Cartesian coordinates of the reactants, transition states, and products for the reaction of **G13-6-Rea** (G13 = B, Al, Ga, In, and Tl) with CH_4 and C_2H_4 at the BP86-D3(BJ)/def2-TZVP level of theory.

Table S1

E_{HOMO} and E_{LUMO} (in eV) represent the energies of the highest occupied molecular orbital and the lowest unoccupied molecular orbital, respectively. μ, η and ω represent the electronic chemical potential, the chemical hardness, and electrophilicity index of **G13-6-Rea**, whose definitions can be obtained from eq.(3), eq.(4), and eq.(5) in the text, respectively. The calculations were performed at the BP86-D3(BJ)/def2-TZVP level of theory.

	B-6-Rea	**Al-6-Rea**	**Ga-6-Rea**	**In-6-Rea**	**Tl-6-Rea**
E_{HOMO}	-3.453	-3.680	-4.456	-4.730	-4.515
E_{LUMO}	-2.097	-2.199	-1.924	-1.730	-1.631
μ	1.356	1.481	2.532	2.884	3.002
η	2.775	2.940	3.190	3.073	3.230
ω	2.551	3.224	10.23	12.78	14.54

Table S2

Values of the Fukui function at the carbenic atom (G13) for **G13-6-Rea** calculated through eqs. (a), (b), and (c). The calculations were performed at the BP86-D3(BJ)/def2-TZVP level of theory.

	B-6-Rea	**Al-6-Rea**	**Ga-6-Rea**	**In-6-Rea**	**Tl-6-Rea**
$q_k(N-1)$	0.591	0.663	0.621	0.650	0.651
$q_k(N)$	0.356	0.543	0.480	0.714	-0.236
$q_k(N+1)$	0.921	1.34	1.11	0.916	0.798
f_k^+	-0.235	-0.141	-0.120	-0.266	-0.888
f_k^-	-0.329	-0.703	-0.489	0.065	-0.147
f_k^0	-0.282	-0.142	-0.315	-0.101	-0.517

For nucleophilic attack: $$f_k^+ = q_k(N+1) - q_k(N) \quad \text{(a)}$$

For electrophilic attack: $$f_k^- = q_k(N) - q_k(N-1) \quad \text{(b)}$$

For radical attack: $$f_k^0 = \frac{1}{2}[f_k^+ + f_k^-] \quad \text{(c)}$$

Table S3-S34. Cartesian coordinates of the reactants, transition states, and products for the reaction of **G13-6-Rea** (G13 = B, Al, Ga, In, and Tl) with CH_4 and C_2H_4 at BP86-D3(BJ)/def2-TZVP level of theory.

Table S3

B-6-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.43220900	0.19445000	1.30380900
H	-1.95739400	0.90822000	1.94104500
C	-0.89206400	-0.95866900	1.86450000
H	-0.71750900	-1.05769600	2.93848900
C	-1.31179200	0.44947300	-0.05865700
H	-1.94690100	1.17389200	-0.57402800
N	-0.38569300	-0.28954700	-0.78061400
N	-0.51869200	-1.98569300	1.00958000
B	-0.10856800	-1.60449300	-0.30230600
C	-0.59954000	-3.40225700	1.48586100
C	0.28137900	0.32962600	-1.96875700
C	-0.41845200	-4.33480500	0.28738700
H	-0.51322900	-5.37759800	0.62536200
H	0.56411000	-4.19324300	-0.18284500
H	-1.18477500	-4.14400700	-0.47876800
C	-1.98371400	-3.63671900	2.11305300
H	-2.07288100	-4.68106900	2.44513500
H	-2.77722900	-3.43373100	1.37911600
H	-2.14917200	-2.98445700	2.98168700
C	0.51451700	-3.64856800	2.51570800
H	1.49648300	-3.45869700	2.05902900
H	0.48639900	-4.68953300	2.86998200
H	0.40605000	-2.99300100	3.39230600
C	-0.74029500	0.44846900	-3.11080800
H	-1.12959500	-0.54632900	-3.37094800
H	-0.26938900	0.88672200	-4.00304600
H	-1.58765000	1.09073000	-2.82901400
C	1.44513800	-0.56403200	-2.39988700
H	1.96152100	-0.09645000	-3.25155000
H	1.09354100	-1.56282400	-2.69207300
H	2.16748200	-0.69199700	-1.57984500
C	0.81874700	1.71422700	-1.57095900

H	1.52872000	1.62508500	-0.73577200
H	0.00850700	2.38718500	-1.25800200
H	1.33780100	2.17430400	-2.42408500

Table S4

Al-6-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.31247200	0.01994400	1.14535200
H	-1.83908000	0.73158600	1.77957300
C	-1.18793800	-1.28801300	1.61612400
H	-1.63899200	-1.47855000	2.59928000
C	-0.81701600	0.49052600	-0.07157600
H	-1.00918900	1.55195200	-0.27842100
N	-0.14862400	-0.21121200	-0.98237800
N	-0.58761900	-2.30132400	0.99835700
Al	0.31924900	-2.18283200	-0.81721500
C	-0.60983700	-3.60729200	1.75624000
C	0.26533700	0.57152700	-2.20563600
C	0.09578900	-4.70347400	0.94660200
H	0.06524900	-5.64346100	1.51875500
H	1.14714200	-4.45081300	0.74656400
H	-0.39146900	-4.87064400	-0.02498200
C	-2.06735900	-4.04494700	1.99164500
H	-2.09055900	-5.02069600	2.49884500
H	-2.59372300	-4.14055700	1.03087400
H	-2.62069700	-3.32997000	2.61692400
C	0.13488100	-3.43886300	3.09338000
H	1.16884100	-3.11126900	2.91178200
H	0.16383500	-4.39700000	3.63295300
H	-0.34961000	-2.70018600	3.74772400
C	-0.98680200	1.10861600	-2.92294200
H	-1.65066500	0.27662100	-3.19932700
H	-0.69660400	1.64092700	-3.84075300
H	-1.55656300	1.80888700	-2.29566200

C	1.02819700	-0.33365300	-3.18220000
H	1.31890700	0.25894200	-4.06321400
H	0.41309100	-1.18070900	-3.51894700
H	1.93809200	-0.75031700	-2.72640600
C	1.19649100	1.72539300	-1.78986600
H	2.07628300	1.33008000	-1.26168300
H	0.69484100	2.44687600	-1.12939200
H	1.54224400	2.27087100	-2.68028500

Table S5

Ga-6-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.29465700	-0.00333300	1.12477000
H	-1.82087900	0.70876100	1.75960400
C	-1.17960400	-1.30903800	1.61158800
H	-1.63916700	-1.47435100	2.59736400
C	-0.80502600	0.48510300	-0.09045700
H	-1.00884400	1.55060400	-0.27339200
N	-0.13807200	-0.18496800	-1.01955300
N	-0.58974500	-2.34040200	1.02380500
Ga	0.36442600	-2.24853900	-0.87642900
C	-0.61826900	-3.63186100	1.78709300
C	0.26764500	0.60390200	-2.22964700
C	0.09084100	-4.72556200	0.97778400
H	0.06583800	-5.66951300	1.54241400
H	1.14215600	-4.46827100	0.78319800
H	-0.39798200	-4.89192000	0.00680400
C	-2.07640900	-4.06970000	2.02232800
H	-2.10368400	-5.04151200	2.53722600
H	-2.60118600	-4.17028600	1.06111000
H	-2.62849300	-3.34718500	2.64005300
C	0.12102200	-3.46194400	3.12784000
H	1.15580200	-3.13436900	2.95043100

H	0.14685400	-4.41735100	3.67271400
H	-0.36719600	-2.71925500	3.77476900
C	-0.98436000	1.14678100	-2.94425300
H	-1.65040200	0.31732100	-3.22332100
H	-0.69703300	1.68556200	-3.85938700
H	-1.55114100	1.84229700	-2.30907600
C	1.02760600	-0.30331600	-3.20606000
H	1.32226800	0.28074800	-4.09066100
H	0.40710500	-1.14709800	-3.54127800
H	1.93746900	-0.71826200	-2.74854300
C	1.19906100	1.75814600	-1.81322400
H	2.08080800	1.36235600	-1.28849600
H	0.69570300	2.47247600	-1.14628900
H	1.54120000	2.31094700	-2.70074000

Table S6

In-6-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.23269900	-0.08153900	1.05601800
H	-1.75771700	0.63159500	1.69222900
C	-1.13678200	-1.38054800	1.57417100
H	-1.61160800	-1.49320900	2.56188000
C	-0.75634300	0.44144300	-0.15417200
H	-0.98430700	1.51097800	-0.28788600
N	-0.08992100	-0.16469000	-1.12387300
N	-0.56769500	-2.45273800	1.04656900
In	0.50058000	-2.43880200	-1.04747300
C	-0.63868400	-3.70193700	1.86691500
C	0.27738800	0.68781000	-2.29726700
C	0.06354700	-4.83743100	1.11245800
H	0.01930600	-5.76358700	1.70413100
H	1.12277900	-4.60217600	0.92839500
H	-0.41661400	-5.03129500	0.14135400

C	-2.10823000	-4.10536200	2.09484900
H	-2.16508900	-5.05319100	2.65087800
H	-2.61879600	-4.23631000	1.12942000
H	-2.65537800	-3.34487900	2.66962100
C	0.08120800	-3.49461500	3.21344400
H	1.12471900	-3.19200600	3.04193900
H	0.07999800	-4.42688900	3.79797400
H	-0.40425200	-2.71682100	3.81962000
C	-0.99342300	1.23715000	-2.97369200
H	-1.64912100	0.40783800	-3.27731900
H	-0.73107300	1.82020200	-3.86924300
H	-1.56274800	1.89308200	-2.30013800
C	1.03850100	-0.16629900	-3.31847400
H	1.31534600	0.44771800	-4.18804500
H	0.42384200	-1.00576800	-3.67717900
H	1.96242400	-0.57996000	-2.88669200
C	1.19431100	1.84198400	-1.84851300
H	2.09134100	1.44188700	-1.35337100
H	0.68675400	2.51483100	-1.14297300
H	1.51208700	2.44050100	-2.71546400

Table S7

Tl-6-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.21362200	-0.10829800	1.03208600
H	-1.73861900	0.60525100	1.66861800
C	-1.12539900	-1.40472400	1.56422000
H	-1.60653200	-1.49525300	2.55266500
C	-0.74232900	0.42973000	-0.17619200
H	-0.98042400	1.50081400	-0.28930000
N	-0.07685500	-0.14939300	-1.16021100
N	-0.56527600	-2.49125100	1.06206100
Tl	0.55300600	-2.51580600	-1.11742200

C	-0.64701600	-3.72515400	1.89630500
C	0.27996800	0.71876400	-2.31964900
C	0.05402300	-4.86769600	1.15103200
H	0.01014800	-5.79297500	1.74386500
H	1.11396000	-4.63238900	0.96948200
H	-0.42784400	-5.06438200	0.18104100
C	-2.11859100	-4.12182400	2.12449300
H	-2.18283200	-5.06359100	2.69030400
H	-2.62705600	-4.25902700	1.15870200
H	-2.66260200	-3.35149900	2.68908900
C	0.06934800	-3.50976500	3.24372600
H	1.11441000	-3.21192100	3.07263000
H	0.06267100	-4.43566200	3.83861100
H	-0.41567400	-2.72316100	3.83882700
C	-0.99391100	1.27067900	-2.98871600
H	-1.64774300	0.44180700	-3.29790300
H	-0.73767400	1.86461000	-3.87909900
H	-1.56303500	1.91635500	-2.30512400
C	1.04147100	-0.12614800	-3.34851000
H	1.31836500	0.48913500	-4.21701100
H	0.42484600	-0.96328200	-3.71009900
H	1.96669400	-0.53860100	-2.91767200
C	1.19372800	1.87285800	-1.86352200
H	2.09319900	1.47149800	-1.37361700
H	0.68370100	2.53456000	-1.14925000
H	1.50715000	2.48270700	-2.72437500

Table S8

B-6-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.57403600	0.68681900	0.02627600
C	-0.33668600	-0.25705500	2.30743100

H	0.04438300	-0.16536700	0.79219400
N	-0.12942300	2.09578500	-0.00746700
N	-1.99885100	0.43953900	-0.21173000
C	1.27477500	2.47709200	-0.36603800
C	-1.05552400	3.02027200	0.42214100
C	-2.60348900	-0.92595500	-0.47484000
C	-2.84078100	1.51867400	-0.24856200
C	1.37466300	3.98210100	-0.68756700
C	2.22626600	2.13224500	0.80302000
C	1.66284300	1.66639500	-1.62044400
C	-2.41349100	2.77251500	0.22977000
H	-0.71527600	3.96282900	0.88428000
C	-3.73395200	-1.19950800	0.54126600
C	-1.53893800	-2.03126400	-0.36341300
C	-3.15969200	-0.93710300	-1.91889400
H	-3.86472000	1.37791700	-0.62596400
H	2.38276800	4.20334900	-1.09341400
H	1.23789200	4.62076800	0.20902200
H	0.62555400	4.28374800	-1.44859500
H	2.20707200	1.04536800	1.01864400
H	3.27075600	2.41850600	0.55781100
H	1.93015500	2.67215300	1.72672100
H	1.06871800	1.99096800	-2.49971800
H	1.46430400	0.58690800	-1.44817600
H	2.73932400	1.79741200	-1.85354100
H	-3.15238600	3.56036600	0.43724000
H	-4.18304500	-2.19602100	0.35248500
H	-3.34152000	-1.18859600	1.57819700
H	-4.54516800	-0.44676200	0.47514800
H	-0.69110300	-1.84342400	-1.05149500
H	-2.00387400	-3.00172000	-0.63145300
H	-1.13679600	-2.11468500	0.66315600
H	-3.58253800	-1.93509500	-2.15608300
H	-3.96549300	-0.18992900	-2.06855400
H	-2.35047700	-0.72130600	-2.64653200
H	0.39913800	-1.05642400	2.52157300
H	-0.05044600	0.70410200	2.77105300
H	-1.36925400	-0.55596700	2.56208200

Table S9

Al-6-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.16039600	0.17046000	-0.01587400
C	0.00244700	0.06481400	2.36948600
H	0.68676700	-0.69880900	1.02489700
N	0.02885400	2.12252100	-0.06022500
N	-2.12056700	0.09185900	-0.00569100
C	1.31570400	2.73238500	-0.54099900
C	-0.98307300	2.88045900	0.36281900
C	-2.81453000	-1.17020900	-0.43518100
C	-2.80860100	1.15571000	0.40926900
C	1.36408200	4.26426700	-0.39023100
C	2.46765500	2.10504300	0.27587800
C	1.46946600	2.36204400	-2.03492300
C	-2.28621500	2.43896400	0.67427700
H	-0.81081600	3.96876400	0.45423600
C	-4.34253100	-1.12569600	-0.24822000
C	-2.23436300	-2.33372900	0.40000000
C	-2.49006900	-1.38589800	-1.93210000
H	-3.90201400	1.04824200	0.53320300
H	2.34639900	4.62646900	-0.75449400
H	1.26638100	4.58546900	0.66782900
H	0.58285300	4.77551400	-0.99034200
H	2.45563300	0.99712300	0.18096600
H	3.44968800	2.46789100	-0.09193400
H	2.37655000	2.36347200	1.35071900
H	0.65619100	2.81498600	-2.63916100
H	1.42510000	1.25834300	-2.16511500
H	2.44298100	2.71960100	-2.43023000
H	-2.99356800	3.19747200	1.03823400
H	-4.76924400	-2.09457500	-0.57685800

H	-4.63188100	-0.98185100	0.81375700
H	-4.82243500	-0.33206600	-0.85785200
H	-1.13045600	-2.38958200	0.27829100
H	-2.66304300	-3.30264100	0.07016300
H	-2.45944700	-2.19740400	1.47755100
H	-2.91092400	-2.34818300	-2.29087900
H	-2.91146500	-0.56531000	-2.54913300
H	-1.38903700	-1.40747200	-2.08858100
H	-0.34658400	-0.87299100	2.84557500
H	0.97076000	0.37750800	2.80829000
H	-0.75459900	0.86668800	2.51961200

Table S10

Ga-6-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.14696100	0.15548100	-0.05428600
C	0.02931500	0.03537600	2.36454300
H	0.72995400	-0.74945200	0.85839600
N	0.03777200	2.15127300	-0.07307300
N	-2.15005600	0.08449500	-0.01773900
C	1.33026700	2.75475100	-0.52854300
C	-0.99199900	2.89519500	0.32050000
C	-2.83730400	-1.18289800	-0.42193500
C	-2.82390800	1.16460100	0.36681900
C	1.37758300	4.28643700	-0.36589400
C	2.46918100	2.12386600	0.30369300
C	1.51007700	2.39648700	-2.02274800
C	-2.29844600	2.45043100	0.61350100
H	-0.83052400	3.98616400	0.40369000
C	-4.36462100	-1.13768500	-0.22174300
C	-2.25130700	-2.33325500	0.42723500
C	-2.52774300	-1.42326600	-1.91850100

H	-3.91963000	1.06790500	0.48198400
H	2.36754200	4.65060200	-0.70677200
H	1.25658700	4.59884700	0.69228400
H	0.60937500	4.80242900	-0.97840700
H	2.47038000	1.01900600	0.19595200
H	3.45539500	2.49995000	-0.03850800
H	2.35313600	2.36698400	1.37944000
H	0.70623100	2.85366700	-2.63624900
H	1.46848400	1.29536000	-2.16447700
H	2.48898600	2.75991700	-2.39896600
H	-3.01173700	3.21461700	0.95342300
H	-4.79299400	-2.11351400	-0.52681300
H	-4.64301600	-0.97167400	0.83982300
H	-4.85122400	-0.35707100	-0.84255200
H	-1.15161000	-2.40198200	0.29220400
H	-2.69265900	-3.30492100	0.12352900
H	-2.45875900	-2.17326000	1.50480400
H	-2.95455100	-2.38999900	-2.25783000
H	-2.95485800	-0.61195100	-2.54372100
H	-1.42992800	-1.44764200	-2.08754700
H	-0.30304100	-0.92484900	2.80634100
H	1.01798300	0.32855100	2.76981800
H	-0.71971700	0.83067700	2.56535400

Table S11

In-6-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.00553800	-0.00722000	-0.12893000
C	0.18951800	-0.13238400	2.43811100
H	0.99462500	-1.02896100	0.79887600
N	0.10168000	2.21231300	-0.14981000
N	-2.21598600	0.02170400	-0.09005700

C	1.38909800	2.86962900	-0.52343900
C	-0.98203500	2.90615500	0.17814600
C	-2.95488600	-1.23509000	-0.41202500
C	-2.83883400	1.15115500	0.22582800
C	1.37815300	4.39910400	-0.32313700
C	2.50620900	2.25965000	0.35274400
C	1.66123700	2.55709000	-2.01425700
C	-2.29310000	2.43939200	0.42017500
H	-0.86786700	4.00478700	0.25846500
C	-4.47532700	-1.13156500	-0.17298800
C	-2.38559700	-2.36271200	0.47792200
C	-2.69882100	-1.56235600	-1.90251800
H	-3.93955200	1.10166800	0.33729400
H	2.37344700	4.80376700	-0.59612600
H	1.18313800	4.67929800	0.73287900
H	0.63004300	4.90515000	-0.96764600
H	2.56351100	1.15850400	0.21709000
H	3.49499100	2.68075700	0.07674000
H	2.32260900	2.46459800	1.42693700
H	0.87094200	2.99549000	-2.65809000
H	1.67417400	1.45964800	-2.18795400
H	2.64189000	2.96882400	-2.33208000
H	-3.01851000	3.21471900	0.70732000
H	-4.94285800	-2.10875000	-0.40836000
H	-4.71519700	-0.89377000	0.88419300
H	-4.95568700	-0.37251200	-0.82434100
H	-1.29340100	-2.48582800	0.31624300
H	-2.86881700	-3.33254700	0.23891000
H	-2.55138800	-2.14090600	1.55167300
H	-3.17455200	-2.52520200	-2.18328100
H	-3.10860400	-0.76447900	-2.55578200
H	-1.60904100	-1.64324600	-2.10389100
H	-0.14696100	-1.09520400	2.87074700
H	1.18281800	0.15219800	2.83786500
H	-0.55494500	0.66678400	2.64358200

Table S12

Tl-6-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.05304300	-0.05643400	-0.14857100
C	0.29526600	-0.24438400	2.44783200
H	1.10307500	-1.15358700	0.57458100
N	0.10242600	2.24562000	-0.16371000
N	-2.24939500	0.02260300	-0.10296700
C	1.39274900	2.90569400	-0.51110800
C	-0.99858400	2.92628200	0.12250100
C	-2.99037700	-1.23650800	-0.39779500
C	-2.85948300	1.16722600	0.17031700
C	1.36142900	4.43813100	-0.32568200
C	2.49398000	2.32023600	0.40105700
C	1.70815900	2.58541800	-1.99177800
C	-2.31259400	2.45786000	0.34022200
H	-0.89556700	4.02762800	0.18748000
C	-4.51317600	-1.11276400	-0.17527200
C	-2.44416400	-2.34504800	0.52969700
C	-2.72782100	-1.60836700	-1.87670900
H	-3.96272800	1.12875900	0.26618100
H	2.35955400	4.85005000	-0.57651300
H	1.13534100	4.72543300	0.72208800
H	0.62529500	4.92969200	-0.99453600
H	2.57819200	1.22055100	0.27518200
H	3.48203500	2.75995100	0.15298700
H	2.27339000	2.52504900	1.46814600
H	0.92981000	3.00950000	-2.65921000
H	1.73822100	1.48789300	-2.15885500
H	2.69156400	3.00789400	-2.28620100
H	-3.04456900	3.23918100	0.59276000
H	-4.98735000	-2.09200300	-0.38764000
H	-4.75935000	-0.84279000	0.87258300
H	-4.97997800	-0.36776300	-0.85203100
H	-1.35442800	-2.49414000	0.38000500

H	-2.94445300	-3.31280500	0.31919500
H	-2.60930000	-2.08583500	1.59499800
H	-3.21375400	-2.57286200	-2.13336400
H	-3.12414600	-0.82427500	-2.55441100
H	-1.63865600	-1.70647300	-2.07027300
H	-0.01852000	-1.23034400	2.84626900
H	1.30934200	0.01607600	2.81274800
H	-0.43282300	0.53930800	2.74682900

Table S13

B-6-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.57403600	0.68681900	0.02627600
C	-0.33668600	-0.25705500	2.30743100
H	0.04438300	-0.16536700	0.79219400
N	-0.12942300	2.09578500	-0.00746700
N	-1.99885100	0.43953900	-0.21173000
C	1.27477500	2.47709200	-0.36603800
C	-1.05552400	3.02027200	0.42214100
C	-2.60348900	-0.92595500	-0.47484000
C	-2.84078100	1.51867400	-0.24856200
C	1.37466300	3.98210100	-0.68756700
C	2.22626600	2.13224500	0.80302000
C	1.66284300	1.66639500	-1.62044400
C	-2.41349100	2.77251500	0.22977000
H	-0.71527600	3.96282900	0.88428000
C	-3.73395200	-1.19950800	0.54126600
C	-1.53893800	-2.03126400	-0.36341300
C	-3.15969200	-0.93710300	-1.91889400
H	-3.86472000	1.37791700	-0.62596400
H	2.38276800	4.20334900	-1.09341400
H	1.23789200	4.62076800	0.20902200

H	0.62555400	4.28374800	-1.44859500
H	2.20707200	1.04536800	1.01864400
H	3.27075600	2.41850600	0.55781100
H	1.93015500	2.67215300	1.72672100
H	1.06871800	1.99096800	-2.49971800
H	1.46430400	0.58690800	-1.44817600
H	2.73932400	1.79741200	-1.85354100
H	-3.15238600	3.56036600	0.43724000
H	-4.18304500	-2.19602100	0.35248500
H	-3.34152000	-1.18859600	1.57819700
H	-4.54516800	-0.44676200	0.47514800
H	-0.69110300	-1.84342400	-1.05149500
H	-2.00387400	-3.00172000	-0.63145300
H	-1.13679600	-2.11468500	0.66315600
H	-3.58253800	-1.93509500	-2.15608300
H	-3.96549300	-0.18992900	-2.06855400
H	-2.35047700	-0.72130600	-2.64653200
H	0.39913800	-1.05642400	2.52157300
H	-0.05044600	0.70410200	2.77105300
H	-1.36925400	-0.55596700	2.56208200

Table S14

Al-6-CH_4- Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.16039600	0.17046000	-0.01587400
C	0.00244700	0.06481400	2.36948600
H	0.68676700	-0.69880900	1.02489700
N	0.02885400	2.12252100	-0.06022500
N	-2.12056700	0.09185900	-0.00569100
C	1.31570400	2.73238500	-0.54099900
C	-0.98307300	2.88045900	0.36281900
C	-2.81453000	-1.17020900	-0.43518100

C	-2.80860100	1.15571000	0.40926900
C	1.36408200	4.26426700	-0.39023100
C	2.46765500	2.10504300	0.27587800
C	1.46946600	2.36204400	-2.03492300
C	-2.28621500	2.43896400	0.67427700
H	-0.81081600	3.96876400	0.45423600
C	-4.34253100	-1.12569600	-0.24822000
C	-2.23436300	-2.33372900	0.40000000
C	-2.49006900	-1.38589800	-1.93210000
H	-3.90201400	1.04824200	0.53320300
H	2.34639900	4.62646900	-0.75449400
H	1.26638100	4.58546900	0.66782900
H	0.58285300	4.77551400	-0.99034200
H	2.45563300	0.99712300	0.18096600
H	3.44968800	2.46789100	-0.09193400
H	2.37655000	2.36347200	1.35071900
H	0.65619100	2.81498600	-2.63916100
H	1.42510000	1.25834300	-2.16511500
H	2.44298100	2.71960100	-2.43023000
H	-2.99356800	3.19747200	1.03823400
H	-4.76924400	-2.09457500	-0.57685800
H	-4.63188100	-0.98185100	0.81375700
H	-4.82243500	-0.33206600	-0.85785200
H	-1.13045600	-2.38958200	0.27829100
H	-2.66304300	-3.30264100	0.07016300
H	-2.45944700	-2.19740400	1.47755100
H	-2.91092400	-2.34818300	-2.29087900
H	-2.91146500	-0.56531000	-2.54913300
H	-1.38903700	-1.40747200	-2.08858100
H	-0.34658400	-0.87299100	2.84557500
H	0.97076000	0.37750800	2.80829000
H	-0.75459900	0.86668800	2.51961200

Table S15

Ga-6-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.14696100	0.15548100	-0.05428600
C	0.02931500	0.03537600	2.36454300
H	0.72995400	-0.74945200	0.85839600
N	0.03777200	2.15127300	-0.07307300
N	-2.15005600	0.08449500	-0.01773900
C	1.33026700	2.75475100	-0.52854300
C	-0.99199900	2.89519500	0.32050000
C	-2.83730400	-1.18289800	-0.42193500
C	-2.82390800	1.16460100	0.36681900
C	1.37758300	4.28643700	-0.36589400
C	2.46918100	2.12386600	0.30369300
C	1.51007700	2.39648700	-2.02274800
C	-2.29844600	2.45043100	0.61350100
H	-0.83052400	3.98616400	0.40369000
C	-4.36462100	-1.13768500	-0.22174300
C	-2.25130700	-2.33325500	0.42723500
C	-2.52774300	-1.42326600	-1.91850100
H	-3.91963000	1.06790500	0.48198400
H	2.36754200	4.65060200	-0.70677200
H	1.25658700	4.59884700	0.69228400
H	0.60937500	4.80242900	-0.97840700
H	2.47038000	1.01900600	0.19595200
H	3.45539500	2.49995000	-0.03850800
H	2.35313600	2.36698400	1.37944000
H	0.70623100	2.85366700	-2.63624900
H	1.46848400	1.29536000	-2.16447700
H	2.48898600	2.75991700	-2.39896600
H	-3.01173700	3.21461700	0.95342300
H	-4.79299400	-2.11351400	-0.52681300
H	-4.64301600	-0.97167400	0.83982300
H	-4.85122400	-0.35707100	-0.84255200
H	-1.15161000	-2.40198200	0.29220400
H	-2.69265900	-3.30492100	0.12352900
H	-2.45875900	-2.17326000	1.50480400

H	-2.95455100	-2.38999900	-2.25783000
H	-2.95485800	-0.61195100	-2.54372100
H	-1.42992800	-1.44764200	-2.08754700
H	-0.30304100	-0.92484900	2.80634100
H	1.01798300	0.32855100	2.76981800
H	-0.71971700	0.83067700	2.56535400

Table S16

In-6-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.00553800	-0.00722000	-0.12893000
C	0.18951800	-0.13238400	2.43811100
H	0.99462500	-1.02896100	0.79887600
N	0.10168000	2.21231300	-0.14981000
N	-2.21598600	0.02170400	-0.09005700
C	1.38909800	2.86962900	-0.52343900
C	-0.98203500	2.90615500	0.17814600
C	-2.95488600	-1.23509000	-0.41202500
C	-2.83883400	1.15115500	0.22582800
C	1.37815300	4.39910400	-0.32313700
C	2.50620900	2.25965000	0.35274400
C	1.66123700	2.55709000	-2.01425700
C	-2.29310000	2.43939200	0.42017500
H	-0.86786700	4.00478700	0.25846500
C	-4.47532700	-1.13156500	-0.17298800
C	-2.38559700	-2.36271200	0.47792200
C	-2.69882100	-1.56235600	-1.90251800
H	-3.93955200	1.10166800	0.33729400
H	2.37344700	4.80376700	-0.59612600
H	1.18313800	4.67929800	0.73287900
H	0.63004300	4.90515000	-0.96764600
H	2.56351100	1.15850400	0.21709000

H	3.49499100	2.68075700	0.07674000
H	2.32260900	2.46459800	1.42693700
H	0.87094200	2.99549000	-2.65809000
H	1.67417400	1.45964800	-2.18795400
H	2.64189000	2.96882400	-2.33208000
H	-3.01851000	3.21471900	0.70732000
H	-4.94285800	-2.10875000	-0.40836000
H	-4.71519700	-0.89377000	0.88419300
H	-4.95568700	-0.37251200	-0.82434100
H	-1.29340100	-2.48582800	0.31624300
H	-2.86881700	-3.33254700	0.23891000
H	-2.55138800	-2.14090600	1.55167300
H	-3.17455200	-2.52520200	-2.18328100
H	-3.10860400	-0.76447900	-2.55578200
H	-1.60904100	-1.64324600	-2.10389100
H	-0.14696100	-1.09520400	2.87074700
H	1.18281800	0.15219800	2.83786500
H	-0.55494500	0.66678400	2.64358200

Table S17

Tl-6-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.05304300	-0.05643400	-0.14857100
C	0.29526600	-0.24438400	2.44783200
H	1.10307500	-1.15358700	0.57458100
N	0.10242600	2.24562000	-0.16371000
N	-2.24939500	0.02260300	-0.10296700
C	1.39274900	2.90569400	-0.51110800
C	-0.99858400	2.92628200	0.12250100
C	-2.99037700	-1.23650800	-0.39779500
C	-2.85948300	1.16722600	0.17031700
C	1.36142900	4.43813100	-0.32568200

C	2.49398000	2.32023600	0.40105700
C	1.70815900	2.58541800	-1.99177800
C	-2.31259400	2.45786000	0.34022200
H	-0.89556700	4.02762800	0.18748000
C	-4.51317600	-1.11276400	-0.17527200
C	-2.44416400	-2.34504800	0.52969700
C	-2.72782100	-1.60836700	-1.87670900
H	-3.96272800	1.12875900	0.26618100
H	2.35955400	4.85005000	-0.57651300
H	1.13534100	4.72543300	0.72208800
H	0.62529500	4.92969200	-0.99453600
H	2.57819200	1.22055100	0.27518200
H	3.48203500	2.75995100	0.15298700
H	2.27339000	2.52504900	1.46814600
H	0.92981000	3.00950000	-2.65921000
H	1.73822100	1.48789300	-2.15885500
H	2.69156400	3.00789400	-2.28620100
H	-3.04456900	3.23918100	0.59276000
H	-4.98735000	-2.09200300	-0.38764000
H	-4.75935000	-0.84279000	0.87258300
H	-4.97997800	-0.36776300	-0.85203100
H	-1.35442800	-2.49414000	0.38000500
H	-2.94445300	-3.31280500	0.31919500
H	-2.60930000	-2.08583500	1.59499800
H	-3.21375400	-2.57286200	-2.13336400
H	-3.12414600	-0.82427500	-2.55441100
H	-1.63865600	-1.70647300	-2.07027300
H	-0.01852000	-1.23034400	2.84626900
H	1.30934200	0.01607600	2.81274800
H	-0.43282300	0.53930800	2.74682900

Table S18

B-6-C_2H_4-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
C	-2.20257500	-1.10411300	-0.17240400
H	-3.29153200	-0.93625000	-0.17837900
C	-1.57909300	-1.58344200	0.97238300
H	-2.08490100	-1.58331500	1.95069500
C	-1.43050200	-0.75755300	-1.30785700
H	-1.89292700	-0.54998000	-2.28870200
N	-0.07631900	-0.57387300	-1.12776500
N	-0.26619400	-2.05348800	0.87973200
B	0.49132800	-1.55533000	-0.23838600
C	0.20164700	-3.07177700	1.88489300
C	0.68305500	0.45213700	-1.90672400
C	1.71199600	-3.31039500	1.71910500
H	2.04093700	-4.08977200	2.43757800
H	2.28643900	-2.38233100	1.91350600
H	1.96975100	-3.64804400	0.69743600
C	-0.57840900	-4.39033700	1.68002800
H	-0.30384400	-5.13353300	2.45701100
H	-0.36089800	-4.83406500	0.68746500
H	-1.67222300	-4.21572500	1.74304900
C	-0.04377300	-2.53578500	3.31589200
H	0.43250900	-1.54259100	3.44894300
H	0.39734800	-3.23320900	4.05713300
H	-1.12121400	-2.44302000	3.56071500
C	-0.00830900	1.82118200	-1.71803800
H	-1.05406300	1.80155700	-2.08686100
H	0.53642900	2.61072400	-2.27562600
H	-0.03206900	2.10315600	-0.64532200
C	0.70978500	0.07283200	-3.40479500
H	1.26717000	0.83548300	-3.98724500
H	-0.31216400	0.01122800	-3.83314200
H	1.20709700	-0.90673000	-3.55331200
C	2.11810700	0.52275300	-1.36072100
H	2.63859900	-0.44999900	-1.46872700
H	2.12153800	0.78626000	-0.28251200
H	2.68823200	1.29994000	-1.91014300
C	-0.67603000	-3.51903800	-2.19043900

H	-1.42022400	-4.03334900	-1.56172600
H	-1.05668300	-3.03547500	-3.10402800
C	0.64702600	-3.49030800	-1.86416700
H	1.40130500	-3.05864300	-2.53988800
H	1.04292000	-4.08979600	-1.03063700

Table S19

Al-6-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.24042800	-1.27437200	-0.24545100
H	-3.32610200	-1.10628000	-0.19896200
C	-1.70180800	-2.20963600	0.66273800
H	-2.41195700	-2.62220200	1.40396400
C	-1.49020100	-0.37461000	-1.03105000
H	-2.05458500	0.47671600	-1.45604900
N	-0.17714800	-0.42885400	-1.25733000
N	-0.42643200	-2.59147100	0.73976900
Al	0.79941800	-2.04752700	-0.70350400
C	0.07755800	-3.37003300	1.92211700
C	0.55053300	0.73439400	-1.87016900
C	0.88400300	-4.57506700	1.39012000
H	1.32831800	-5.14995600	2.22869700
H	1.71366300	-4.22558200	0.73803600
H	0.23758900	-5.25761300	0.80067100
C	-1.04546300	-3.88657700	2.84230500
H	-0.59157100	-4.48311200	3.65903000
H	-1.75507500	-4.54810700	2.30270300
H	-1.61943700	-3.06519500	3.31884800
C	1.01068300	-2.43523100	2.72716500
H	1.82141000	-2.04759900	2.07196100
H	1.47739800	-2.97709100	3.57624200
H	0.44707700	-1.56827800	3.12996100

C	-0.38806100	1.82049900	-2.43063700
H	-1.06833100	1.42073200	-3.21151000
H	0.22587700	2.61493000	-2.90060500
H	-1.00003100	2.30507200	-1.64204100
C	1.43271300	0.19351200	-3.01676600
H	2.03798100	1.00908700	-3.46355900
H	0.81184000	-0.26083500	-3.81627400
H	2.13250700	-0.57994200	-2.63231300
C	1.44771800	1.34971300	-0.77060300
H	2.12541900	0.57387900	-0.35156100
H	0.83184700	1.75560000	0.05853700
H	2.07046800	2.17160800	-1.18177400
C	-0.22152900	-3.41096400	-2.30625600
H	-0.85640400	-4.15969600	-1.80765500
H	-0.69822900	-2.78664200	-3.07778000
C	1.20738400	-3.45114400	-2.17130500
H	1.84277100	-2.99316800	-2.94988700
H	1.68788600	-4.33296700	-1.71180100

Table S20

Ga-6-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.30053100	-1.19937800	-0.17178000
H	-3.37748400	-0.99538300	-0.08526800
C	-1.76682800	-2.15275100	0.72133100
H	-2.46559400	-2.53085000	1.49125900
C	-1.55474800	-0.31275500	-0.97745800
H	-2.10891700	0.56294100	-1.36489200
N	-0.25791300	-0.39523000	-1.26549700
N	-0.51093800	-2.59177300	0.76331800
Ga	0.65504400	-2.10144800	-0.77981200
C	0.01761900	-3.37794200	1.92180900

C	0.49251800	0.74125000	-1.88577800
C	0.72102200	-4.63571100	1.36757600
H	1.16714700	-5.22910500	2.19205300
H	1.53853100	-4.34933700	0.67444900
H	0.00573800	-5.28070200	0.81739500
C	-1.08134800	-3.81375600	2.91123100
H	-0.61741400	-4.41563300	3.71830800
H	-1.85176700	-4.44773200	2.42485300
H	-1.58543100	-2.95136300	3.39423600
C	1.04521500	-2.48719300	2.65888800
H	1.83642700	-2.15151200	1.95493600
H	1.52792800	-3.04452300	3.48870100
H	0.55363900	-1.58594800	3.08020900
C	-0.42311000	1.89012500	-2.35275100
H	-1.16298900	1.55204200	-3.10792600
H	0.20072900	2.67410200	-2.82715900
H	-0.96750100	2.36861200	-1.51260900
C	1.27191100	0.19485600	-3.10154500
H	1.87883500	0.99715000	-3.56941500
H	0.57964300	-0.21350400	-3.86600000
H	1.96293300	-0.61417800	-2.78742800
C	1.48497800	1.27646400	-0.82696000
H	2.14251200	0.45584600	-0.46843400
H	0.94146300	1.68975800	0.04778700
H	2.12457100	2.07703300	-1.25382700
C	0.06083800	-3.47451700	-2.34039600
H	-0.46499200	-4.39211800	-2.02504400
H	-0.30818000	-3.03196400	-3.28162300
C	1.51653600	-3.38417300	-2.06072700
H	2.18177900	-2.88939900	-2.79070100
H	2.02739700	-4.22431300	-1.55728900

Table S21

In-6-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.22471500	-0.76836500	0.31518400
H	-3.23208000	-0.41369200	0.57802700
C	-1.75623700	-1.85900800	1.08098100
H	-2.44470900	-2.17963900	1.88639300
C	-1.54671300	0.01520500	-0.64504700
H	-2.09850400	0.91904900	-0.96768600
N	-0.34626500	-0.17550900	-1.18066600
N	-0.60851900	-2.51979500	0.97738100
In	0.72092700	-2.05273700	-0.72151800
C	-0.19139700	-3.55593800	1.96895800
C	0.29889500	0.83144200	-2.07519600
C	0.16905500	-4.84159500	1.19220700
H	0.52458400	-5.63065300	1.88659500
H	0.97947400	-4.65474900	0.45775900
H	-0.70953500	-5.22896800	0.63757700
C	-1.28675800	-3.89066000	3.00217800
H	-0.90873900	-4.68117900	3.68110300
H	-2.20883200	-4.27825000	2.52128900
H	-1.55591300	-3.01790800	3.63220500
C	1.05672600	-3.02083300	2.71020400
H	1.86074000	-2.76374400	1.98768800
H	1.45356400	-3.78073400	3.41523100
H	0.80911000	-2.10424900	3.28449400
C	-0.62039000	2.02036700	-2.42224800
H	-1.54300000	1.69522400	-2.94643800
H	-0.07683300	2.70668000	-3.10217000
H	-0.91013700	2.60688800	-1.52605700
C	0.70382600	0.11653900	-3.38342800
H	1.22563100	0.81799900	-4.06673400
H	-0.18698000	-0.28810700	-3.90528800
H	1.39333700	-0.72941900	-3.18369800
C	1.55966600	1.36135800	-1.35203200
H	2.23645900	0.52288500	-1.08063100
H	1.28243900	1.89113900	-0.41730100
H	2.12137100	2.06477000	-2.00137500

C	1.05408700	-3.57380600	-2.33548500
H	0.81127700	-4.64189400	-2.17508700
H	0.95906000	-3.30554800	-3.40532800
C	2.37035200	-3.10141800	-1.66404800
H	3.07061600	-2.48503900	-2.25854700
H	2.92433100	-3.82012200	-1.03142800

Table S22

Tl-6-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.95925800	-0.40925300	0.73783000
H	-2.83710200	0.09014900	1.17381900
C	-1.60282400	-1.62214900	1.36774100
H	-2.26547900	-1.90161200	2.21024000
C	-1.39254200	0.26275700	-0.36772400
H	-1.92034000	1.19678300	-0.64336300
N	-0.34255000	-0.05948300	-1.10969900
N	-0.61079300	-2.45873700	1.09802000
Tl	0.84500600	-1.96375800	-0.61114300
C	-0.38426800	-3.71959000	1.86126800
C	0.11272000	0.76133600	-2.26839900
C	-0.46835100	-4.89938800	0.86522500
H	-0.24564100	-5.86000700	1.37430100
H	0.25497200	-4.77393200	0.03272200
H	-1.48303400	-4.96434900	0.42115300
C	-1.41679800	-3.94502800	2.98625500
H	-1.18060700	-4.89764600	3.50161400
H	-2.45220700	-4.02741300	2.59577800
H	-1.38893200	-3.14001400	3.74949100
C	1.02715100	-3.65002400	2.48875600
H	1.80368700	-3.47942700	1.71447600
H	1.26930300	-4.59564900	3.01661600

H	1.09092200	-2.81533800	3.21687800
C	-0.74506100	2.02456400	-2.49466600
H	-1.80371000	1.77922300	-2.71905300
H	-0.34206100	2.57812100	-3.36648900
H	-0.71752200	2.71201100	-1.62401100
C	0.04052300	-0.12332100	-3.53467400
H	0.43116000	0.42255100	-4.41842200
H	-1.00716900	-0.42359600	-3.74250500
H	0.63707400	-1.05093000	-3.40965600
C	1.57291000	1.19402800	-2.00188800
H	2.22761800	0.31546400	-1.82533000
H	1.63135100	1.84136200	-1.10274500
H	1.97953600	1.75733900	-2.86720000
C	2.12368000	-3.28564500	-1.90025100
H	2.11537400	-4.38394200	-1.76082500
H	2.25950600	-3.03156100	-2.96909600
C	3.01992200	-2.46123400	-0.87683900
H	3.71497300	-1.72601600	-1.32645000
H	3.53813500	-3.06065700	-0.10373600

Table S23

B-6-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.36340500	-0.64101400	0.14475300
H	-3.32355600	-0.17325700	0.39929900
C	-1.80297800	-1.60257700	1.00826900
H	-2.28692200	-1.78187400	1.98267800
C	-1.51982700	-0.03405000	-0.80615500
H	-1.79149500	0.96244500	-1.19217500
N	-0.35681300	-0.57632200	-1.17501600
N	-0.65455100	-2.22475200	0.73135000
B	-0.23529300	-2.10121000	-0.78555200

C	0.07670000	-3.00026800	1.79135100
C	0.65872000	0.22574700	-1.94003000
C	1.57409700	-2.63080000	1.71542600
H	2.15030300	-3.22763800	2.45223800
H	1.72132900	-1.55611500	1.94881800
H	1.98016200	-2.82202500	0.70549400
C	-0.13128200	-4.51501900	1.54738500
H	0.40250600	-5.10610600	2.32056200
H	0.24635600	-4.82649500	0.55570100
H	-1.20937800	-4.77219700	1.59935300
C	-0.42514600	-2.66418500	3.21304000
H	-0.37028800	-1.57601900	3.42442900
H	0.21974000	-3.18356400	3.95046200
H	-1.46343300	-3.00891500	3.39799700
C	0.37114100	1.74229300	-1.88122300
H	-0.55366300	2.02857800	-2.42331300
H	1.20741100	2.28260300	-2.36923200
H	0.29702800	2.10871500	-0.83621400
C	0.64157600	-0.21551000	-3.42404400
H	1.38590100	0.36614000	-4.00695400
H	-0.35935800	-0.04007000	-3.86958300
H	0.88138400	-1.28933100	-3.53580100
C	2.04607800	-0.02050600	-1.30846300
H	2.28914400	-1.09848200	-1.29165200
H	2.07022200	0.35519900	-0.26474200
H	2.82716000	0.51424300	-1.88731800
C	-0.82857400	-3.17812800	-1.80832900
H	-1.37785600	-4.06075900	-1.43315100
H	-1.16331700	-2.86826300	-2.81500900
C	0.68829000	-3.14679600	-1.54543200
H	1.33806200	-2.84499300	-2.38599000
H	1.12748200	-4.01842500	-1.02842600

Table S24

Al-6-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.05359100	-0.42124100	0.60776500
H	-2.95365600	0.07055200	1.00206200
C	-1.57600800	-1.54078300	1.31069000
H	-2.13402300	-1.80038500	2.23119000
C	-1.39898900	0.21031000	-0.47077500
H	-1.81793600	1.18415700	-0.78079600
N	-0.31992700	-0.23437700	-1.11385000
N	-0.51581600	-2.29836100	1.00577100
Al	0.28613500	-2.06638900	-0.75439300
C	-0.15413700	-3.38401800	1.99239500
C	0.37309900	0.63438700	-2.13095200
C	1.11345000	-4.10576400	1.50501700
H	1.40347600	-4.88667900	2.23700400
H	1.96267600	-3.40263900	1.39188300
H	0.94575400	-4.60569500	0.53001000
C	-1.30987100	-4.40743300	2.08268100
H	-1.03710000	-5.23682800	2.76745000
H	-1.52570000	-4.83788500	1.08345800
H	-2.24404200	-3.95057400	2.46955400
C	0.13535800	-2.75888100	3.37656800
H	0.95628800	-2.01589900	3.30496600
H	0.44367300	-3.54598100	4.09524600
H	-0.75232000	-2.24950400	3.80439900
C	-0.30959300	2.00049300	-2.33817700
H	-1.34333800	1.90428000	-2.73107600
H	0.27268300	2.57308700	-3.08763900
H	-0.33645600	2.60840900	-1.41002000
C	0.38824400	-0.11776700	-3.48109200
H	0.91532600	0.48479800	-4.24933900
H	-0.64505300	-0.30999300	-3.83580800
H	0.90907500	-1.09107400	-3.40074700
C	1.81589900	0.86791300	-1.62477500
H	2.32390700	-0.09974900	-1.43520500
H	1.80775000	1.44736200	-0.67815200

H	2.40427900	1.43501000	-2.37569100
C	0.48073000	-3.49148100	-2.07369000
H	0.32904500	-4.55422800	-1.79130900
H	0.28631000	-3.38760200	-3.16061900
C	1.86736700	-2.88139900	-1.56907500
H	2.44342600	-2.35826600	-2.36093100
H	2.54726100	-3.59958600	-1.06919900

Table S25

Ga-6-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.43866500	-0.29069900	0.46287100
H	-3.39795400	0.11825800	0.81005600
C	-1.97809900	-1.45473700	1.11299400
H	-2.59426200	-1.80132000	1.96246500
C	-1.70625900	0.50419800	-0.44347300
H	-2.13618700	1.49911000	-0.65968300
N	-0.54719500	0.19987800	-1.02352900
N	-0.87215200	-2.14344300	0.83894600
Ga	0.09708000	-1.67560500	-0.83690200
C	-0.38520800	-3.24219200	1.73526300
C	0.23337600	1.21261900	-1.80605200
C	-0.24667900	-4.53068400	0.89364400
H	0.13092700	-5.36275500	1.52305100
H	0.46414500	-4.39327900	0.05593700
H	-1.22567000	-4.83019100	0.46693900
C	-1.33151100	-3.52373100	2.91917500
H	-0.90042900	-4.34226500	3.52982800
H	-2.33674900	-3.85604300	2.58584300
H	-1.45073700	-2.64446600	3.58557800
C	0.99578100	-2.81276900	2.28401800
H	1.68971600	-2.57803700	1.45096300

H	1.44221300	-3.62335400	2.89671400
H	0.89986700	-1.90749100	2.91875400
C	-0.48611100	2.57033300	-1.92940200
H	-1.45595000	2.48679300	-2.46278900
H	0.15432000	3.25802900	-2.51730700
H	-0.66276600	3.04816700	-0.94354600
C	0.47584800	0.64876500	-3.22408100
H	1.06916800	1.36629300	-3.82756000
H	-0.48586100	0.46356700	-3.74466200
H	1.03574400	-0.30581200	-3.19004400
C	1.58171500	1.42030300	-1.07698000
H	2.10927100	0.45254400	-0.95131900
H	1.41815500	1.85748400	-0.07013900
H	2.23642300	2.10624400	-1.65368100
C	0.48011500	-2.91941200	-2.33235400
C	1.77328100	-2.46867100	-1.53784500
H	2.30730600	-3.27199600	-0.99294500
H	0.23080200	-3.99588800	-2.26454800
H	0.42892600	-2.58554100	-3.38661500
H	2.50540800	-1.86726200	-2.11201200

Table S26

In-6-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.11037500	0.34415700	1.45261500
H	-1.56979200	1.01247500	2.19525800
C	-1.00307600	-1.00693600	1.84453800
H	-1.39858900	-1.21799000	2.85980400
C	-0.71102400	0.96529200	0.25041200
H	-0.91454400	2.05568000	0.21320500
N	-0.13419300	0.43683600	-0.82366300
N	-0.50262700	-2.04323100	1.18031100

In	0.29182700	-1.73680400	-0.86521700
C	-0.51900400	-3.38911000	1.84902300
C	0.18230300	1.34516100	-1.97843900
C	0.12891900	-4.41123200	0.90011000
H	0.13135200	-5.41979900	1.36071500
H	1.18005800	-4.13640100	0.67489600
H	-0.42927100	-4.47671700	-0.05686900
C	-1.97901500	-3.81608300	2.12906000
H	-2.00647700	-4.82959900	2.58021700
H	-2.56508100	-3.83944100	1.18730800
H	-2.48642400	-3.12378700	2.83202300
C	0.29721500	-3.33640000	3.16184500
H	1.33886100	-3.01205900	2.96003800
H	0.33193600	-4.33948300	3.63514600
H	-0.14387800	-2.63560500	3.90011300
C	-1.12564200	1.94881800	-2.54162200
H	-1.82219100	1.14400900	-2.85478000
H	-0.91015700	2.58469700	-3.42522700
H	-1.64629200	2.58152600	-1.79360200
C	0.86516600	0.51420600	-3.07763500
H	1.11226600	1.15368400	-3.94905800
H	0.20049800	-0.30053100	-3.43274600
H	1.80842800	0.06165700	-2.70796500
C	1.14934800	2.46277300	-1.52216600
H	2.07792100	2.02587600	-1.10045900
H	0.69645700	3.11804800	-0.75005400
H	1.42825700	3.10628200	-2.38209700
C	0.31288400	-3.11510400	-2.56655600
C	1.76921100	-2.87568400	-1.99986600
H	2.25984100	-3.75949500	-1.54858400
H	-0.07257500	-4.14830800	-2.46601800
H	0.13744800	-2.74775400	-3.59636300
H	2.47117100	-2.35867900	-2.68208400

Table S27

Tl-6-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.42056300	0.24729500	1.27141900
H	-2.04298900	0.87165100	1.92882700
C	-1.19123400	-1.06440300	1.72986700
H	-1.64511200	-1.28691000	2.71879800
C	-0.90888800	0.89889100	0.13249200
H	-1.17173100	1.97594700	0.06761000
N	-0.15479000	0.42298400	-0.84890000
N	-0.50581300	-2.05093000	1.16833600
Tl	0.33420000	-1.80542400	-0.94134200
C	-0.36412700	-3.34237500	1.92016100
C	0.32309300	1.37049300	-1.91063500
C	0.45992600	-4.32422000	1.07005200
H	0.59051500	-5.28398900	1.60984800
H	1.46782200	-3.91582500	0.84982100
H	-0.05364500	-4.54552900	0.11104000
C	-1.76294800	-3.95464500	2.17233400
H	-1.66998400	-4.94086200	2.67259700
H	-2.30178600	-4.09910100	1.21373100
H	-2.38694900	-3.30906300	2.82375700
C	0.37354400	-3.08938000	3.25597200
H	1.36135100	-2.61895800	3.07182900
H	0.53907500	-4.04504200	3.79538000
H	-0.20404100	-2.42237300	3.92821500
C	-0.88881500	2.03218300	-2.61002500
H	-1.56138400	1.25904200	-3.03458100
H	-0.54613300	2.68834400	-3.43670800
H	-1.48148700	2.65993700	-1.91368400
C	1.12470300	0.57966400	-2.95853200
H	1.49979800	1.26043800	-3.74936100
H	0.49044900	-0.18877300	-3.44784300
H	2.00055800	0.07836500	-2.49701100
C	1.24008500	2.44026300	-1.27303800
H	2.09603000	1.96041000	-0.75524600

H	0.69527300	3.06028600	-0.53182500
H	1.64219600	3.12246400	-2.05064000
C	-0.32502100	-3.13683300	-2.68458900
C	1.22755600	-3.12480100	-2.40509100
H	1.69218000	-4.04417100	-2.00212200
H	-0.76482700	-4.14833000	-2.56750700
H	-0.57181800	-2.76263100	-3.69906900
H	1.88683200	-2.63898900	-3.14863300
