Supporting Information

Theoretical Investigations in the Reactions of Group 15 Analogues of the Monocationic Five-Membered N-Heterocyclic Carbenes: Interplay of Electrophilicity, Basicity, and Aromaticity Governing the Reactivity

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Contents:

Table S1. E_{HOMO-2} and E_{LUMO} (in eV) represent the energies of the highest occupied molecular orbital-2 and the lowest unoccupied molecular orbital, respectively. μ, η and ω respectively represent the electronic chemical potential, the chemical hardness, and electrophilicity index of **G15-Rea**, whose definitions can be obtained from Figure 1. The calculations were performed at the BP86/def2-TZVP level of theory.

Table S2. Values of the Fukui function at the carbenic atom (G15) for **G15-Rea** calculated through eqs. (A), (B), and (C) fof_k^+ f_k^- f_k^0 respectively. The calculations were performed at the BP86/def2-TZVP level of theory.

Table S3-S27. Cartesian coordinates of the reactants, transition states, and products for the reaction of **G15-Rea** (G15 = N, P, As, Sb, and Bi) with CH_4 and C_2H_4 at BP86/def2-TZVP level of theory.

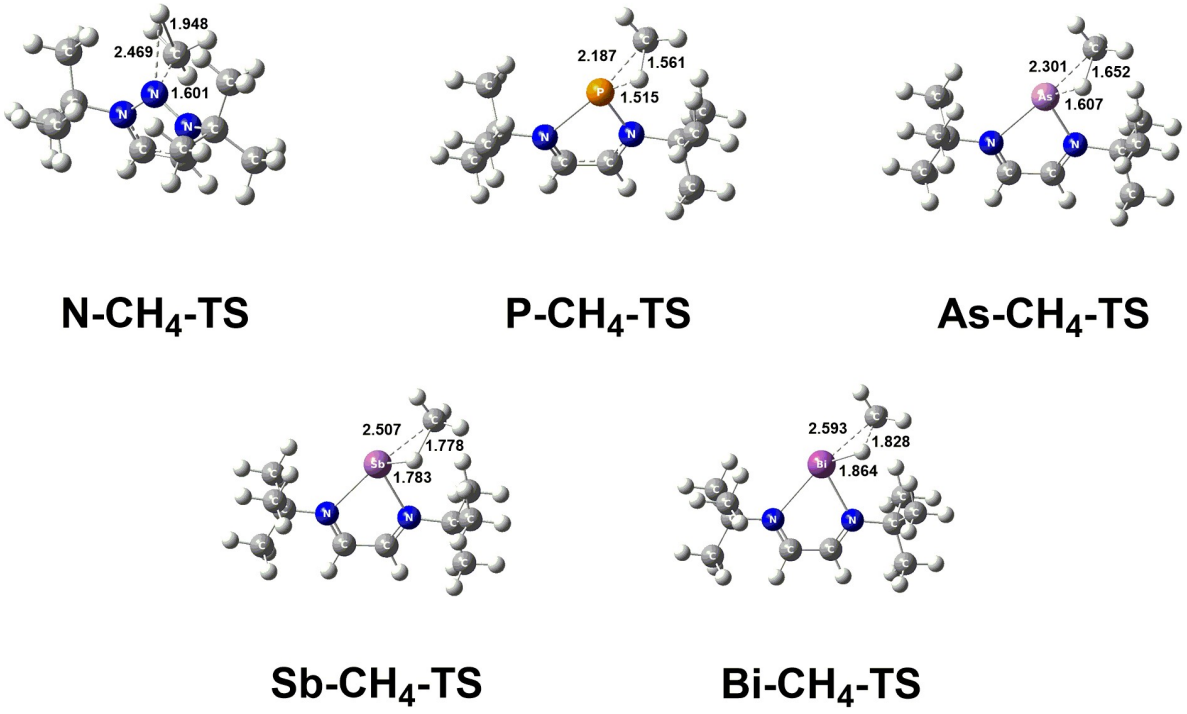

Figure S1. The optimized **G15-CH_4-TS** (G15 = N, P, As, Sb, and Bi) structures (Å) at the BP86/def2-TZVP level of theory. The hydrogen is omitted for clarity.

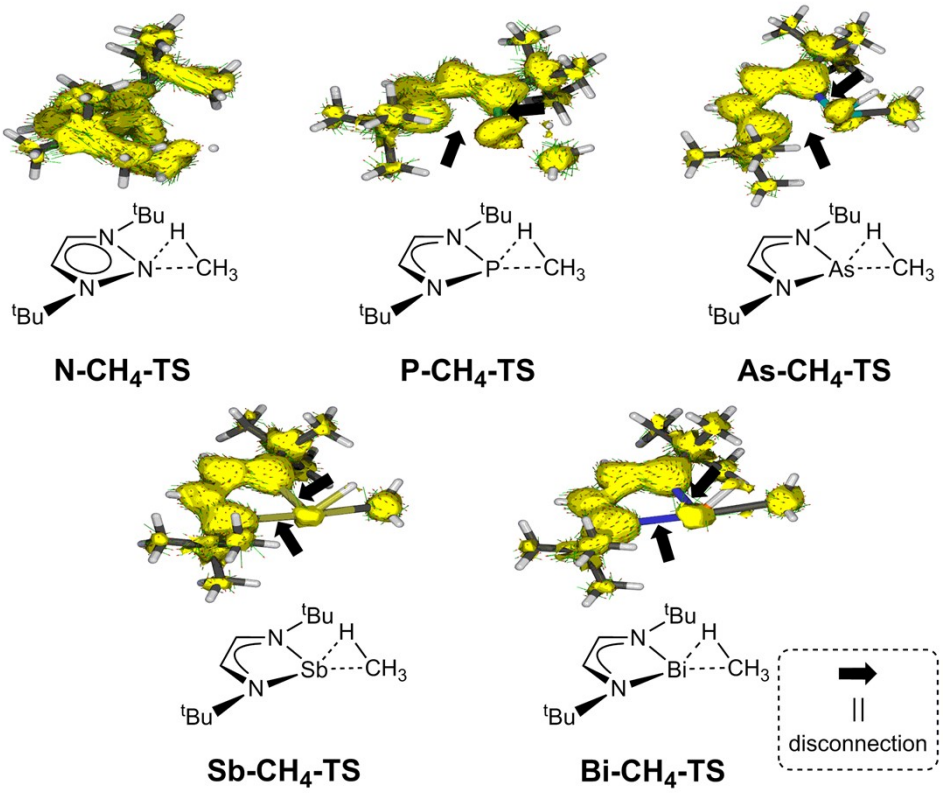

Figure S2. ACID plots for the **G15-CH$_4$-TS** (G15 = N, P, As, Sb, and Bi) molecules. For more information see the text.

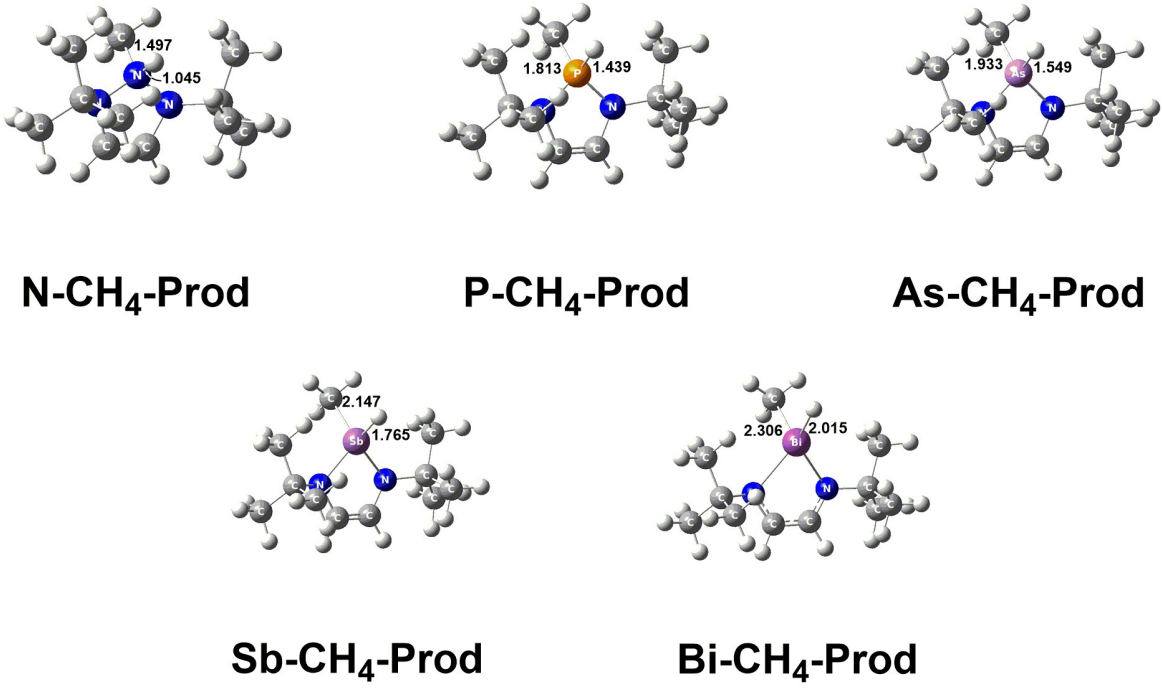

Figure S3. The optimized **G15-CH_4-Prod** (G15 = N, P, As, Sb, and Bi) structures (Å) at the BP86/def2-TZVP level of theory. The hydrogen is omitted for clarity.

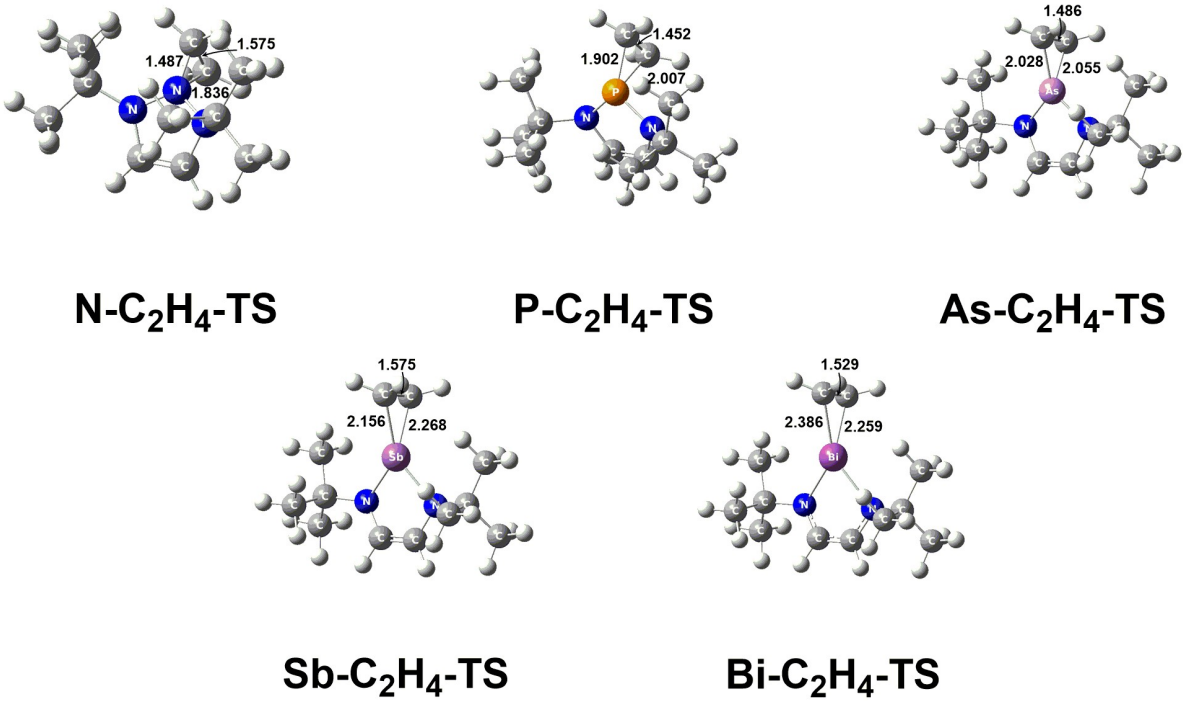

Figure S4. The optimized **G15-C_2H_4-TS** (G15 = N, P, As, Sb, and Bi) structures (Å) at the BP86/def2-TZVP level of theory. The hydrogen is omitted for clarity.

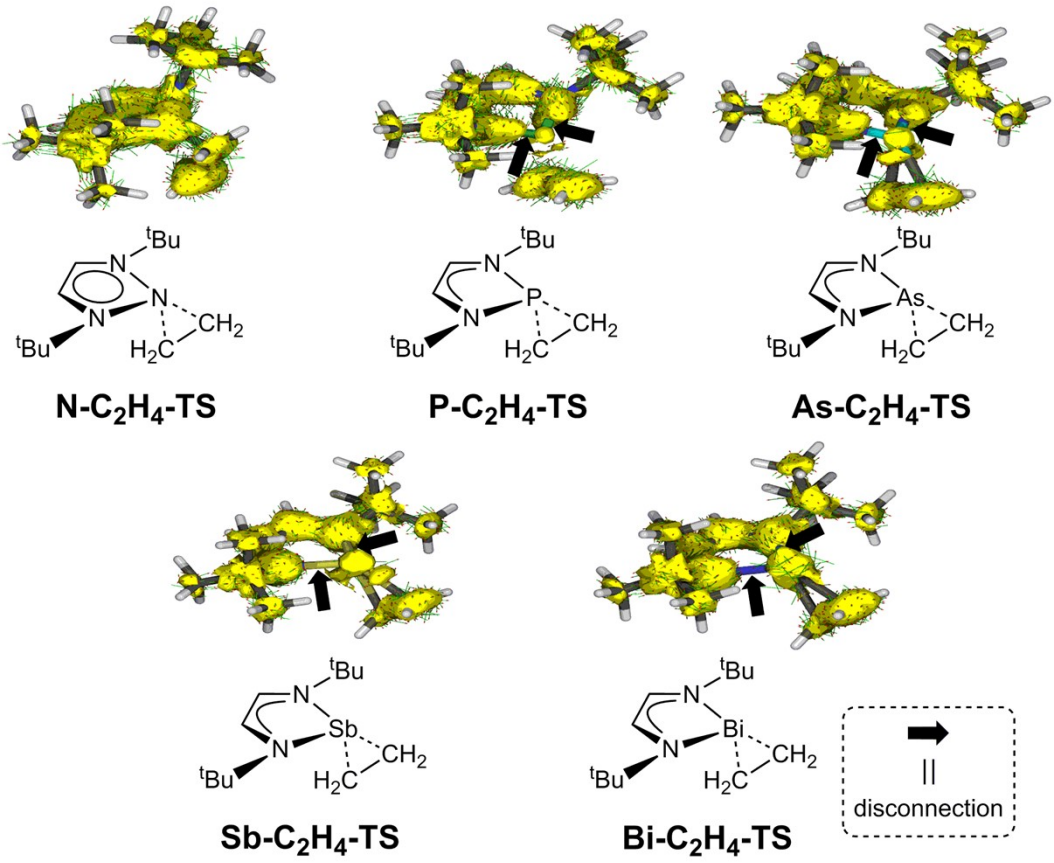

Figure S5. ACID plots for the **G15-C_2H_4-TS** (G15 = N, P, As, Sb, and Bi) molecules. For more information see the text.

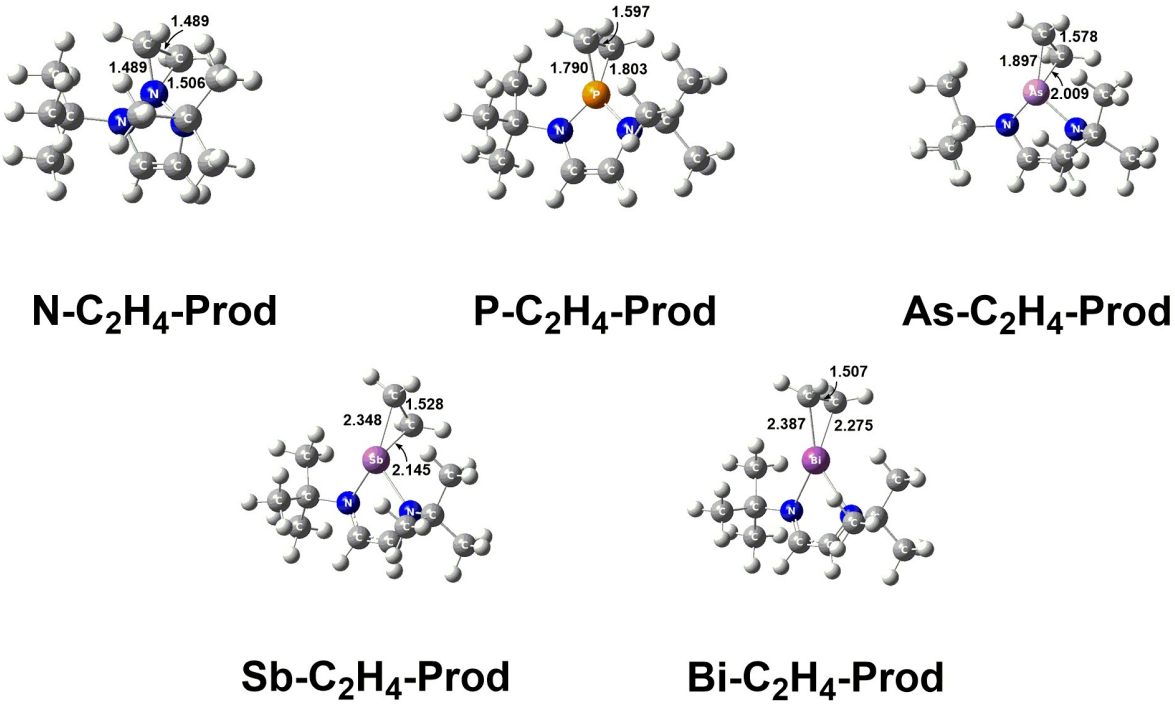

Figure S6. The optimized **G15-C_2H_4-Prod** (G15 = N, P, As, Sb, and Bi) structures (Å) at the BP86/def2-TZVP level of theory. The hydrogen is omitted for clarity.

Table S1

E_{HOMO-2} and E_{LUMO} (in eV) represent the energies of the highest occupied molecular orbital-2 and the lowest unoccupied molecular orbital, respectively. The electronic chemical potential (μ), the chemical hardness (η), and electrophilicity index (ω) of **G15-Rea** were obtained using eqs. (i), (ii), and (iii), respectively. Also see Figure 1. The calculations were performed at the BP86/def2-TZVP level of theory. See the text.

	N-Rea	**P-Rea**	**As-Rea**	**Sb-Rea**	**Bi-Rea**
E_{HOMO-2}	-11.89	-11.72	-11.65	-11.41	-11.37
E_{LUMO}	-6.450	-6.861	-6.979	-7.036	-6.975
μ	18.34	18.58	18.63	18.45	18.35
η	5.440	4.859	4.671	4.374	4.395
ω	30.92	35.53	37.15	38.90	38.29

(i) $\mu = -(E_{HOMO-2} + E_{LUMO})/2$.

(ii) $\eta = E_{LUMO} - E_{HOMO-2}$.

(iii) $\omega = \mu^2/2\eta$.

Table S2

Values of the Fukui function at the carbenic atom (G15) for **G15-Rea** calculated through eqs. (A), (B), and (C) for [illegible], respectively. The calculations were performed at the BP86/def2-TZVP level of theory. See the text.

	N-Rea	**P-Rea**	**As-Rea**	**Sb-Rea**	**Bi-Rea**
$q_k(N-1)$	0.254	1.376	1.417	1.447	1.504
$q_k(N)$	-0.012	1.004	1.010	1.076	1.048
$q_k(N+1)$	-0.267	0.591	0.587	0.624	0.582
[illegible]	-0.255	-0.413	-0.423	-0.452	-0.466
f_k^-	-0.266	-0.372	-0.407	-0.371	-0.456
[illegible]	-0.261	-0.393	-0.415	-0.412	-0.461

For nucleophilic attack: $f_k^+ = q_k(N+1) - q_k(N)$

(A)

For electrophilic attack: $f_k^- = q_k(N) - q_k(N-1)$

(B)

For radical attack: $f_k^0 = \frac{1}{2}[f_k^+ + f_k^-]$

(C)

(All were calculated at BP86/def2-TZVP level of theory)

Table S3

N-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.02505800	-0.72478400	0.55244900
C	0.79665900	-1.59446900	1.27360900
H	0.43435900	-2.55029100	1.66163200
C	2.04083800	-0.98987200	1.36770400
H	2.96276400	-1.32157100	1.85292400
N	1.91912500	0.19560300	0.69566100
N	0.70171100	0.35744400	0.20226600
C	-1.43570400	-0.85000400	0.12874900
C	-1.97517600	-2.18212500	0.66739900
H	-1.43884400	-3.05642800	0.24531100
H	-3.03557300	-2.27419800	0.36202900
H	-1.95090300	-2.23011900	1.77524800
C	-2.19147600	0.34471700	0.74045300
H	-1.79112400	1.30823100	0.36960700
H	-2.13764200	0.33465700	1.84799300
H	-3.25862600	0.28136600	0.45001400
C	-1.46739300	-0.81818900	-1.41102500
H	-0.89448200	-1.66208100	-1.84608000
H	-1.05958200	0.13364300	-1.80337100
H	-2.51800300	-0.90791300	-1.75068400
C	2.95994000	1.28711200	0.46271200
C	4.26897500	0.84766900	1.13287700
H	5.02561000	1.63847000	0.96461000
H	4.67400300	-0.08754400	0.69520300
H	4.16218900	0.72891900	2.23048200
C	2.41492600	2.57945400	1.09957700
H	3.15091100	3.39321500	0.94690500
H	2.25958400	2.45961200	2.19096900
H	1.45972500	2.88793200	0.63199700
C	3.13566300	1.43118700	-1.06083200
H	3.88814100	2.21873500	-1.26266600
H	2.18774400	1.72826300	-1.55010600
H	3.49708900	0.48800700	-1.51846600

Table S4

P-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.22084800	-0.53554000	0.36379400
C	0.66916700	-1.29835600	1.07283400
H	0.38523700	-2.27078800	1.49451800

C	1.90936600	-0.69269900	1.17160600
H	2.79062500	-1.09611000	1.68611300
N	1.94151200	0.52042400	0.53596900
P	0.44643500	0.94563100	-0.19853200
C	-1.65733600	-0.96596500	0.10371800
C	-2.35854500	-1.13975200	1.46606900
H	-1.89317200	-1.93842300	2.07798900
H	-3.41559900	-1.42653500	1.29819500
H	-2.34716200	-0.19612400	2.04810000
C	-2.34932100	0.13468000	-0.71739100
H	-1.86329700	0.28755800	-1.70441500
H	-2.38493600	1.10214400	-0.17283900
H	-3.39742500	-0.16420600	-0.91545700
C	-1.62376600	-2.28711200	-0.69096200
H	-1.14417200	-3.10735300	-0.11990000
H	-1.08645800	-2.16474800	-1.65307200
H	-2.66144200	-2.60436300	-0.91545700
C	3.18357900	1.39878500	0.49012300
C	4.30308000	0.60712400	-0.21556200
H	5.20969100	1.24042600	-0.28476600
H	4.00592400	0.31948500	-1.24429700
H	4.58285000	-0.30974700	0.34120600
C	3.56857900	1.75828000	1.93946200
H	4.45604500	2.42165400	1.92732400
H	3.83405400	0.86290000	2.53673800
H	2.74575700	2.29510300	2.45338000
C	2.84541800	2.67084900	-0.30477800
H	3.74078200	3.32169400	-0.34730000
H	2.03719100	3.26165500	0.17639100
H	2.55867500	2.44407600	-1.35365100

Table S5

As-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.27537300	-0.52258500	0.31732200
C	0.64155700	-1.24068000	1.02025000
H	0.38988300	-2.22143500	1.44638700
C	1.88211800	-0.62325400	1.13596800
H	2.74483600	-1.04938200	1.66604100
N	1.96021200	0.59010800	0.52591200
As	0.37818400	1.10255200	-0.30456400
C	-1.68880100	-1.00919700	0.07098100
C	-2.38227800	-1.19929200	1.43642500
H	-1.88519400	-1.97552900	2.05217600
H	-3.42859000	-1.52610900	1.27417100
H	-2.40278600	-0.25193600	2.01217900
C	-2.42477000	0.05877300	-0.75505500
H	-1.94725000	0.21893400	-1.74578300
H	-2.49305000	1.02739700	-0.21435400

H	-3.46360600	-0.27250100	-0.95029000
C	-1.61619200	-2.33526300	-0.71507300
H	-1.10529000	-3.13353400	-0.14016300
H	-1.08708200	-2.20191600	-1.68029700
H	-2.64336000	-2.69005300	-0.93182500
C	3.21877800	1.43347500	0.52883900
C	4.34234600	0.63197900	-0.16162800
H	5.26359700	1.24680700	-0.19624400
H	4.06589500	0.36693700	-1.20217800
H	4.58725400	-0.29987900	0.38649200
C	3.57875900	1.76448800	1.99252400
H	4.48086700	2.40772100	2.01204200
H	3.80923400	0.85410400	2.58146900
H	2.75534300	2.31086000	2.49537300
C	2.92988200	2.72566400	-0.25299100
H	3.83584200	3.36292100	-0.26634200
H	2.12260100	3.32527800	0.22029700
H	2.66691700	2.51919200	-1.31291600

Table S6

Sb-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.38523900	-0.44739100	0.32406800
C	0.58153900	-1.12137900	0.98543000
H	0.36411100	-2.09084000	1.45884600
C	1.85133000	-0.53473400	1.03736500
H	2.69707100	-1.01302900	1.55425800
N	2.00783200	0.65824500	0.42202400
Sb	0.26394100	1.36641500	-0.48969400
C	-1.79186600	-0.97677900	0.19893600
C	-2.39261700	-1.13347600	1.61314700
H	-1.83724400	-1.87681100	2.21949200
H	-3.43993100	-1.48696500	1.53387800
H	-2.39429200	-0.16730600	2.15737100
C	-2.60936900	0.04430400	-0.60974600
H	-2.20206700	0.17481500	-1.63697200
H	-2.66119400	1.02902700	-0.09428500
H	-3.65420500	-0.30478700	-0.72748200
C	-1.75042500	-2.32921300	-0.54587500
H	-1.18213000	-3.09582600	0.01802800
H	-1.29208800	-2.22027200	-1.54972400
H	-2.78215400	-2.71185400	-0.67716200
C	3.32737200	1.38837600	0.40869500
C	4.37784200	0.50462600	-0.29915200
H	5.34416700	1.04488100	-0.34866700
H	4.06464600	0.26114600	-1.33467100
H	4.55621200	-0.44404700	0.24570700
C	3.74191400	1.69525400	1.86451700
H	4.69220400	2.26538100	1.86683300

H	3.90948500	0.77025300	2.45181100
H	2.97240100	2.30436400	2.38073200
C	3.13224600	2.69996000	-0.37012800
H	4.08053900	3.27165900	-0.40617700
H	2.38295100	3.36057700	0.11992600
H	2.83750600	2.51006900	-1.42617800

Table S7

Bi-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.44221700	-0.38993000	0.38704600
C	0.55042700	-1.05866600	0.99983000
H	0.34546800	-2.01080100	1.51515600
C	1.84793800	-0.51726400	0.96780300
H	2.68992900	-1.03262300	1.45725000
N	2.04446000	0.64768400	0.32565100
Bi	0.21277400	1.48395600	-0.57175900
C	-1.85857000	-0.89454000	0.37104300
C	-2.37084200	-1.00191700	1.82485700
H	-1.79108900	-1.74090600	2.41341200
H	-3.42798200	-1.33463000	1.82375700
H	-2.31671200	-0.02230700	2.34173800
C	-2.70854400	0.12196800	-0.41029100
H	-2.36521300	0.21407900	-1.46512400
H	-2.70427500	1.11997600	0.08257600
H	-3.76694100	-0.20272400	-0.45237100
C	-1.89530300	-2.26705300	-0.33774000
H	-1.30561800	-3.02991600	0.20904000
H	-1.50091100	-2.19423900	-1.37162200
H	-2.94071000	-2.63109200	-0.39097600
C	3.39719700	1.29877800	0.24128600
C	4.36839700	0.34711800	-0.49261800
H	5.35912600	0.83293300	-0.59599000
H	3.99625300	0.10018100	-1.50764700
H	4.51922500	-0.59903200	0.06478600
C	3.89457700	1.61269200	1.67011700
H	4.87293300	2.13077300	1.61857200
H	4.03840700	0.69125000	2.26916900
H	3.18176500	2.27150700	2.20640200
C	3.23910500	2.60413400	-0.55706300
H	4.21155700	3.12680200	-0.64951900
H	2.54797300	3.31198600	-0.04694800
H	2.88790100	2.40646700	-1.59467400

Table S8

N-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.11180200	-0.07286200	-0.49752400
C	-0.70038100	-0.75693500	-1.60006200
H	-1.38621800	-1.27751000	-2.27779000
C	0.70034000	-0.75695500	-1.60007000
H	1.38615500	-1.27754900	-2.27780500
N	1.11179200	-0.07289300	-0.49753600
N	0.00000800	0.58934600	0.05633400
C	-2.39581400	-0.19152800	0.28651400
C	-2.14940700	-1.23554300	1.39996300
H	-1.86482900	-2.21937600	0.97495300
H	-3.08066800	-1.37152300	1.98597400
H	-1.35457900	-0.89685700	2.09335200
C	-2.74786500	1.17540100	0.89414900
H	-3.02105000	1.91417000	0.11393500
H	-1.91895200	1.58994500	1.50961400
H	-3.62332500	1.05378200	1.56156300
C	-3.49671700	-0.66291200	-0.67744200
H	-3.31395300	-1.68678900	-1.06231800
H	-3.62198400	0.03283900	-1.53181400
H	-4.45745300	-0.69378100	-0.12732900
C	2.39581000	-0.19159700	0.28648700
C	3.49668900	-0.66301200	-0.67748200
H	4.45743100	-0.69390800	-0.12737900
H	3.62196700	0.03273800	-1.53185400
H	3.31389300	-1.68688300	-1.06235700
C	2.14938500	-1.23560700	1.39993800
H	3.08064800	-1.37161500	1.98594000
H	1.86477500	-2.21943200	0.97493000
H	1.35457300	-0.89689900	2.09333600
C	2.74790500	1.17532100	0.89412100
H	3.62337200	1.05367800	1.56152200
H	1.91901200	1.58988500	1.50959900
H	3.02110000	1.91408500	0.11390500
C	0.00002400	2.05673900	-0.58516400
H	0.00001600	1.73095900	-1.66193000
H	-0.92344100	2.63946500	-0.43030500
H	0.92350600	2.63944100	-0.43031200
H	0.00003700	2.76159300	1.23158100

Table S9

P-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.21839500	0.21914600	0.94078100
C	0.57198300	-0.03631200	1.97343300
H	0.19905400	-0.68975200	2.77321800

C	1.91738900	0.48399800	2.07470100
H	2.46884400	0.33976400	3.02576000
N	2.39157900	1.05911700	1.01832000
P	0.46232300	1.35837200	-0.36162000
C	-1.59057200	-0.54097700	0.90770100
C	-1.54976500	-1.76538100	1.85135700
H	-0.71101600	-2.45332200	1.62120300
H	-2.48988900	-2.33065100	1.70110600
H	-1.52461300	-1.49570500	2.92621700
C	-2.69802500	0.41273300	1.39790300
H	-2.87239500	1.26641500	0.72139900
H	-2.46697200	0.80447500	2.40921100
H	-3.64878100	-0.15282300	1.46732200
C	-1.84697600	-1.07901000	-0.51486500
H	-1.00519600	-1.70634800	-0.86916100
H	-2.04484000	-0.29149200	-1.26487300
H	-2.75387100	-1.71483100	-0.48793400
C	3.74244400	1.64028600	0.90645000
C	4.55936500	1.55019900	2.20701100
H	5.55555700	2.00846500	2.04867800
H	4.73062400	0.49931100	2.52071200
H	4.07441100	2.09859900	3.04147600
C	3.54931200	3.12171900	0.48946300
H	4.54202400	3.59080400	0.33756000
H	3.01309000	3.69125600	1.27537200
H	2.97937500	3.20189600	-0.45710300
C	4.44329500	0.86117700	-0.23654000
H	5.44411600	1.30025700	-0.42210300
H	3.85745900	0.91628800	-1.17544900
H	4.57761400	-0.20607700	0.03268300
C	-1.39947200	2.32293800	-0.98627000
H	-2.28470200	1.84287300	-1.45185200
H	-1.68671900	2.85321400	-0.06102800
H	-0.90646300	3.00545700	-1.70517000
H	-0.67209200	0.97530900	-1.29008300

Table S10

As-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.21862200	0.15132000	0.96558200
C	0.62794100	-0.14120700	1.93105100
H	0.30831600	-0.83980800	2.71779700
C	1.98196200	0.37912100	2.01267600
H	2.58687100	0.09024700	2.89592600
N	2.40672600	1.12077300	1.04513000
As	0.47230700	1.44491800	-0.43559300
C	-1.60147900	-0.54694800	0.98243000
C	-1.65692600	-1.65523400	2.05642900
H	-0.89146600	-2.44297300	1.90226700

H	-2.64686700	-2.14469200	1.97638600
H	-1.58464600	-1.26467100	3.09180200
C	-2.67240700	0.50869700	1.32497800
H	-2.74927800	1.30620100	0.56744400
H	-2.46730800	0.97594400	2.30940500
H	-3.66062500	0.01080500	1.38638700
C	-1.83687700	-1.21788100	-0.38678600
H	-1.02673900	-1.93539900	-0.62605100
H	-1.92492100	-0.49580400	-1.21819100
H	-2.78985500	-1.78162500	-0.34727500
C	3.76234700	1.70303800	0.96824800
C	4.65211700	1.35413000	2.17380000
H	5.64685400	1.82427900	2.04410900
H	4.81778400	0.26062900	2.26779500
H	4.23158000	1.73620900	3.12733600
C	3.56864700	3.23807200	0.86473600
H	4.55708600	3.72601500	0.74808400
H	3.08837200	3.64292700	1.77849300
H	2.94539400	3.50878400	-0.01081000
C	4.38600200	1.16029900	-0.34318200
H	5.38531100	1.61615400	-0.49275200
H	3.75664300	1.40864700	-1.22111900
H	4.51046100	0.05932500	-0.30027900
C	-1.49769200	2.18759000	-1.36576700
H	-2.28956900	1.55866500	-1.81659600
H	-1.90392400	2.80805300	-0.54723900
H	-1.00482400	2.81290900	-2.13615500
H	-0.55958500	0.83388300	-1.50551100

Table S11

Sb-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.20859700	0.09625900	1.00099500
C	0.68141100	-0.23807200	1.90193200
H	0.40764800	-0.96784500	2.68066700
C	2.04434300	0.27766300	1.94484700
H	2.70847900	-0.13009600	2.73262400
N	2.41602300	1.16240200	1.08005100
Sb	0.50328700	1.61063000	-0.55476200
C	-1.60390600	-0.52884700	1.07668800
C	-1.72255400	-1.54646500	2.23007600
H	-1.03034900	-2.40620200	2.11876000
H	-2.75073200	-1.95724100	2.21188300
H	-1.58069200	-1.08532500	3.22895400
C	-2.61145700	0.61297500	1.32731000
H	-2.60239600	1.36470000	0.51874700
H	-2.39880600	1.12554900	2.28736900
H	-3.63479100	0.19150600	1.38514200
C	-1.87226000	-1.27047500	-0.24955700

H	-1.12417500	-2.07160200	-0.41539900
H	-1.86173800	-0.59374700	-1.12203400
H	-2.87417700	-1.74161100	-0.20506400
C	3.77995600	1.74401600	1.02939200
C	4.72250400	1.19564300	2.11470800
H	5.71492800	1.67736200	2.01334900
H	4.87977400	0.10116200	2.01856300
H	4.35554400	1.41705200	3.13849500
C	3.60271200	3.27471000	1.19418700
H	4.58981500	3.77234600	1.11236400
H	3.17171100	3.52317800	2.18513800
H	2.94256300	3.69522800	0.40874800
C	4.34189200	1.42277300	-0.37876300
H	5.34704100	1.87726600	-0.48758500
H	3.69368000	1.83343600	-1.17936700
H	4.43820900	0.32881300	-0.53181000
C	-1.64582400	2.00705900	-1.78430900
H	-2.27589500	1.21676400	-2.23226900
H	-2.22124300	2.60741400	-1.05597400
H	-1.19167800	2.64538900	-2.56818900
H	-0.42114600	0.71762300	-1.79092400

Table S12

Bi-CH_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.14049100	0.88195100	-0.01465800
C	0.30847800	1.88796200	0.01094500
H	0.70908500	2.91592200	0.03023000
C	-1.14970700	1.77223100	0.00305100
H	-1.71303600	2.72642000	-0.02855800
N	-1.71757800	0.61253900	0.03069000
Bi	0.12376200	-1.28634100	-0.07386500
C	2.63893900	1.14316400	0.00607000
C	2.97245100	2.64874600	-0.00272600
H	2.60461600	3.16303600	-0.91435900
H	4.07478500	2.75403300	0.00452700
H	2.59365400	3.17790700	0.89574600
C	3.19404200	0.51794300	1.30419000
H	3.00579500	-0.57015700	1.35269200
H	2.74395400	0.99380000	2.19901800
H	4.29035100	0.67430600	1.34828200
C	3.25202300	0.49534800	-1.25325200
H	2.83123300	0.94240700	-2.17638600
H	3.08328500	-0.59657200	-1.28438500
H	4.34672700	0.66706800	-1.25642600
C	-3.19048700	0.42879100	0.02219000
C	-3.98244500	1.74690200	-0.03446400
H	-5.06716100	1.52199000	-0.03680800

H	-3.76685400	2.32502200	-0.95702700
H	-3.78558000	2.39199900	0.84691400
C	-3.53346500	-0.34674600	1.31899700
H	-4.61951900	-0.56720600	1.34483000
H	-3.28012600	0.24793800	2.21990400
H	-2.98923000	-1.31186500	1.37264300
C	-3.51620600	-0.44100600	-1.21783400
H	-4.60408000	-0.65154400	-1.24891300
H	-2.98446600	-1.41428700	-1.18466200
H	-3.23738200	0.07826500	-2.15699600
C	2.21638600	-2.79907200	0.16377100
H	3.09549400	-2.73136200	-0.50158500
H	2.49776800	-2.62256300	1.21789100
H	1.69002700	-3.76527500	0.03526000
H	1.44649600	-1.90576600	-1.23318600

Table S13

N-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.16351200	-0.36686500	0.27199400
C	0.80376100	-1.30340200	0.73202600
H	0.48415000	-2.31808500	0.98997900
C	2.05996500	-0.82115300	0.65172100
H	3.00072700	-1.35189100	0.82943400
N	2.09728700	0.50120700	0.12793800
N	0.66499200	0.79259300	-0.16466500
C	-1.39008200	-0.04863500	1.11504300
C	-1.02442600	0.55338600	2.48391400
H	-0.29887400	-0.08454900	3.02813500
H	-1.93436700	0.64509800	3.11010900
H	-0.60256100	1.57789900	2.40107800
C	-2.29614000	0.90651400	0.31692200
H	-2.58115200	0.47380300	-0.66317400
H	-1.83426900	1.90493600	0.14942600
H	-3.22602800	1.09481800	0.88900000
C	-2.10915100	-1.40189800	1.29581600
H	-1.55277100	-2.08665200	1.96581800
H	-2.27203000	-1.90202200	0.32043800
H	-3.09811800	-1.22309000	1.76184400
C	2.88313900	1.59058900	0.84382700
C	4.33725800	1.07485200	0.87403500
H	4.99826700	1.88668100	1.23631000
H	4.67753400	0.77735900	-0.13773300
H	4.46474600	0.21870800	1.56551100
C	2.37266800	1.84378000	2.27401700
H	3.05418500	2.54299600	2.79857200
H	2.32904100	0.90474900	2.86216900
H	1.36886900	2.31934400	2.29162700
C	2.81680100	2.87582700	-0.00107200

H	3.43919700	3.65989000	0.47357200
H	1.79031700	3.30048000	-0.06653800
H	3.20279600	2.70974400	-1.02698500
H	0.37105800	1.64541400	0.36391700
C	0.49323200	0.99631600	-1.63814200
H	0.82101200	0.06399300	-2.13008600
H	-0.57465100	1.19054400	-1.84285800
H	1.12674200	1.84549000	-1.95054600

Table S14

P-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.27185000	-0.16845500	0.66739200
C	0.72101800	-1.11040900	1.08144200
H	0.41233700	-2.12586900	1.35123600
C	1.98809400	-0.64813400	0.99303000
H	2.90610100	-1.21613900	1.17709500
N	2.08549800	0.69155000	0.50290600
P	0.52161200	1.24084800	0.18356500
C	-1.70963800	-0.25305300	1.15005700
C	-1.75164800	0.06657100	2.65770900
H	-1.10624400	-0.62893200	3.23172700
H	-2.78569900	-0.03133100	3.04548900
H	-1.41379500	1.10374600	2.86656400
C	-2.55469000	0.75907900	0.35626700
H	-2.56451300	0.52767500	-0.72848400
H	-2.21495700	1.80751000	0.50909400
H	-3.60302500	0.72451000	0.71252500
C	-2.22934100	-1.67687800	0.87280200
H	-1.71863100	-2.44141100	1.49127300
H	-2.11356300	-1.94736300	-0.19598300
H	-3.30671800	-1.72747300	1.12716700
C	3.28998900	1.56871000	0.79778000
C	4.56043600	0.79764600	0.39055000
H	5.44141900	1.45992500	0.50580800
H	4.51114300	0.46916000	-0.66706500
H	4.74088000	-0.08855300	1.03081600
C	3.30732500	1.90681000	2.30188500
H	4.20295500	2.51033600	2.55250800
H	3.33521000	0.98536100	2.91826100
H	2.41406200	2.49546700	2.60021500
C	3.18254300	2.85123500	-0.04611100
H	4.04372300	3.51187900	0.17533900
H	2.27290000	3.44402000	0.19703700
H	3.20240200	2.63291100	-1.13344200
H	0.15114400	2.40159900	0.95096700
C	0.23178000	1.70467000	-1.54561700

H	0.85730900	2.58212900	-1.80403300
H	0.50024100	0.84418500	-2.18974800
H	-0.83618900	1.96523800	-1.68563400

Table S15

As-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.31103000	-0.21774700	0.61908400
C	0.73584100	-1.07924600	1.05588000
H	0.47382500	-2.09787400	1.36448000
C	1.99806200	-0.59411300	0.97489600
H	2.90511400	-1.16348900	1.20845800
N	2.14534500	0.72644300	0.46161900
As	0.46150200	1.38268100	0.19703800
C	-1.72557400	-0.35339500	1.13843900
C	-1.76572300	-0.04487000	2.64862000
H	-1.08862900	-0.71835400	3.21224300
H	-2.79091100	-0.18258700	3.04778700
H	-1.46480600	1.00331600	2.86154600
C	-2.61088200	0.63253600	0.35651500
H	-2.60323600	0.41457600	-0.73108800
H	-2.30644400	1.69132000	0.52344700
H	-3.65947400	0.56193600	0.70666300
C	-2.19701400	-1.79495900	0.85808600
H	-1.64421700	-2.54324000	1.46004300
H	-2.08834000	-2.05132800	-0.21475600
H	-3.26685900	-1.88935600	1.13141200
C	3.33556400	1.59149900	0.81384300
C	4.61327500	0.82201000	0.42094100
H	5.49472000	1.47729400	0.56877700
H	4.58446200	0.51289100	-0.64308500
H	4.77275000	-0.07751200	1.04807100
C	3.32774300	1.91210700	2.32200900
H	4.21959400	2.51011300	2.59821000
H	3.34060000	0.98349100	2.92799500
H	2.43095100	2.50055200	2.61199900
C	3.24267100	2.88200300	-0.01871300
H	4.10153400	3.54370100	0.20854700
H	2.33105200	3.47381000	0.22687800
H	3.26062600	2.66818700	-1.10699400
H	0.05395000	2.59145400	1.07682900
C	0.14154700	1.90802500	-1.63576200
H	0.42711600	1.05908500	-2.28516500
H	-0.93290600	2.14803400	-1.75191400
H	0.75781900	2.79977400	-1.86048700

Table S16

Sb-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.38761000	-0.52832200	-0.43128100
C	-0.68036700	-1.72095100	-0.71360000
H	-1.27206500	-2.61218700	-0.96106200
C	0.68038200	-1.72103600	-0.71302500
H	1.27219500	-2.61234800	-0.96004400
N	1.38755600	-0.52836900	-0.43096000
Sb	-0.00017200	0.84515700	0.20057800
C	-2.80038600	-0.54981700	0.08112400
C	-2.88168400	-1.28676200	1.43378900
H	-2.50576700	-2.32615800	1.34444400
H	-3.92869000	-1.33466100	1.79582400
H	-2.28158500	-0.77075800	2.21410300
C	-3.24083400	0.91549900	0.23281900
H	-3.20416800	1.45379600	-0.73661300
H	-2.60860500	1.45550000	0.97977000
H	-4.27719800	0.97975600	0.61896000
C	-3.68563300	-1.24350400	-0.97850400
H	-3.45351100	-2.32272800	-1.07464100
H	-3.56974100	-0.76680400	-1.97236300
H	-4.74922500	-1.16710100	-0.67636600
C	2.80042000	-0.54993500	0.08123100
C	3.68494200	-1.24464800	-0.97829800
H	4.74864200	-1.16894600	-0.67636300
H	3.56922300	-0.76819100	-1.97229000
H	3.45193300	-2.32371200	-1.07405500
C	2.88195000	-1.28580500	1.43442800
H	3.92923300	-1.33447400	1.79559400
H	2.50482300	-2.32487500	1.34654100
H	2.28320200	-0.76817300	2.21467600
C	3.24147700	0.91531700	0.23178300
H	4.27959800	0.97963100	0.61317900
H	2.61275800	1.45483900	0.98194800
H	3.20030300	1.45380100	-0.73735000
H	-0.00146900	1.42721100	1.86735400
C	0.00081500	2.60886400	-1.02521000
H	0.00264700	2.29039000	-2.08424300
H	-0.91059800	3.18778800	-0.78142200
H	0.91074900	3.18892500	-0.77860900

Table S17

Bi-CH_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z

N	-1.43209500	0.85844500	0.44290800
C	-0.70593900	1.98346100	0.42571900
H	-1.22425200	2.95096300	0.29732500
C	0.70628500	1.98365500	0.42578200
H	1.22430800	2.95121100	0.29684700
N	1.43246800	0.85865400	0.44337300
Bi	-0.00002300	-0.91127700	-0.24140900
C	-2.87277700	0.88517800	0.02570200
C	-3.03935600	1.42247900	-1.41088400
H	-2.63560800	2.44975100	-1.51742700
H	-4.11245300	1.45474300	-1.68624100
H	-2.52340600	0.77012300	-2.14767700
C	-3.38229200	-0.56389800	0.12043700
H	-3.27818300	-0.96411200	1.14917800
H	-2.83418300	-1.22994100	-0.58955400
H	-4.45083400	-0.62878300	-0.16604300
C	-3.64001600	1.77070000	1.04223300
H	-3.35057900	2.83794100	0.96513600
H	-3.46315400	1.43031900	2.08183300
H	-4.72668500	1.70680900	0.83379600
C	2.87280800	0.88525900	0.02541700
C	3.64065000	1.77205000	1.04042700
H	4.72711200	1.70866100	0.83083800
H	3.46511500	1.43239900	2.08049800
H	3.35047300	2.83905600	0.96290900
C	3.03756100	1.42110900	-1.41186100
H	4.11026100	1.45396200	-1.68871200
H	2.63270500	2.44790200	-1.51900700
H	2.52093900	0.76739100	-2.14702100
C	3.38277400	-0.56362500	0.12152800
H	4.45204500	-0.62805000	-0.16239300
H	2.83669000	-1.23041000	-0.58931900
H	3.27653900	-0.96345700	1.15022800
H	-0.00335100	-2.17166700	-1.81415800
C	0.00077600	-2.34740700	1.56333400
H	0.00297100	-1.74190300	2.48679500
H	-0.91470800	-2.95933300	1.46069100
H	0.91472900	-2.96107800	1.45749000

Table S18

N-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.46040000	0.46461600	1.74246800
C	0.44244300	-0.22036800	2.62087800
H	0.07347400	-0.91313100	3.38185900
C	1.72248000	0.11187200	2.30969300
H	2.65770900	-0.22596000	2.76481100
N	1.71041000	1.03807500	1.25138900

N	0.38454300	1.46395800	1.20241100
C	-1.30493900	-0.40638200	0.78604500
C	-2.09480600	-1.34929800	1.71671900
H	-1.44434100	-2.09336100	2.21674100
H	-2.82818300	-1.91693900	1.11085800
H	-2.65290200	-0.78083800	2.48754400
C	-2.29864900	0.47610700	0.01084900
H	-1.81059000	1.08303700	-0.77847500
H	-2.87847100	1.13562000	0.68869700
H	-3.02371000	-0.17832100	-0.51265300
C	-0.41816700	-1.21007300	-0.17984100
H	0.33007000	-1.81988000	0.36615700
H	0.10997300	-0.55057500	-0.89760900
H	-1.04558900	-1.90483000	-0.77445200
C	2.83119600	1.49381200	0.35712600
C	2.41967400	1.35276900	-1.12402000
H	3.25711100	1.68704300	-1.76836500
H	1.53995100	1.96894000	-1.39722600
H	2.19775800	0.29714700	-1.37641700
C	4.01959700	0.54865000	0.63454200
H	4.83847100	0.80285900	-0.06646400
H	3.75072800	-0.51349400	0.46762000
H	4.41994000	0.66768700	1.66098200
C	3.26219000	2.94182400	0.69613700
H	4.16367100	3.20390900	0.10707100
H	3.52491000	3.03892100	1.76899900
H	2.49401400	3.70198800	0.44943300
C	0.07992900	3.02601400	2.11912000
H	1.03621000	3.43227900	2.47621300
H	-0.73889500	2.85774500	2.83130100
C	-0.12457800	2.76540300	0.69315900
H	0.55694500	3.21981400	-0.04254900
H	-1.15121500	2.67329400	0.31068300

Table S19

P-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.32124500	-0.16442100	-0.53700500
C	0.68351000	-1.12178500	-1.38547700
H	1.31137900	-1.79230100	-1.98702900
C	-0.68054700	-1.12706700	-1.38351600
H	-1.30492800	-1.80243100	-1.98327400
N	-1.32323200	-0.17465400	-0.53321600
P	-0.00401500	0.79968800	-0.02491000
C	2.49832800	-0.55164700	0.34780900
C	3.60851100	-1.07962100	-0.58312900
H	3.32987800	-2.03592200	-1.06919500
H	4.52151500	-1.27561000	0.01356200

H	3.86078000	-0.33983900	-1.36903600
C	2.97586100	0.72490400	1.05752600
H	2.19163100	1.13336200	1.73263600
H	3.27775900	1.50638100	0.32993400
H	3.85456500	0.50004900	1.69376900
C	2.07807400	-1.62438300	1.36815300
H	1.66928100	-2.52268600	0.86218200
H	1.30783100	-1.23450500	2.06715800
H	2.94754000	-1.94579200	1.97660600
C	-2.49486800	-0.57083000	0.35484600
C	-2.06349400	-1.63998300	1.37430800
H	-2.92882000	-1.96821700	1.98501600
H	-1.29463000	-1.24384000	2.07131000
H	-1.64882200	-2.53507500	0.86743200
C	-3.60338300	-1.10770200	-0.57298200
H	-4.51325900	-1.31054800	0.02618700
H	-3.31864300	-2.06197900	-1.05948400
H	-3.86344200	-0.37015400	-1.35845100
C	-2.98045400	0.70214000	1.06552500
H	-3.85560700	0.47058800	1.70425700
H	-3.29047900	1.48100100	0.33854900
H	-2.19759400	1.11693800	1.73835500
C	-0.01135500	2.17039600	-1.49093700
H	-0.95686800	2.14427500	-2.05520600
H	0.93272400	2.15149900	-2.05788800
C	-0.01145300	2.69875000	-0.13794100
H	-0.93851900	3.07925200	0.32812900
H	0.91400100	3.08633800	0.32549400

Table S20

As-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.31986100	-0.59584600	-0.34499200
C	0.67985300	-1.84820800	-0.22483400
H	1.29506600	-2.74277100	-0.07208800
C	-0.68152700	-1.84772400	-0.22467300
H	-1.29742900	-2.74183400	-0.07198600
N	-1.32063100	-0.59492600	-0.34569400
As	0.00024700	0.68858500	0.00111800
C	2.77381700	-0.45894400	0.05523900
C	3.56343100	-1.50643300	-0.76359200
H	3.32010900	-2.54766700	-0.47376700
H	4.64678800	-1.36377100	-0.58004600
H	3.37500400	-1.38882400	-1.84922900
C	3.24939200	0.94729100	-0.34476500
H	2.73305300	1.74324300	0.23297900
H	3.11164200	1.12980200	-1.42974100
H	4.32848000	1.05439400	-0.11908200

C	2.94695200	-0.68795800	1.56935600
H	2.58154300	-1.68943600	1.87495500
H	2.39611400	0.07537900	2.15921700
H	4.01726800	-0.62146500	1.85003700
C	-2.77449500	-0.45783000	0.05535900
C	-2.94808500	-0.69059000	1.56885700
H	-4.01825500	-0.62209200	1.84960700
H	-2.39530400	0.06960300	2.16095500
H	-2.58555300	-1.69389900	1.87184400
C	-3.56481800	-1.50265800	-0.76630200
H	-4.64806000	-1.36069300	-0.58151700
H	-3.32113600	-2.54480300	-0.48005100
H	-3.37698600	-1.38155000	-1.85165700
C	-3.24917800	0.94971500	-0.34093300
H	-4.32846000	1.05633600	-0.11595100
H	-3.11090100	1.13517900	-1.42535200
H	-2.73334400	1.74386400	0.23972600
C	0.00091300	2.36290600	-0.89122000
H	-0.91447400	2.66167200	-1.43313100
H	0.91540700	2.65937500	-1.43583700
C	0.00334600	2.58255300	0.67219800
H	-0.91709600	2.96580800	1.14620700
H	0.92617100	2.96352800	1.14368400

Table S21

Sb-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.38758000	-0.82481100	-0.30685300
C	0.68723500	-2.00399000	-0.11916700
H	1.26556500	-2.91723700	0.08323500
C	-0.68834600	-2.00359700	-0.11950800
H	-1.26717000	-2.91658600	0.08268100
N	-1.38803400	-0.82402200	-0.30779200
Sb	0.00019100	0.75522200	0.01447800
C	2.84375800	-0.70335100	0.01812000
C	3.59462000	-1.77371400	-0.80956700
H	3.37361200	-2.80183300	-0.46009800
H	4.68581500	-1.61694900	-0.69531300
H	3.34157900	-1.70109000	-1.88597800
C	3.28560500	0.69917300	-0.43001100
H	2.76339900	1.48611800	0.16451000
H	3.09086700	0.86013200	-1.50994700
H	4.36811200	0.85256500	-0.25105000
C	3.10011800	-0.89963600	1.52785100
H	2.74013800	-1.89088900	1.87115800
H	2.58331800	-0.11895600	2.12535600
H	4.18372000	-0.83803200	1.75487900
C	-2.84411800	-0.70256400	0.01817100
C	-3.10074800	-0.90437700	1.52701600

H	-4.18442200	-0.84285200	1.75371700
H	-2.58380500	-0.12647300	2.12791000
H	-2.74177600	-1.89723800	1.86665100
C	-3.59561600	-1.76958900	-0.81332900
H	-4.68674500	-1.61332400	-0.69778100
H	-3.37423900	-2.79902600	-0.46797700
H	-3.34314300	-1.69274600	-1.88958500
C	-3.28530300	0.70180100	-0.42471000
H	-4.36814200	0.85436800	-0.24706000
H	-3.08900700	0.86719300	-1.50372500
H	-2.76417300	1.48614400	0.17416900
C	0.00063400	2.73539800	-0.83968800
H	-0.91571100	3.02934800	-1.38496700
H	0.91662000	3.02883800	-1.38582100
C	0.00140600	2.90913900	0.72623900
H	-0.91878800	3.31334300	1.18577200
H	0.92235700	3.31255400	1.18489300

Table S22

Bi-C_2H_4-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.42797800	-1.03238600	-0.32592500
C	0.70522700	-2.15681400	-0.10782400
H	1.24593700	-3.08069700	0.15896300
C	-0.70646900	-2.15636800	-0.10799500
H	-1.24779100	-3.07991800	0.15872400
N	-1.42858600	-1.03156800	-0.32667200
Bi	0.00016300	0.74176100	0.02314200
C	2.88843600	-0.98297600	0.00364200
C	3.59542000	-2.08851900	-0.82122800
H	3.32437000	-3.10583400	-0.47462200
H	4.69213700	-1.98273600	-0.70166300
H	3.35218400	-2.00258300	-1.89895000
C	3.39562200	0.39917100	-0.44278300
H	2.91089400	1.21343400	0.14571900
H	3.21325300	0.56940300	-1.52311000
H	4.48364700	0.49674800	-0.25825100
C	3.12787900	-1.19059500	1.51525500
H	2.72566600	-2.16484400	1.86085100
H	2.64696600	-0.38703000	2.11246600
H	4.21306500	-1.17599600	1.74040900
C	-2.88898900	-0.98195700	0.00373300
C	-3.12858400	-1.19418900	1.51465100
H	-4.21380800	-1.17950200	1.73960700
H	-2.64728400	-0.39295600	2.11464000
H	-2.72731700	-2.16984300	1.85727800
C	-3.59658800	-2.08462400	-0.82454000
H	-4.69322900	-1.97927100	-0.70391500
H	-3.32516500	-3.10311200	-0.48162500

H	-3.35396100	-1.99496000	-1.90209400
C	-3.39566300	0.40178500	-0.43835700
H	-4.48395500	0.49853600	-0.25496200
H	-3.21227100	0.57580300	-1.51791600
H	-2.91182300	1.21395500	0.15371700
C	0.00088300	2.83252600	-0.83467100
H	-0.91549900	3.10674700	-1.38934600
H	0.91695200	3.10592600	-1.39025400
C	0.00172300	3.03624200	0.68100800
H	-0.91932200	3.44960800	1.12868500
H	0.92371200	3.44856000	1.12771100

Table S23

N-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.38391400	0.40023100	1.76707900
C	0.54281200	-0.35355800	2.53878200
H	0.18598100	-1.16641000	3.17702400
C	1.80110300	0.13163800	2.45779200
H	2.67829200	-0.20521700	3.01675400
N	1.89181400	1.27731700	1.61947000
N	0.45849500	1.55397600	1.38816400
C	-1.34895800	-0.28532100	0.79332400
C	-1.70967700	-1.63403500	1.45654600
H	-0.85121600	-2.33336500	1.48333100
H	-2.50722100	-2.11255500	0.85531100
H	-2.10391700	-1.49595800	2.48335800
C	-2.64572000	0.54869600	0.69802800
H	-3.04351600	0.77498000	1.70728200
H	-3.41624300	-0.02976500	0.15041000
H	-2.53448800	1.50254100	0.14409300
C	-0.73510100	-0.55354100	-0.59033700
H	0.17783800	-1.17606100	-0.51225500
H	-0.48733800	0.37468800	-1.14238100
H	-1.46539700	-1.10936100	-1.21248700
C	2.94801100	1.36563800	0.51185500
C	2.51658800	0.69000000	-0.79976600
H	3.35394000	0.73175300	-1.52533400
H	1.65246000	1.18945100	-1.28108100
H	2.26740100	-0.37742700	-0.63955100
C	4.18997900	0.63600600	1.07242100
H	5.02755700	0.78455200	0.36325800
H	4.02918300	-0.45544700	1.17019200
H	4.50452200	1.05063600	2.05119400
C	3.33390900	2.84624500	0.29952100
H	4.22644100	2.90381900	-0.35490700
H	3.58750600	3.32950300	1.26399200
H	2.55339200	3.45347900	-0.20160400
C	-0.00802800	2.86320000	1.97067100

H	0.81083800	3.44632300	2.41905600
H	-0.94991000	2.76866600	2.53242600
C	-0.01988800	2.64699700	0.49692900
H	0.76610100	3.09629700	-0.12319400
H	-0.96756300	2.42904200	-0.01165000

Table S24

P-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.27308200	-0.10397800	1.23478200
C	0.74259300	-1.07731500	1.46410000
H	0.45393600	-2.10130700	1.71739500
C	2.00125900	-0.58984100	1.40452700
H	2.92285500	-1.14515000	1.60033000
N	2.07539600	0.80564100	1.12352400
P	0.49618500	1.36176600	0.89577500
C	-1.71892800	-0.48944900	0.96460200
C	-2.08807500	-1.66127800	1.89744800
H	-1.56098300	-2.59941100	1.63464900
H	-3.17178700	-1.86764500	1.79631800
H	-1.88347100	-1.41721900	2.95927300
C	-2.63711800	0.70192700	1.29252200
H	-2.48062700	1.56363100	0.61237600
H	-2.51626800	1.03367600	2.34365800
H	-3.69259400	0.39425900	1.15762200
C	-1.85737300	-0.90816000	-0.51279200
H	-1.18028100	-1.75313800	-0.75232000
H	-1.62025200	-0.07035600	-1.20075300
H	-2.89572400	-1.23403200	-0.72502300
C	3.37619300	1.48311600	0.72223200
C	3.63850200	1.21661700	-0.77355200
H	4.60511100	1.66467100	-1.08067000
H	2.84564700	1.65529200	-1.41416700
H	3.68695200	0.12838900	-0.98145400
C	4.51199800	0.89556600	1.58507100
H	5.43977700	1.46803500	1.38824200
H	4.73346000	-0.16135100	1.33836200
H	4.28418800	0.97380900	2.66713600
C	3.27807500	2.99248900	1.00871800
H	4.25029000	3.46968600	0.77639800
H	3.05326000	3.19193700	2.07606400
H	2.52744600	3.50204100	0.37111400
C	-0.11521400	2.99159600	1.31452500
H	0.59527800	3.74946900	1.68810200
H	-1.11661900	3.08577800	1.76954500
C	-0.05574500	2.64614800	-0.24388200
H	0.69032800	3.18660500	-0.85378900
H	-1.01852000	2.52513700	-0.77229400

Table S25

As-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.40321300	-0.29426700	0.58521500
C	-0.68679100	-1.35502200	1.15609700
H	-1.25899300	-2.22584500	1.50478300
C	0.68658300	-1.35511200	1.15609300
H	1.25866100	-2.22599400	1.50481800
N	1.40314000	-0.29439100	0.58531400
As	0.00004600	0.79659300	-0.13011200
C	-2.65392400	-0.59540900	-0.22240000
C	-3.69035600	-1.17801500	0.76731300
H	-3.40019400	-2.17939700	1.14312700
H	-4.66042900	-1.29612600	0.24462800
H	-3.84099100	-0.50326800	1.63325600
C	-3.17398800	0.74177700	-0.77418200
H	-2.46455900	1.17902000	-1.51151500
H	-3.35351100	1.47270800	0.04082200
H	-4.13147800	0.59059200	-1.31058000
C	-2.36145400	-1.58659600	-1.36465400
H	-1.94642400	-2.53984100	-0.97908900
H	-1.63596400	-1.15876100	-2.09008900
H	-3.28979900	-1.82544100	-1.92183500
C	2.65381100	-0.59553200	-0.22236000
C	2.36105000	-1.58551400	-1.36560300
H	3.28943200	-1.82447200	-1.92268000
H	1.63620000	-1.15644100	-2.09094800
H	1.94520900	-2.53885800	-0.98115500
C	3.68976200	-1.17958100	0.76698500
H	4.65986200	-1.29765000	0.24434800
H	3.39905400	-2.18119400	1.14175800
H	3.84056200	-0.50574600	1.63360800
C	3.17467800	0.74184700	-0.77293900
H	4.13220000	0.59058400	-1.30925700
H	3.35437500	1.47204200	0.04268600
H	2.46564900	1.18000800	-1.51011500
C	0.00019100	2.34777300	1.17706100
H	0.93519700	2.44850100	1.75549200
H	-0.93481900	2.44875000	1.75543900
C	0.00028400	2.84955100	-0.22207100
H	0.93219700	3.20431100	-0.69674500
H	-0.93151300	3.20455400	-0.69679800

Table S26

Sb-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.41164200	-0.71897700	-0.46812900
C	0.69682700	-1.85000100	-0.58323300
H	1.20968900	-2.82512600	-0.51732600
C	-0.71483500	-1.84713700	-0.58562600
H	-1.23374400	-2.81869300	-0.51764500
N	-1.42406000	-0.71159000	-0.48017000
Sb	-0.00348800	0.83667700	0.25425100
C	2.82538000	-0.77460400	0.04628600
C	3.67044100	-1.54306200	-0.99990800
H	3.33456200	-2.59274100	-1.11802600
H	4.72667200	-1.56914200	-0.66549700
H	3.62916400	-1.04740100	-1.99019500
C	3.31980500	0.67985300	0.13683400
H	2.77537200	1.24240100	0.93124800
H	3.19998600	1.20443200	-0.83292900
H	4.39315600	0.71679600	0.40922100
C	2.90063700	-1.46059000	1.42687700
H	2.58539800	-2.52274100	1.38024600
H	2.26102600	-0.93936900	2.17004600
H	3.94209600	-1.44028400	1.80620700
C	-2.83302300	-0.75372900	0.04551600
C	-2.86649400	-1.19144200	1.52583500
H	-3.90573300	-1.42400800	1.83447100
H	-2.48933600	-0.39032900	2.19616600
H	-2.25652500	-2.10362700	1.68984200
C	-3.64287600	-1.74209700	-0.83281800
H	-4.72375100	-1.52987600	-0.71343900
H	-3.48180400	-2.79730400	-0.53305000
H	-3.38646500	-1.62742600	-1.90488000
C	-3.39594800	0.66763700	-0.12007900
H	-4.40450700	0.75088800	0.33090900
H	-3.46047200	0.95773100	-1.18750800
H	-2.75661500	1.41220500	0.41386900
C	0.01611100	2.37958100	-1.23656800
H	-0.90652300	2.48776500	-1.83973700
H	0.92596200	2.44404100	-1.86499000
C	0.04955800	3.17719900	0.06724300
H	-0.86221300	3.68066200	0.43387100
H	0.99591500	3.62494000	0.41828100

Table S27

Bi-C_2H_4-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.42095300	-1.12102300	-0.34230500
C	0.70960300	-2.18602200	-0.02146700
H	1.21585000	-3.09487600	0.36004100

C	-0.73172100	-2.18100500	-0.02012800
H	-1.24284600	-3.08546000	0.36544800
N	-1.43566800	-1.11164500	-0.34389500
Bi	0.00314800	0.80576300	0.06173200
C	2.88671100	-1.06922400	-0.03823800
C	3.57387000	-2.21381600	-0.82766500
H	3.29750600	-3.21258000	-0.43376500
H	4.67333000	-2.11304300	-0.73248400
H	3.31242800	-2.17034900	-1.90373500
C	3.39329200	0.28926900	-0.55359000
H	2.91992500	1.13059000	0.00690200
H	3.18856600	0.41436900	-1.63570200
H	4.48489800	0.39131000	-0.39333100
C	3.14944000	-1.21224500	1.47637400
H	2.75328800	-2.16856600	1.87471500
H	2.68391700	-0.38116600	2.04782400
H	4.23909500	-1.19111300	1.67725200
C	-2.90017100	-1.04825700	-0.03783700
C	-3.16415600	-1.19455500	1.47622800
H	-4.25365100	-1.16555400	1.67699700
H	-2.69225000	-0.36934800	2.05085000
H	-2.77588400	-2.15542900	1.87128900
C	-3.59665200	-2.18500600	-0.83083300
H	-4.69524100	-2.07631800	-0.73427600
H	-3.32693300	-3.18700200	-0.44056500
H	-3.33575800	-2.13968700	-1.90695300
C	-3.39677200	0.31570000	-0.54895900
H	-4.48775900	0.42484000	-0.38907100
H	-3.19098900	0.44265400	-1.63065100
H	-2.91761700	1.15203100	0.01414600
C	0.02185400	2.87539700	-0.88399600
H	-0.89197900	3.14723300	-1.44441800
H	0.93692400	3.12736000	-1.45159900
C	0.03275400	3.13112200	0.60153900
H	-0.88259200	3.56001300	1.04649600
H	0.96122400	3.54229900	1.03568500