Supporting Information

Examining the Reactivity of Oxygen-Bridged Intramolecular Group 13 Element/Phosphorus and Boron/Group 15 Element Frustrated Lewis Pairs in 1,2-Addition Reactions with CS_2

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Figure S2. The electron density deformations for the transition states (**B/G15-TS**) are plotted, showing $\Delta\rho_1$ and $\Delta\rho_2$ associated with $\Delta E_{Orb(1)}$ and $\Delta E_{Orb(2)}$ for the singlet–singlet model. In the subplots, red and blue contours represent negative and positive density deformations, with a contour value of $|\Delta\rho| = 0.002$ a.u. for all transition states. All calculations were conducted at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level.

Figure S3. The electron density deformations for the transition states (**B/G15-TS**) are plotted, showing $\Delta\rho_1$ and $\Delta\rho_2$ associated with $\Delta E_{Orb(1)}$ and $\Delta E_{Orb(2)}$ for the triplet–triplet model. In the subplots, red and blue contours represent negative and positive density deformations, with

a contour value of $|\Delta\rho| = 0.002$ a.u. for all transition states. All calculations were conducted at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level.

Table S1. The **G13/P-TS** ASM was analyzed through ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP calculations.[a]

Entry	**B/P-TS**	**Al/P-TS**	**Ga/P-TS**	**In/P-TS**	**Tl/P-TS**
ΔE_{ACT}[b]	7.5	–9.9	–7.8	–6.4	–2.4
$\Delta E_{DEF,CS2}$	24.1	5.1	5.1	6.8	10.4
$\Delta E_{DEF,\ G13/P\text{-}Rea}$	2.8	4.2	3.7	1.8	2.0
ΔE_{INT}	–19.4	–19.2	–16.6	–15.0	–14.8

(a) All in kcal mol^{-1}.

(b) $\Delta E_{ACT} = \Delta E_{DEF,CS2} + \Delta E_{DEF,G13/P\text{-}Rea} + \Delta E_{INT}$.

Table S2. Based on the B3LYP-D3(BJ)/def2-TZVP level of theory, the energy difference (in eV) between the FMOs of the bent O-bridged intramolecular **B/G15-Rea** FLPs and CS_2 for the 1,2-addition reactions is presented in eq. (2).

System	**Energy difference** $\lvert CS_2$ **(LUMO)** $-$ **FLP (HOMO)** $\rvert$	**Energy difference** $\lvert$ **FLP (LUMO)** $-CS_2$ **(HOMO)** $\rvert$
B/N-Rea + CS_2	3.847	7.066
B/P-Rea + CS_2	4.271	7.155
B/As-Rea + CS_2	4.555[(a)]	7.182
B/Sb-Rea + CS_2	4.450[(a)]	7.290[(b)]
B/Bi-Rea + CS_2	4.410[(a)]	7.432[(c)]

(a) According to Figure S1, this value is obtained from $\lvert CS_2$ (LUMO) – FLP (HOMO–1) $\rvert$.

(b) According to Figure S1, this value is obtained from $\lvert$ FLP (LUMO+1) – CS_2 (HOMO) $\rvert$.

(c) According to Figure S1, this value is obtained from $\lvert$ FLP (LUMO+2) – CS_2 (HOMO) $\rvert$.

Table S3. Results from the EDA-NOCV analysis, conducted at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level, show the chemical bonding between **B/G15-Rea** and CS_2 at the transition state (**B/15-TS**). This analysis covers singlet and triplet spin states, with energy values reported in kcal/mol.

Fragments	B/N-TS		B/P-TS		B/As-TS		B/Sb-TS		B/Bi-TS	
	B/N-Rea (S) + CS_2 (S)	B/N-Rea (T) + CS_2 (T)	B/P-Rea (S) + CS_2 (S)	B/P-Rea (T) + CS_2 (T)	B/As-Rea (S) + CS_2 (S)	B/As-Rea (T) + CS_2 (T)	B/Sb-Rea (S) + CS_2 (S)	B/Sb-Rea (T) + CS_2 (T)	B/Bi-Rea (S) + CS_2 (S)	B/Bi-Rea (T) + CS_2 (T)
ΔE_{INT} [a]	-20.3	-156.2	-19.4	-169.7	-18.0	-149.5	-21.2	-129.1	-18.5	-146.6
ΔE_{Pauli}	154.2	231.5	84.7	82.9	112.8	96.7	182.5	164.6	175.5	218.9
ΔE_{Elstat} [b]	-74.3 (42.6 %)	-139.3 (35.9 %)	-48.2 (46.3 %)	-46.0 (18.2 %)	-60.5 (46.2 %)	-65.3 (26.5 %)	-94.2 (46.3 %)	-110.3 (37.5 %)	-97.3 (50.2 %)	-121.0 (33.1 %)
ΔE_{Orb} [b]	-84.5 (48.4 %)	-232.2 (60.0 %)	-43.4 (41.7 %)	-194.2 (76.9 %)	-58.2 (44.5 %)	-168.8 (68.5 %)	-97.7 (48.0 %)	-171.6 (58.5 %)	-83.7 (43.2 %)	- 231.5 (63.3 %)
$\Delta E_{Orb\ (1)}$ [c]	-48.2 (57.1 %)	-133.4 (57.3 %)	-35.7 (82.3 %)	- 120.3 (61.9 %)	-47.6 (81.9 %)	- 104.1 (61.7 %)	- 79.5 (81.3 %)	- 94.1 (54.8 %)	- 69.8 (83.4 %)	- 107.6(46.5 %)
$\Delta E_{Orb\ (2)}$ [c]	-24.4 (28.9 %)	-12.5 (5.4 %)	-3.0 (6.9 %)	-12.4 (6.4 %)	-3.5 (5.9 %)	- 17.4 (10.3 %)	- 6.7(6.9 %)	- 30.3 (17.7 %)	-4.2 (5.0 %)	- 29.3 (12.7 %)
ΔE_{Rest} [c]	-11.8 (14.0 %)	-86.9 (37.3 %)	-4.7 (10.8 %)	-61.5 (31.7 %)	-7.1 (12.2 %)	-47.2 (28.0 %)	- 11.5 (11.7 %)	- 47.2 (27.5 %)	- 9.8 (11.7 %)	- 94.6 (40.9 %)
ΔE_{Disper} [b]	-15.6 (9.0 %)	-15.6 (4.0 %)	-12.5 (12.0 %)	-12.5 (4.9 %)	-12.2 (9.3 %)	-12.2 (4.9 %)	-11.7 (5.8 %)	- 11.7 (4.0 %)	- 13.0 (6.7 %)	- 13.0 (3.6 %)

(a) $\Delta E_{INT} = \Delta E_{Elstat} + \Delta E_{Pauli} + \Delta E_{Orb} + \Delta E_{Disper}$.

(b) The values in parentheses offer the percentage contribution to the total attractive interactions ($\Delta E_{Elstat} + \Delta E_{Orb} + \Delta E_{Disper}$).

(c) The values in parentheses offer the percentage contribution to the total orbital interactions (ΔE_{Orb}).

Table S4. The **B/G15-TS** ASM was analyzed through ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP calculations.[a]

Entry	**B/N-TS**	**B/P-TS**	**B/As-TS**	**B/Sb-TS**	**B/Bi-TS**
ΔE_{ACT}[b]	15.0	7.5	10.7	17.6	82.1
$\Delta E_{DEF,CS2}$	28.1	24.1	28.0	35.6	94.0
$\Delta E_{DEF,\ B/G15\text{-}Rea}$	7.2	2.8	0.7	3.2	6.6
ΔE_{INT}	–20.3	–19.4	–18.0	–21.2	–18.5

(a) All in kcal mol^{-1}.

(b) $\Delta E_{ACT} = \Delta E_{DEF,CS2} + \Delta E_{DEF,B/G15\text{-}Rea} + \Delta E_{INT}$.

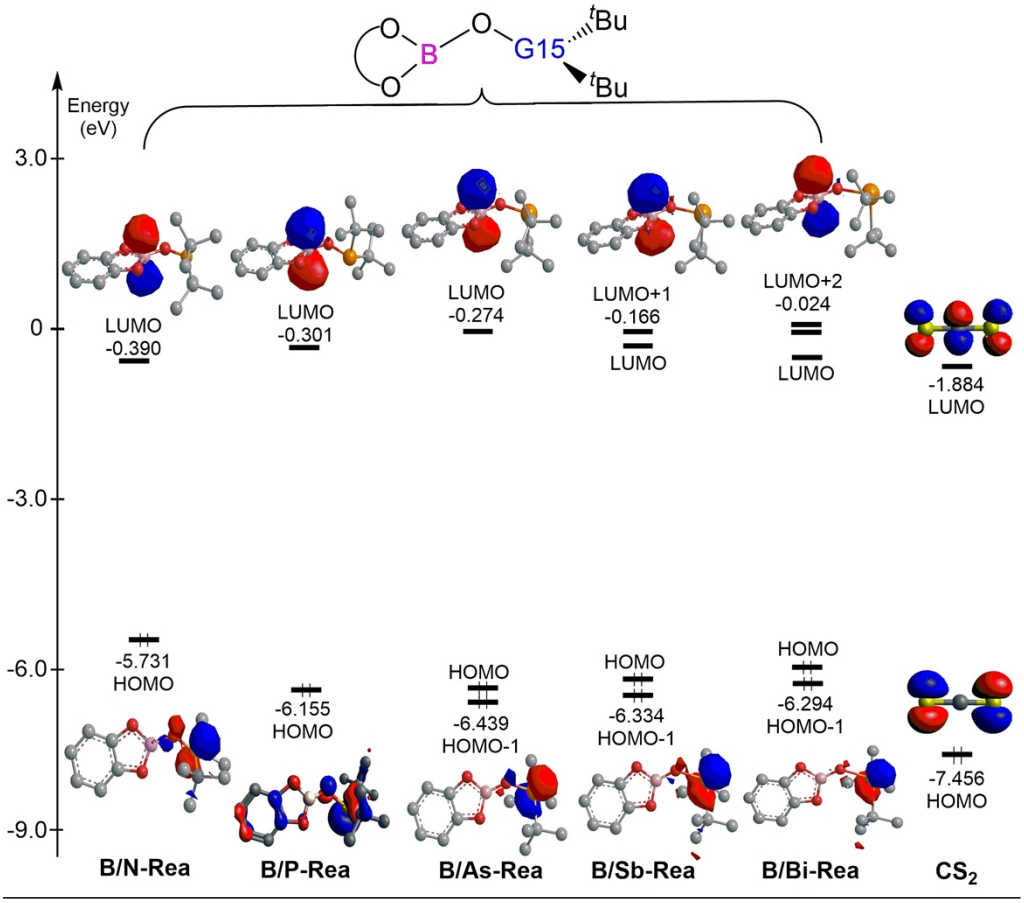
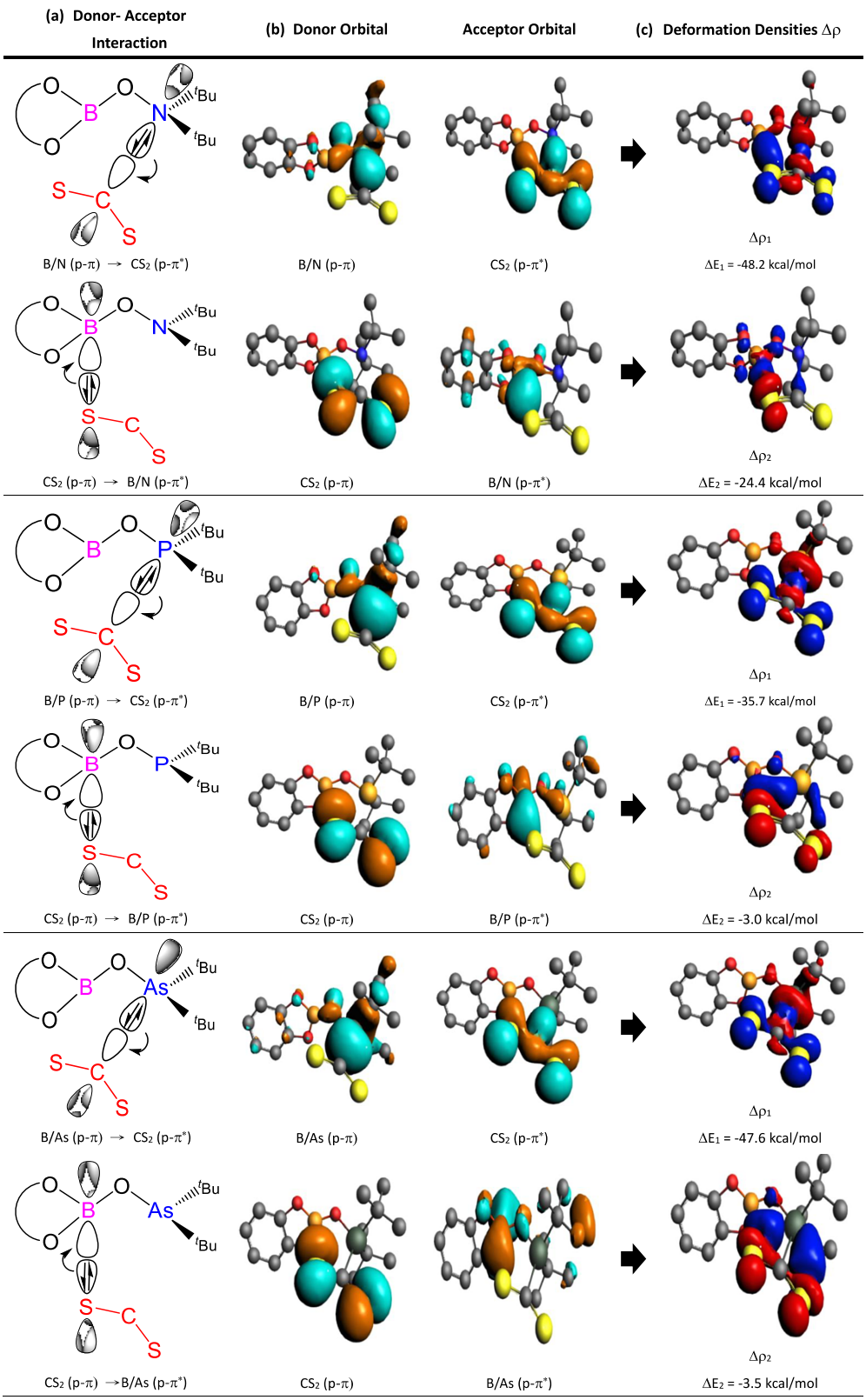


Figure S1. The HOMOs and LUMOs, including their energy values (in eV), for the bent O-bridged intramolecular **B/G15-Rea** FLP-type molecules and CS_2 are listed.


(a) Donor- Acceptor Interaction
(b) Donor Orbital
Acceptor Orbital
(c) Deformation Densities Δρ
B/N (p-π) → CS2 (p-π*)
B/N (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -48.2 kcal/mol
CS2 (p-π) → B/N (p-π*)
CS2 (p-π)
B/N (p-π*)
Δρ2
ΔE2 = -24.4 kcal/mol
B/P (p-π) → CS2 (p-π*)
B/P (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -35.7 kcal/mol
CS2 (p-π) → B/P (p-π*)
CS2 (p-π)
B/P (p-π*)
Δρ2
ΔE2 = -3.0 kcal/mol
B/As (p-π) → CS2 (p-π*)
B/As (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -47.6 kcal/mol
CS2 (p-π) →B/As (p-π*)
CS2 (p-π)
B/As (p-π*)
Δρ2
ΔE2 = -3.5 kcal/mol

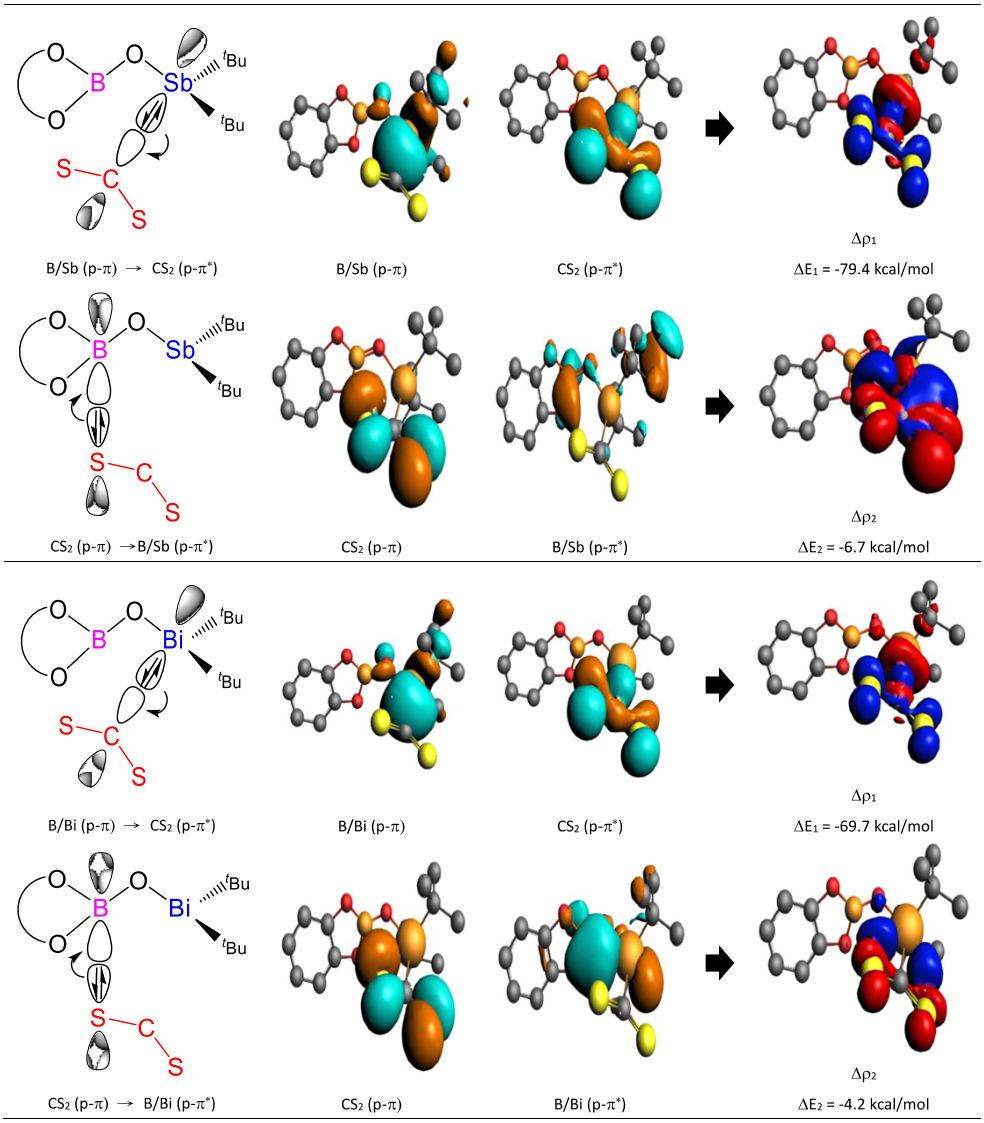
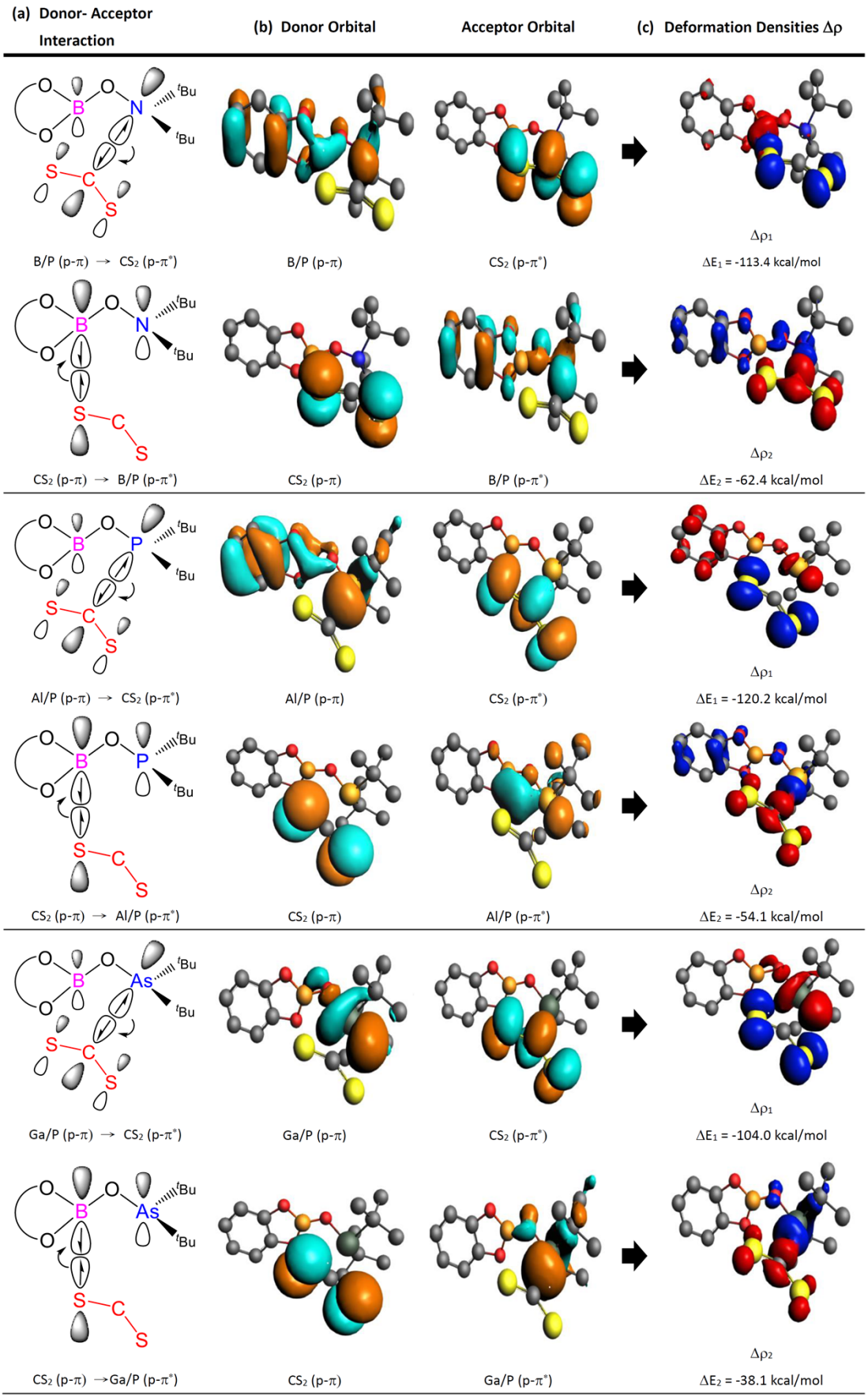


Figure S2. The electron density deformations for the transition states (**B/G15-TS**) are plotted, showing $\Delta\rho_1$ and $\Delta\rho_2$ associated with $\Delta E_{\mathrm{Orb}(1)}$ and $\Delta E_{\mathrm{Orb}(2)}$ for the singlet–singlet model. In the subplots, red and blue contours represent negative and positive density deformations, with a contour value of $|\Delta\rho| = 0.002$ a.u. for all transition states. All calculations were conducted at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level.


(a) Donor- Acceptor Interaction
(b) Donor Orbital
Acceptor Orbital
(c) Deformation Densities Δρ
B/P (p-π) → CS2 (p-π*)
B/P (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -113.4 kcal/mol
CS2 (p-π) → B/P (p-π*)
CS2 (p-π)
B/P (p-π*)
Δρ2
ΔE2 = -62.4 kcal/mol
Al/P (p-π) → CS2 (p-π*)
Al/P (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -120.2 kcal/mol
CS2 (p-π) → Al/P (p-π*)
CS2 (p-π)
Al/P (p-π*)
Δρ2
ΔE2 = -54.1 kcal/mol
Ga/P (p-π) → CS2 (p-π*)
Ga/P (p-π)
CS2 (p-π*)
Δρ1
ΔE1 = -104.0 kcal/mol
CS2 (p-π) →Ga/P (p-π*)
CS2 (p-π)
Ga/P (p-π*)
Δρ2
ΔE2 = -38.1 kcal/mol

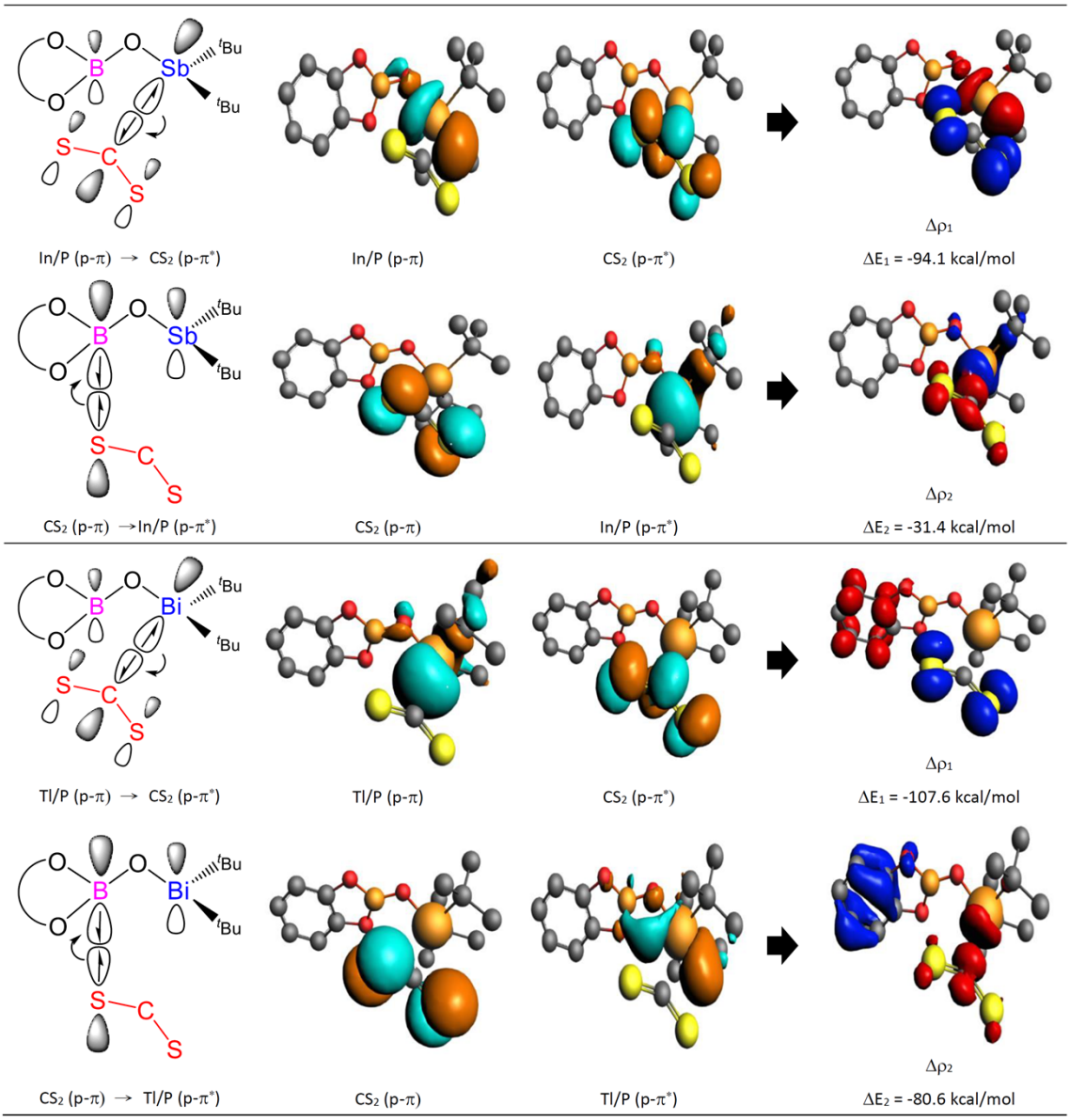


Figure S3. The electron density deformations for the transition states (**B/G15-TS**) are plotted, showing $\Delta\rho_1$ and $\Delta\rho_2$ associated with $\Delta E_{\mathrm{Orb}(1)}$ and $\Delta E_{\mathrm{Orb}(2)}$ for the triplet–triplet model. In the subplots, red and blue contours represent negative and positive density deformations, with a contour value of $|\Delta\rho| = 0.002$ a.u. for all transition states. All calculations were conducted at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level.

(All were calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory)

Table S1
B/P-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	1.40843400	-0.83888500	2.88123500
C	0.57401600	-0.18521800	2.62356300
C	-1.59648700	1.54629800	1.92025800
C	-0.66160400	-0.25165400	3.29056400
C	0.68897900	0.75696800	1.61406300
C	-0.37459000	1.60277700	1.27088200
C	-1.72285200	0.59454300	2.94724900
H	-0.79421500	-0.97996800	4.09349100
H	-2.66924600	0.51544500	3.48642400
H	-2.41575600	2.21064300	1.64168100
O	1.76437100	1.03915400	0.81221500
O	0.02394600	2.42397000	0.24453500
B	1.35278600	2.07580800	-0.02817200
O	2.14492700	2.60719200	-0.96101400
P	2.52820800	4.04823900	-1.76262900
C	3.21354300	5.01537800	-0.27101600
C	0.83575900	4.76457600	-2.27487900
C	-0.07720600	5.36319300	-1.19872300
H	0.36572700	6.25121400	-0.72597500
H	-0.32532100	4.63092200	-0.42071400
H	-1.02388400	5.68535500	-1.66726300
C	1.17137800	5.83963200	-3.32867000
H	1.80539800	5.43563600	-4.13326100
H	1.68808800	6.70688000	-2.89274400
H	0.23748900	6.20769200	-3.78580000
C	0.10477300	3.60401000	-2.97796600
H	0.74774700	3.10575400	-3.72175300
H	-0.77813000	3.99785500	-3.50900300
H	-0.24460100	2.85041900	-2.25935900
C	2.41724200	4.87671900	1.03249600

H	2.90897200	5.46667000	1.82485500
H	2.39900200	3.83501400	1.38709800
H	1.38363100	5.22974600	0.94506900
C	3.35606800	6.49214700	-0.66889300
H	3.86113100	6.60554500	-1.64211100
H	3.96813600	7.01970100	0.08191800
H	2.38568900	7.00566000	-0.72305400
C	4.61851800	4.41648100	-0.05500300
H	5.25317500	4.54344700	-0.94550500
H	4.56406000	3.34092500	0.17321900
H	5.11317400	4.91905300	0.79360000

Table S2
Al/P-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	2.13500600	-0.20375300	3.52773000
C	1.08404800	-0.24120700	3.23481700
C	-1.63009400	-0.29399400	2.44415700
C	0.20695500	-1.20405600	3.75373100
C	0.59862600	0.69061800	2.32224700
C	-0.76388900	0.66374300	1.92676100
C	-1.13498400	-1.23066300	3.36257200
H	0.57986400	-1.93902900	4.47070600
H	-1.80754900	-1.98662300	3.77419000
H	-2.67423400	-0.29722400	2.12572000
O	1.36013900	1.67869400	1.75075500
O	-1.13734300	1.63094600	1.02535200
Al	0.28826300	2.56794500	0.70264700
O	0.52580600	3.92637500	-0.26598400
P	2.01512600	4.62912100	-0.68340800
C	2.00627300	6.06597700	0.56719700
C	1.57242500	5.25436900	-2.41835500
C	0.46103200	6.30422400	-2.50010000
H	0.78433700	7.27706000	-2.10353400
H	-0.43731400	5.98306100	-1.95263000
H	0.17492200	6.46106300	-3.55465700
C	2.86885200	5.78004600	-3.05826200
H	3.68133100	5.03851300	-2.99210000
H	3.21999400	6.71068300	-2.59033200
H	2.69394800	5.99214700	-4.12656500
C	1.12616900	3.98878900	-3.17791400
H	1.88080100	3.18737300	-3.11387700
H	0.98405700	4.23093500	-4.24438200
H	0.17503200	3.60062700	-2.78591400
C	0.64888800	6.74842900	0.77155300
H	0.69732400	7.41134900	1.65252000
H	-0.14522900	6.00830500	0.94880900

H	0.35253100	7.36163000	-0.08740100
C	3.08139000	7.08492400	0.16473800
H	4.04235300	6.59685800	-0.06903300
H	3.26127400	7.78665500	0.99643400
H	2.77653700	7.67997300	-0.70855700
C	2.42667400	5.39583000	1.89214500
H	3.40151100	4.89100500	1.80550200
H	1.69463700	4.64191700	2.22903900
H	2.49762800	6.15433400	2.68962500

Table S3
Ga/P-Rea

Atomic	Coordinates (Angstroms)		
	X	Y	Z
H	-0.08179100	-0.04964000	1.64239700
C	-0.20063800	0.02234100	2.72588000
C	-0.50953000	0.19347100	5.49631600
C	-0.77555600	-1.03474900	3.43828600
C	0.22645200	1.17885500	3.39079600
C	0.07448200	1.26585600	4.77323100
C	-0.93338900	-0.95342900	4.82768000
H	-1.10597700	-1.93284200	2.91148000
H	0.67689100	2.01590200	2.85396600
H	-1.38086300	-1.76627600	5.40283600
O	0.46694100	2.36066400	5.49663000
O	-0.62821800	0.35072500	6.85092400
Ga	0.07238600	1.98791600	7.23260800
O	0.29525800	2.96298600	8.68136300
P	0.40613800	2.26428000	10.23278600
C	2.24116900	1.73905800	10.21793400
C	3.26827900	2.86239200	10.05880400
C	2.49097900	0.93948000	11.50825000
C	2.36757300	0.77257300	9.02282700
H	3.02919000	3.50392700	9.19754900
H	3.32693100	3.49426800	10.95575000
H	4.27243500	2.43452700	9.89294400
H	2.43870600	1.57218200	12.40490600
H	3.49706400	0.48792200	11.48008700
H	1.75918200	0.12433200	11.62474700
H	2.37290500	1.30851400	8.05535800
H	1.57076900	0.01061500	9.00707200
H	3.33220500	0.24084000	9.06769100
C	0.18621800	3.87431400	11.21590900
C	0.63319900	3.64854100	12.66667300
C	-1.34087200	4.09629700	11.18402800
C	0.87487800	5.10428500	10.61209900

H	1.72804800	3.59866500	12.75735700
H	0.20857200	2.72336800	13.09017000
H	0.28837400	4.48706300	13.29482900
H	-1.59786100	5.00592400	11.75242600
H	-1.88470100	3.24862800	11.62912100
H	-1.70126200	4.22997800	10.15237800
H	0.64827900	5.19973200	9.54102100
H	0.50961200	6.01279300	11.12091500
H	1.96450300	5.07623600	10.73153000

Table S4
In/P-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	-0.41511600	-0.18718700	1.39648800
C	-0.43507800	-0.11665800	2.48652500
C	-0.47946400	0.06127400	5.28599400
C	-0.85377100	-1.20773700	3.25458000
C	-0.04059800	1.07213100	3.10831500
C	-0.05284200	1.17341100	4.50304600
C	-0.88099500	-1.11764900	4.64974600
H	-1.16284100	-2.13591600	2.76823300
H	0.28603200	1.93806400	2.52894700
H	-1.20796000	-1.95489300	5.26968700
O	0.32543300	2.32152500	5.12558600
O	-0.49844300	0.16796600	6.64067900
In	0.10546100	2.05440300	7.13740700
O	0.47644400	3.17990700	8.72501200
P	0.47139200	2.38899400	10.23170200
C	2.28416700	1.79687300	10.31549300
C	3.35231600	2.89258800	10.28603600
C	2.42051000	0.92113700	11.57255700
C	2.46552900	0.89246200	9.07965600
H	3.18767500	3.58665600	9.44826600
H	3.36941700	3.47317400	11.21862500
H	4.35284500	2.44263000	10.16182700
H	2.32761800	1.50614400	12.49768500
H	3.41114100	0.43582800	11.58600600
H	1.65661500	0.12764100	11.59490300
H	2.55303200	1.48399000	8.15008100
H	1.65183300	0.15466400	8.96930000
H	3.40695900	0.32431400	9.15896100
C	0.23053500	3.94035000	11.30153400
C	0.58113300	3.62354300	12.76131300
C	-1.28533700	4.20759000	11.18959900
C	0.98697400	5.17973600	10.80758800

H	1.66654300	3.53806000	12.91582400
H	0.10783100	2.68937100	13.10584800
H	0.21907000	4.43650000	13.41312200
H	-1.55438500	5.09278500	11.79003700
H	-1.87693200	3.35337300	11.55402300
H	-1.57626200	4.40595100	10.14650500
H	0.82977400	5.33569600	9.73102800
H	0.61468400	6.07118200	11.34089100
H	2.06602600	5.11263500	10.99089900

Table S5
Tl/P-Rea

Atomic	Coordinates (Angstroms)		
	X	Y	Z
H	-2.54910300	0.46285300	1.81420900
C	-1.89976400	0.35130200	2.68565000
C	-0.21014500	0.07471400	4.91364500
C	-1.35120300	-0.89556200	3.00148000
C	-1.62038800	1.46391400	3.48279500
C	-0.77159900	1.34933900	4.59253200
C	-0.52018000	-1.03487100	4.11583800
H	-1.56797300	-1.76693900	2.37927600
H	-2.04245000	2.44547100	3.25893400
H	-0.08486000	-1.99906400	4.38502900
O	-0.48660000	2.42212400	5.35191100
O	0.60894000	-0.05595100	5.97524100
Tl	0.75231000	1.81965100	7.00518600
O	1.71480200	2.75041800	8.58660400
P	1.08051700	2.15971500	10.06343700
C	2.71329700	1.73854600	10.93237500
C	3.68228800	2.90981000	11.11860300
C	2.38038600	1.07723800	12.27989700
C	3.36525600	0.68477800	10.01413600
H	3.82786000	3.46243700	10.17853000
H	3.33371200	3.61302400	11.88803900
H	4.66670000	2.52983700	11.44385700
H	1.95963100	1.78807600	13.00394500
H	3.30099200	0.66031700	12.72239500
H	1.66358000	0.24936000	12.15780900
H	3.67250100	1.12523600	9.05490900
H	2.68261500	-0.15646500	9.80920800
H	4.26366900	0.27407000	10.50417300
C	0.33584000	3.78417200	10.71745200
C	0.04947100	3.65026900	12.21924800
C	-1.00400100	3.89503600	9.95956000
C	1.17051200	5.03676900	10.42131500

H	0.97062300	3.69269100	12.81834600
H	-0.47466300	2.70961800	12.45729500
H	-0.59658200	4.48134600	12.54934600
H	-1.55489300	4.78754000	10.30038300
H	-1.64394000	3.01448200	10.12752900
H	-0.84750100	4.00791400	8.87425300
H	1.48851500	5.05934900	9.36902800
H	0.56304100	5.93803700	10.61453600
H	2.06575100	5.10191300	11.05162800

Table S6
B/P-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	0.352072589006	0.812886013260	4.651581429384
C	0.028921376407	0.452858950580	3.673402463738
C	-0.795972271644	-0.462311479358	1.097963477628
C	-0.810883904682	-0.668839019183	3.532963243574
C	0.436733341025	1.091226397030	2.513304717617
C	0.029960956821	0.640452616556	1.244603103548
C	-1.214662541248	-1.116813628577	2.272490223082
H	-1.149156048113	-1.197003848586	4.427372011661
H	-1.864853899409	-1.991048768620	2.192985518311
H	-1.103444512056	-0.802146585713	0.107515402289
O	1.238555609842	2.186056403656	2.378207707847
O	0.564738113490	1.442383935322	0.280402501454
B	1.385090253142	2.403318678926	0.970810607346
O	1.135425670552	3.792947908641	0.554910337069
P	2.142293475048	4.609872201039	-0.356538476406
C	2.519402572192	6.156602206659	0.611629978987
C	1.341628740801	4.737529946124	-2.035066355980
C	-0.125261090456	5.163389602953	-1.841100089670
H	-0.216443407825	6.190056200448	-1.461312687511
H	-0.654081344539	4.485514459165	-1.157352118323
H	-0.626460846522	5.125804729012	-2.821321761920
C	2.083527569979	5.715054257847	-2.956907212760
H	3.157746794178	5.489066445129	-3.010334773093
H	1.956981554437	6.758211260790	-2.635660847461
H	1.659703863730	5.626586350075	-3.970016395759
C	1.381631028113	3.310171261814	-2.621532966482
H	2.409880986868	2.989242764224	-2.837263661956
H	0.820873869106	3.317146840174	-3.569573802094
H	0.910518044120	2.572912499921	-1.954929506715
C	1.188666155245	6.851623191870	0.952460178460
H	1.395232088333	7.664731292105	1.666324205929
H	0.474349025448	6.159233373372	1.419509302069
H	0.720884021285	7.302155916633	0.065938871384
C	3.460350387973	7.114754202361	-0.131648539908
H	4.380217581748	6.611189658314	-0.457854076771
H	3.733099610458	7.931070138343	0.556312525772
H	2.981687252473	7.567228980139	-1.009898812111
C	3.189748913681	5.656598318303	1.908827957353
H	4.164295406797	5.189978745368	1.707886263750
H	2.557996846526	4.937047384007	2.448848024934

H	3.357592864756	6.525230174958	2.564713252818
C	3.626990750949	3.535617451982	-0.446400743750
S	3.368367015665	2.097214849620	0.427116884013
S	4.950232536301	4.038990723321	-1.303768361346

Table S7
Al/P-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-2.048838817026	0.200160125352	0.083540808883
C	-1.219998491847	0.170602421405	0.794062219454
C	0.920349954879	0.038963711458	2.627875877044
C	-0.677213103810	-1.061754232513	1.147229701084
C	-0.692026928873	1.342630716315	1.358238059965
C	0.367526451330	1.277441985982	2.265884128376
C	0.403050518645	-1.128434497921	2.072779363634
H	-1.116992012340	2.311036221466	1.083063909892
H	0.771601123102	2.194847833375	2.700910385529
H	1.748036075026	-0.033463087444	3.336721228168
O	-1.112149149614	-2.261305704507	0.659454402580
O	0.863131640612	-2.382821612934	2.351906805001
Al	-0.087693971196	-3.499052934254	1.375398597170
O	0.850854311500	-4.535606285476	0.254071213956
P	0.891875694061	-6.106919247611	0.338718989913
C	-0.277855909924	-6.591588738990	1.684282156028
S	-1.084144918678	-5.278683641129	2.466426299387
S	-0.468602565949	-8.191279758798	2.031280320353
C	2.635151279778	-6.533066072320	0.854323887630
C	0.225912006364	-6.710887460270	-1.297715504046
C	3.602941087566	-5.762828847640	-0.064142481450
C	2.773099506124	-5.997011217571	2.295622648705
C	2.928512312297	-8.038753459165	0.811504840682
C	0.279686445061	-8.236091039982	-1.457967280348
C	-1.238382350540	-6.222416987303	-1.337566986504
C	1.026205519490	-6.019083858035	-2.418323336477
H	2.118859494123	-6.531689063553	2.998778502947
H	2.562359772532	-4.918464208096	2.358842518776
H	3.814480871914	-6.149421039433	2.619626133732
H	3.369744985743	-4.688896542752	-0.090556386519
H	3.598506491452	-6.151088433956	-1.092362461193
H	4.623122147070	-5.886159399872	0.332984461592
H	2.193901859591	-8.617861660565	1.387127790594
H	2.948483869285	-8.422566365714	-0.218151163174
H	3.925473611232	-8.210011955470	1.248094493349
H	1.076651992534	-4.930739633824	-2.273397641061
H	2.048123227245	-6.415690026340	-2.499285729246
H	0.518860379571	-6.214796759116	-3.376128456606
H	1.311994862181	-8.610656399489	-1.506624533393
H	-0.215324848062	-8.498969308623	-2.406816576964

H	-0.238434983949	-8.754801180432	-0.639404591128
H	-1.311679903494	-5.130238044574	-1.226539851948
H	-1.663063126027	-6.488503484658	-2.318033538511
H	-1.853845408979	-6.701700825023	-0.562258225854

Table S8
Ga/P-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-1.950991386654	0.478661860252	0.392591094500
C	-1.075593538878	0.328076192688	1.027925157986
C	1.172045434473	-0.117595284006	2.661868215124
C	-0.650909398377	-0.974384712489	1.286105199988
C	-0.377461097516	1.410019233996	1.583541556819
C	0.738371874550	1.188831594218	2.394331184943
C	0.486438181001	-1.200522725202	2.112606918742
H	-0.712735537702	2.429628020501	1.378623911032
H	1.278804754218	2.034908461274	2.825784005659
H	2.040576951025	-0.312815905580	3.294681025091
O	-1.282792169487	-2.072296182215	0.777899477454
O	0.847631160150	-2.496343367747	2.328240113370
Ga	-0.340718674519	-3.533882676314	1.366801485551
O	0.556330758723	-4.555783930375	0.036800884651
P	0.739777609440	-6.103345129725	0.228280460573
C	-0.445352118172	-6.643444278721	1.544600927815
S	-1.318124730067	-5.388599256374	2.356098996166
S	-0.596994096588	-8.251614610332	1.863452690602
C	2.477516549691	-6.358952802799	0.872574483612
C	0.250925912500	-6.867946383649	-1.406437014538
C	3.444182507660	-5.731228675562	-0.148652867912
C	2.544598556936	-5.569666042395	2.197752490407
C	2.836212833058	-7.828880593088	1.124640286249
C	0.689327654869	-8.331110768901	-1.547380047545
C	-1.284962392004	-6.753014651320	-1.482611887878
C	0.874985981048	-6.006511345224	-2.522055497440
H	1.856516194345	-5.976347780368	2.953232416500
H	2.336479395259	-4.497314755927	2.070683859221
H	3.566599231429	-5.663183690701	2.597266584445
H	3.151162013259	-4.704297176766	-0.408084956826
H	3.514650069621	-6.327940319206	-1.069244152273
H	4.449136473040	-5.696094433626	0.300597182678
H	2.153340155083	-8.301798697586	1.842161869481
H	2.834397277230	-8.425884580494	0.204008481411
H	3.854601324165	-7.864287047894	1.543936747340
H	0.583811784345	-4.952042763085	-2.430044216921
H	1.971385541900	-6.065606402885	-2.531064291154
H	0.512429565889	-6.386812270992	-3.490113088858
H	1.781862546309	-8.423756193867	-1.623556890265
H	0.259116569092	-8.734003317766	-2.478339698931

H	0.338090628779	-8.947327173890	-0.708995121793
H	-1.625559223800	-5.722053813786	-1.305650699526
H	-1.604933730634	-7.041568751013	-2.496055048723
H	-1.781925394683	-7.419486871057	-0.765329226825

Table S9
In/P-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-1.898321039567	0.797976928267	0.586177911585
C	-1.003725473209	0.584143460119	1.175272666575
C	1.274180258739	-0.024840814120	2.686108600664
C	-0.670715525248	-0.754407564032	1.405452231503
C	-0.204162576346	1.613723985139	1.685660464856
C	0.932478411349	1.309820408059	2.439070288942
C	0.491564673307	-1.066868037808	2.177005625767
H	-0.475303717485	2.654452274568	1.491849488656
H	1.558331251782	2.111007286789	2.839968893921
H	2.155601834844	-0.286432629212	3.276064160819
O	-1.444419462939	-1.757358063250	0.909664569115
O	0.810194572921	-2.363648681850	2.410675686387
In	-0.609365630136	-3.538249761668	1.483962148221
O	0.373636555226	-4.670524996293	-0.043929666692
P	0.661135227866	-6.187867096658	0.175854447130
C	-0.495761157612	-6.843180280326	1.474695857127
S	-1.494366192918	-5.720725427680	2.342425854605
S	-0.531317490782	-8.465468956391	1.750823713847
C	2.400406870625	-6.324093533686	0.861136004289
C	0.274481941600	-7.015720238378	-1.460232134327
C	3.346435436293	-5.683978950632	-0.171786880229
C	2.406084334550	-5.479179852219	2.153185990635
C	2.841930673687	-7.757654207032	1.180647510063
C	0.858790384312	-8.427431298915	-1.594034662115
C	-1.263132002489	-7.052075009725	-1.566147373199
C	0.829019114542	-6.099548562259	-2.569818682051
H	1.703060193798	-5.868891908829	2.904664233849
H	2.186614518272	-4.415896446634	1.975880721504
H	3.414820403633	-5.532546033448	2.591953787035
H	2.995560610807	-4.689663632490	-0.481726688103
H	3.469826580112	-6.315595025782	-1.063211910489
H	4.339056845897	-5.566043758748	0.290638888153
H	2.202079712790	-8.225871702189	1.939437120451
H	2.851002132917	-8.404343466126	0.294578846672
H	3.869432022178	-7.717732390055	1.576978931728
H	0.429889742445	-5.080306145427	-2.489516038205
H	1.925495801126	-6.044378694956	-2.556633396515
H	0.527392313440	-6.520264420930	-3.542099238953
H	1.956956777087	-8.411597777692	-1.640407463171
H	0.496925932895	-8.864441894477	-2.538762165014

H	0.547144835611	-9.081454968836	-0.769172413096
H	-1.704329675867	-6.059715052296	-1.389723431995
H	-1.535479343398	-7.362586904679	-2.587038127012
H	-1.706877676656	-7.768155157213	-0.862121372934

Table S10
Tl/P-Prod

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.90537200	0.96100900	0.67790000
C	-1.01201400	0.73129000	1.26245900
C	1.25964000	0.08359100	2.75796200
C	-0.69545400	-0.61719000	1.47478200
C	-0.20138100	1.74736700	1.77911000
C	0.93390700	1.42349400	2.52586400
C	0.46736100	-0.95151700	2.24142600
H	-0.46199500	2.79229500	1.59357600
H	1.57201400	2.21250700	2.93161800
H	2.14021400	-0.19302400	3.34190900
O	-1.47907900	-1.58401800	0.94916300
O	0.79628200	-2.23819000	2.45664100
Tl	-0.69614000	-3.50122200	1.52342100
O	0.37495000	-4.70767400	-0.11271300
P	0.66198400	-6.21195500	0.13170200
C	-0.49287400	-6.88302300	1.43086400
S	-1.53695200	-5.79771000	2.28119700
S	-0.51471000	-8.50208800	1.73413500
C	2.39767800	-6.34854800	0.83080800
C	0.28861200	-7.08863000	-1.48693300
C	3.35297400	-5.76252000	-0.22625800
C	2.40803500	-5.44917800	2.08560100
C	2.82789100	-7.77045700	1.21263300

C	0.89289700	-8.49451700	-1.59144200
C	-1.24762900	-7.14763600	-1.60003700
C	0.83523800	-6.18920400	-2.61373600
H	1.69213500	-5.79516800	2.84707500
H	2.20279900	-4.39294600	1.85766700
H	3.41194900	-5.49716400	2.53600100
H	3.01247200	-4.77858600	-0.57837000
H	3.46904200	-6.43277800	-1.09047300
H	4.34703300	-5.63624600	0.23098400
H	2.19546000	-8.19456000	2.00363200
H	2.81544900	-8.46014400	0.35880600
H	3.86202300	-7.72385100	1.59144300
H	0.42385300	-5.17335500	-2.55408000
H	1.93106700	-6.12071400	-2.59753000
H	0.54230300	-6.63321600	-3.57856300
H	1.99158000	-8.46563600	-1.62273000
H	0.55015200	-8.95061500	-2.53464500
H	0.57834500	-9.14070300	-0.76173900
H	-1.70268100	-6.15919400	-1.43697200
H	-1.51135300	-7.47431600	-2.61827800
H	-1.68545100	-7.86167900	-0.89040700

Table S11
B/P-TS

Atomic	Coordinates (Angstroms) X	Y	Z
H	-0.00404900	-0.01451900	0.00119900
C	-0.00165100	-0.00847800	1.09196300
C	0.04244700	0.00985400	3.95698500
C	-1.18062100	0.14313700	1.84197500
C	1.17731500	-0.14708600	1.80597200
C	1.19734900	-0.13936000	3.20770400
C	-1.15930300	0.15235100	3.24207000
H	-2.13247000	0.25845300	1.31917000
H	-2.09453400	0.27484700	3.79244500
H	0.07353800	0.01816600	5.04731800
O	2.45944300	-0.30479400	1.33857900
O	2.49412300	-0.29955800	3.63426300
B	3.26023400	-0.35279000	2.47163500
O	4.59787000	-0.56706000	2.42530300
P	5.85221300	0.14340500	3.25625800
C	7.20163000	-0.03068000	1.95416100
C	6.07728000	-0.99212900	4.75171300
C	5.76535400	-2.46027300	4.43285200
H	6.45975500	-2.88908600	3.69882000
H	4.74260400	-2.57925500	4.04927000
H	5.84761400	-3.05179600	5.36045800
C	7.50329100	-0.83652400	5.30251200
H	7.76553000	0.22021100	5.46332100

H	8.25673000	-1.29088400	4.64376500
H	7.56532100	-1.34726300	6.27770200
C	5.07355000	-0.46547800	5.79889600
H	5.30250100	0.57118400	6.08571900
H	5.13469200	-1.09431400	6.70277700
H	4.03928500	-0.50003700	5.42919300
C	7.54554800	-1.48549000	1.61340100
H	8.23673300	-1.50378100	0.75347700
H	6.64751600	-2.05617000	1.33491200
H	8.04495500	-1.99904700	2.44720200
C	8.44602700	0.73919700	2.43166100
H	8.19760800	1.77070900	2.72217000
H	9.17531500	0.78436200	1.60618300
H	8.94115500	0.25555200	3.28345300
C	6.63345800	0.67345800	0.70429700
H	6.33678800	1.71094000	0.91924600
H	5.75784300	0.14545000	0.30313700
H	7.41265900	0.69600900	-0.07500200
C	5.20231200	2.48031300	3.66446200
S	3.88834100	2.65761700	2.75726100
S	6.27920500	3.10384300	4.67938400

Table S12
Al/P-TS

Atomic	Coordinates (Angstroms) X	Y	Z
P	-0.09630200	-0.01842900	0.10273400
C	0.42329400	0.07897700	3.10450800
O	1.52000300	-0.14029600	-0.22624700
Al	2.84095400	0.24703000	0.79047200
S	1.88525300	-0.56592500	2.95686900
O	4.41673500	-0.51439600	0.87059400
O	3.41211200	1.87939600	1.10075200
C	4.75623100	1.77988100	1.32609300
C	5.30471700	0.47292800	1.20108400
C	6.66387500	0.26006100	1.41362700
C	7.48340500	1.34784100	1.75000800
C	6.94506400	2.63152400	1.87258000
C	5.57605800	2.85374800	1.66202600
C	-0.51385600	1.59112400	-0.81469100
C	0.19959200	1.74291000	-2.16330800
C	-0.01678100	2.69806000	0.13993100
C	-2.03500900	1.70916200	-0.97656300
C	-0.74369000	-1.55272900	-0.79526600
C	-2.23484700	-1.71414300	-0.45900600
C	-0.51309600	-1.55610400	-2.30929900
C	0.03886700	-2.71790100	-0.15705400
S	-0.88130800	0.67165000	3.70700800
H	0.05217400	2.76869100	-2.54235500

H	7.06499500	-0.75038900	1.31214300
H	8.55098600	1.18552200	1.91624800
H	7.59217600	3.47190200	2.13481800
H	5.13580200	3.84883800	1.75301900
H	-0.18536400	1.04975000	-2.92141100
H	1.28021800	1.57167400	-2.06004100
H	-2.56586200	1.51983500	-0.02905800
H	-2.42413700	1.01374000	-1.73427300
H	-2.29453100	2.73041600	-1.30237300
H	-0.50385500	2.63493600	1.12539400
H	-0.25129900	3.68633000	-0.28987300
H	1.07345900	2.66232900	0.29191700
H	-0.75157300	-2.55265400	-2.71989200
H	0.53603100	-1.33282900	-2.55265800
H	-1.15484900	-0.82760000	-2.82485600
H	-2.40729300	-1.68307400	0.62890800
H	-2.59367800	-2.68985900	-0.82729300
H	-2.85693300	-0.93720200	-0.92405600
H	-0.05692400	-2.72019900	0.94091600
H	1.10771600	-2.66782400	-0.40718300
H	-0.35875500	-3.67562700	-0.53182400

Table S13
Ga/P-TS

Atomic	Coordinates (Angstroms) X	Y	Z
P	-0.04955700	-0.04278900	0.04456000
O	1.54297000	-0.23352000	-0.39545700
Ga	2.88594400	0.19530600	0.71072700
O	4.57300000	-0.50754800	0.82101000
O	3.46246000	1.90228100	1.07659800
C	4.79545800	1.80357500	1.34572300
C	5.38823000	0.51701200	1.21012400
C	6.74556300	0.34216000	1.47629200
C	7.51930600	1.44157000	1.87150200
C	6.93748100	2.70568700	2.00475000
C	5.57288800	2.88998600	1.74541400
C	-0.47440700	1.57216600	-0.86018000
C	0.18275400	1.70251900	-2.23926200
C	0.08251100	2.67241000	0.06884100
C	-1.99856500	1.72105300	-0.95785300
C	-0.79974200	-1.56297300	-0.79502900
C	-2.27027200	-1.67349400	-0.35979600
C	-0.67007600	-1.58271400	-2.32100500
C	-0.01538500	-2.74899500	-0.19903600
H	0.02741500	2.72521100	-2.62350300
H	7.17975300	-0.65369700	1.36701000
H	8.58377700	1.30478800	2.07591100
H	7.54660700	3.55841800	2.31372400

H	5.09817700	3.86825400	1.84505500
H	-0.23970700	1.00365900	-2.97199600
H	1.26519300	1.52233900	-2.18069200
H	-2.49242500	1.54823400	0.01237400
H	-2.43463700	1.03123300	-1.69476200
H	-2.24909100	2.74646200	-1.27767800
H	-0.37227700	2.62671800	1.07054200
H	-0.14274200	3.66350000	-0.35947500
H	1.17582000	2.61307800	0.18701800
H	-0.97625900	-2.57038400	-2.70738800
H	0.36898600	-1.40463200	-2.63455300
H	-1.31370300	-0.83031700	-2.79854200
H	-2.36914300	-1.63231200	0.73685100
H	-2.68306900	-2.63889600	-0.69747800
H	-2.89680800	-0.87926400	-0.78785000
H	-0.03865700	-2.74027300	0.90275400
H	1.03555400	-2.73595300	-0.51913400
H	-0.46904500	-3.69511600	-0.53793500

Table S14
In/P-TS

Atomic	Coordinates (Angstroms) X	Y	Z
P	-0.07701100	-0.11844500	-0.03743200
O	1.47609800	-0.37068900	-0.56958000
In	2.99079400	0.13045300	0.65470000
O	4.93684500	-0.46137000	0.89691300
O	3.71257900	2.01479000	1.05095400
C	5.02302900	1.89916400	1.37479400
C	5.65541400	0.61984000	1.29769500
C	7.00360900	0.49482800	1.64919600
C	7.73418100	1.61521200	2.05860700
C	7.11673100	2.86755000	2.13358800
C	5.76557400	3.00639200	1.80022100
C	-0.49458100	1.51434700	-0.91801700
C	0.07783500	1.61651800	-2.33643200
C	0.16458900	2.59219100	-0.03035200
C	-2.01394400	1.72915400	-0.91665100
C	-0.93916200	-1.60722200	-0.82747900
C	-2.38543800	-1.65658300	-0.30850400
C	-0.89787100	-1.63330800	-2.35820100
C	-0.17082700	-2.82348700	-0.27346200
H	-0.04208300	2.64810900	-2.70944900
H	7.46385900	-0.49357500	1.58704300
H	8.78936900	1.50530200	2.32000400
H	7.68628300	3.74309800	2.45446100

H	5.26098300	3.97332700	1.85619900
H	-0.43060200	0.94639200	-3.04090000
H	1.14929700	1.37181200	-2.34792700
H	-2.44971700	1.57984500	0.08473600
H	-2.52594500	1.05599500	-1.61930400
H	-2.24219500	2.76314100	-1.22578200
H	-0.21381600	2.55764000	1.00297000
H	-0.05713100	3.59294300	-0.43727300
H	1.26277100	2.50469600	0.00480100
H	-1.26638400	-2.60739400	-2.72423100
H	0.12806500	-1.49817300	-2.73097800
H	-1.53588400	-0.85479400	-2.80005600
H	-2.41955600	-1.60934500	0.79172300
H	-2.85650900	-2.60460600	-0.61838200
H	-3.00209400	-0.83772700	-0.70313200
H	-0.13382100	-2.81379700	0.82806100
H	0.86068800	-2.84964900	-0.65088700
H	-0.67840000	-3.75145100	-0.58514600

Table S15
Tl/P-TS

Atomic	Coordinates (Angstroms) X	Y	Z
P	0.00000000	0.00000000	0.00000000
O	1.59960300	0.00000000	-0.47691700
Tl	3.02102600	0.69603700	0.88042200
O	5.10753500	0.60780900	1.34759300
O	3.34499200	2.76541300	1.49473600
C	4.58380100	2.87780600	1.97808200
C	5.49672500	1.76823500	1.90291300
C	6.79946400	1.90083700	2.40501800
C	7.23052700	3.11184400	2.95018000
C	6.33933600	4.18297000	3.07701800
C	5.02597700	4.07143700	2.61219500
C	-0.64283600	1.53414200	-0.92443900
C	-0.00851700	1.75102200	-2.30208100
C	-0.21510600	2.70055300	0.00391500
C	-2.17405000	1.48670700	-1.01709800
C	-0.51069100	-1.62370000	-0.83746700
C	-1.97692000	-1.90130100	-0.47115500
C	-0.32551500	-1.65281000	-2.35812100
C	0.37472300	-2.70119900	-0.17790400
H	-0.27142100	2.75831500	-2.67336800
H	7.47192800	1.04630000	2.30831400
H	8.26206100	3.20955000	3.29967100
H	6.67363300	5.13328200	3.50423500

H	4.33061900	4.91009500	2.68521800
H	-0.35670100	1.02876800	-3.05131300
H	1.08667600	1.66996400	-2.24572500
H	-2.62227800	0.97301000	-0.15246800
H	-2.50122100	0.99514200	-1.94639800
H	-2.59725400	2.50334600	-1.01534000
H	-0.85030500	2.72412600	0.90335400
H	-0.32610000	3.67066900	-0.50496600
H	0.84646800	2.65717500	0.29470500
H	-0.56133100	-2.65963000	-2.74420200
H	0.71281200	-1.41361500	-2.63030900
H	-0.99227400	-0.94195600	-2.86537700
H	-2.13049100	-1.84921500	0.61890500
H	-2.26068900	-2.91418700	-0.79999000
H	-2.66504100	-1.20632700	-0.96990000
H	0.51721800	-2.51608500	0.89881800
H	1.36746500	-2.73881500	-0.64773200
H	-0.09774900	-3.69143400	-0.28451900

Table S16
B/N-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	1.06910700	-1.29081300	1.97014600
C	0.39157800	-0.43989900	2.05210600
C	-1.36654700	1.81359500	2.24370400
C	-0.74698500	-0.46675700	2.87639400
C	0.61937500	0.72672000	1.34019600
C	-0.24239500	1.82727400	1.43569600
C	-1.60657000	0.63413300	2.97061900
H	-0.96329800	-1.36733000	3.45506900
H	-2.48201600	0.57849100	3.62104100
H	-2.02792800	2.67876900	2.30768300
O	1.63959600	1.02744000	0.47527300
O	0.22823200	2.83265200	0.62336800
B	1.39192100	2.33016200	0.04048200
O	2.22368200	2.89821400	-0.85077900
N	2.21666400	4.26022400	-1.28824500
C	2.97212100	5.06962900	-0.29942200
C	0.98029600	4.65859200	-2.03043200
C	-0.09642200	5.38840600	-1.20045600
H	0.26629800	6.35158000	-0.81568700
H	-0.43480300	4.77633200	-0.35682900
H	-0.96651100	5.60281200	-1.84117000
C	1.40415700	5.55284200	-3.21692900
H	2.20703400	5.06464400	-3.78745600
H	1.75345400	6.54204700	- 2.90316300

H	0.54219300	5.70938700	-3.88349500
C	0.35673100	3.39348700	-2.65053300
H	1.10980200	2.80606900	-3.19341200
H	-0.42472100	3.70134500	-3.35970100
H	-0.12323700	2.74989700	-1.90202300
C	2.33728900	5.12503000	1.10752600
H	2.95732500	5.75237500	1.76601600
H	2.28713600	4.13041200	1.57233600
H	1.32354800	5.54336500	1.09025800
C	3.16220400	6.50327000	-0.81558300
H	3.64607600	6.51024300	-1.80127000
H	3.81762800	7.03769700	-0.11249000
H	2.22150200	7.06540400	-0.87496600
C	4.37510300	4.43901300	-0.18336500
H	4.84504700	4.38166500	-1.17601900
H	4.32842200	3.42391100	0.23089600
H	5.00838800	5.05260500	0.47552700

Table S17
B/As-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	1.28506300	-0.93838600	2.87214400
C	0.49597000	-0.23222000	2.60998000
C	-1.55379400	1.63466700	1.89537800
C	-0.74487000	-0.21895100	3.27092500
C	0.67800100	0.69990000	1.60074000
C	-0.32764600	1.61235800	1.25180100
C	-1.74739700	0.69359200	2.92209800
H	-0.92815900	-0.93706500	4.07314300
H	-2.69991400	0.67613400	3.45608200
H	-2.32746300	2.35005300	1.61248000
O	1.77259800	0.91047200	0.80609500
O	0.12702000	2.40500100	0.22837400
B	1.43665500	1.97295200	-0.04261100
O	2.26676800	2.45489800	-0.96268800
As	2.62081300	4.02771800	-1.84737000
C	3.29320900	5.05394200	-0.22826600
C	0.77183200	4.74044600	-2.31766700
C	-0.08657200	5.32646000	-1.19607600
H	0.37630400	6.21120400	-0.73620800
H	-0.29446700	4.58560500	-0.41474200
H	-1.05571800	5.65153000	-1.61647100
C	1.07173200	5.81981100	-3.37240600
H	1.66798900	5.42405800	-4.21034500
H	1.61194900	6.68032600	- 2.94800200

H	0.12374900	6.20113500	-3.79004100
C	0.03881100	3.56547800	-2.98139600
H	0.64919500	3.08688600	-3.76495000
H	-0.88612500	3.93216200	-3.46035500
H	-0.24520700	2.80037400	-2.24621500
C	2.48342000	4.83612500	1.05101000
H	2.93045400	5.42583400	1.87101300
H	2.50879300	3.78386900	1.37123500
H	1.43507500	5.14090600	0.95299600
C	3.34864800	6.53861500	-0.60776900
H	3.86712900	6.69971200	-1.56801000
H	3.90917400	7.09944600	0.16051200
H	2.34840800	6.98953000	-0.67930500
C	4.71936800	4.51773000	-0.02215500
H	5.35468700	4.69283700	-0.90481600
H	4.71409100	3.43608000	0.18415400
H	5.19089800	5.02371000	0.83861300

Table S18
B/Sb-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	1.16527200	-0.95701800	2.99223000
C	0.40855400	-0.23927700	2.67220300
C	-1.55393900	1.65562900	1.80665000
C	-0.85199400	-0.15762800	3.28995400
C	0.65468100	0.63943100	1.62902600
C	-0.30915100	1.56642200	1.20579500
C	-1.81211100	0.76880900	2.86722500
H	-1.08437000	-0.83255200	4.11665400
H	-2.78161900	0.80565500	3.36877200
H	-2.29441900	2.38123100	1.46645300
O	1.78037500	0.77810300	0.86511700
O	0.20346200	2.29761800	0.16612100
B	1.51151100	1.81295300	-0.04490800
O	2.37793600	2.24132600	-0.95091200
Sb	2.75564400	3.95757800	-1.98986900
C	3.43572300	5.09257000	-0.17884400
C	0.68300800	4.73319200	-2.39535200
C	-0.09249600	5.27653900	-1.19761200
H	0.40248800	6.14370100	-0.73661700
H	-0.24568700	4.50598100	-0.43176000
H	-1.08983200	5.61741900	-1.53526500
C	0.92381800	5.84411900	-3.42691000
H	1.46739700	5.48157700	-4.31555100
H	1.48851100	6.69215600	- 3.00509300

H	-0.04488900	6.24378500	-3.77930800
C	-0.07835100	3.56738100	-3.03547700
H	0.46401600	3.13364500	-3.89246500
H	-1.05458600	3.92368900	-3.41423000
H	-0.27616400	2.76759800	-2.30768300
C	2.61058200	4.76698100	1.06481700
H	2.99217800	5.34980500	1.92399500
H	2.69429000	3.70468100	1.33912700
H	1.54646200	5.00707000	0.94617700
C	3.38056900	6.58473100	-0.51812500
H	3.92766600	6.82204200	-1.44695800
H	3.85303700	7.17354000	0.28991700
H	2.34921900	6.95145400	-0.62779800
C	4.88903800	4.65017100	0.03295500
H	5.52647300	4.88409400	-0.83541400
H	4.95925700	3.56749900	0.22532800
H	5.31891500	5.17123700	0.90854300

Table S19
B/Bi-Rea

Atomic	Coordinates (Angstroms) X	Y	Z
H	0.97740300	-1.13370900	2.89587200
C	0.28762400	-0.34187300	2.60004200
C	-1.49722300	1.74580600	1.79917900
C	-0.97071400	-0.18252200	3.20755500
C	0.62199400	0.55726900	1.59948500
C	-0.25577800	1.57958700	1.20770100
C	-1.84417900	0.83836900	2.81646900
H	-1.27008000	-0.87126900	4.00070200
H	-2.81447200	0.93459500	3.30863600
H	-2.17004600	2.54513500	1.48434700
O	1.76514700	0.63266400	0.85587000
O	0.32960500	2.30997800	0.20824500
B	1.60036600	1.72671600	-0.01447000
O	2.50904800	2.12284000	-0.88693600
Bi	2.81489300	3.93110900	-2.02731400
C	3.51311400	5.15846300	-0.14891200
C	0.61689200	4.70171400	-2.39857900
C	-0.10330900	5.26392200	-1.17940100
H	0.41280900	6.13709500	-0.75352500
H	-0.22131700	4.50470500	-0.39587200
H	-1.11540600	5.60205400	-1.47690000
C	0.83643000	5.78817500	-3.45499500
H	1.35814200	5.40890400	-4.35075400
H	1.40869700	6.64587500	- 3.06245300

H	-0.13872400	6.18380400	-3.79769900
C	-0.14868900	3.51526300	-2.98275000
H	0.36219200	3.07424400	-3.85540500
H	-1.14802800	3.84644700	-3.32587800
H	-0.30075900	2.72674100	-2.23186200
C	2.69515900	4.80208100	1.08680000
H	3.06266700	5.38235300	1.95519300
H	2.79750800	3.73760300	1.34546000
H	1.62627800	5.02238300	0.96762700
C	3.40095800	6.64002700	-0.50476500
H	3.94644000	6.89185800	-1.43109700
H	3.84259600	7.25816100	0.30045500
H	2.35632900	6.96399200	-0.62540100
C	4.97580900	4.75498000	0.04624500
H	5.59888200	4.99852600	-0.83053100
H	5.07648500	3.67646600	0.24849000
H	5.40573200	5.29440400	0.91203100

Table S20
B/N-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	0.35887500	1.12576800	4.55681100
C	0.03261000	0.73788400	3.59031000
C	-0.79943000	-0.25077300	1.04568500
C	-0.87579200	-0.33340400	3.48658800
C	0.50497100	1.28912900	2.41005600
C	0.09471700	0.80208300	1.15616200
C	-1.28315800	-0.81742500	2.24087400
H	-1.26532300	-0.79262600	4.39805900
H	-1.98763700	-1.65076700	2.18927900
H	-1.10956100	-0.61919000	0.06628500
O	1.37813900	2.32071300	2.24083900
O	0.69805800	1.51718300	0.16659800
B	1.55787100	2.48365400	0.81984900
O	1.29788500	3.87003600	0.39813900
N	2.18541500	4.57674500	-0.39289400
C	2.47362100	5.90697400	0.50763100
C	1.42811800	4.68219000	-1.83471300
C	-0.07557000	4.86796500	-1.59955900
H	-0.32330900	5.78705900	-1.06267600
H	-0.51074300	4.01366200	-1.07136300
H	-0.53894800	4.93452300	-2.59510800
C	1.96973200	5.82223100	-2.69140800
H	3.06180400	5.79913600	-2.77362600
H	1.64212800	6.80417600	- 2.32747500

H	1.54960500	5.69383500	-3.70002400
C	1.61613600	3.33362800	-2.54376100
H	2.64684700	3.16722900	-2.87622800
H	0.97534500	3.35080200	-3.43711000
H	1.28486500	2.49434600	-1.91944300
C	1.13391400	6.58128000	0.81018500
H	1.31603400	7.32136200	1.60276200
H	0.38836900	5.86699800	1.17476700
H	0.74015300	7.12806600	-0.05582800
C	3.42096100	6.93250800	-0.11642100
H	4.42390600	6.53402400	-0.29138600
H	3.50226300	7.74893400	0.61715500
H	3.04601200	7.36888900	-1.04516700
C	3.09278600	5.38833300	1.81250300
H	4.07394900	4.92545800	1.64616700
H	2.43954700	4.67628900	2.33029800
H	3.24562700	6.25660600	2.46909700
C	3.51640400	3.76337100	-0.55719900
S	3.44644400	2.27821400	0.25169100
S	4.77054000	4.32669400	-1.44680300

Table S21
B/As-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-0.19252100	0.52529200	4.63918300
C	-0.28901300	0.25356700	3.58719300
C	-0.52064700	-0.42923100	0.81501500
C	-0.72424600	-1.01958300	3.18037300
C	0.02178600	1.15683900	2.58408900
C	-0.09435000	0.82190000	1.22742400
C	-0.83728900	-1.35377500	1.82549900
H	-0.97583600	-1.76346000	3.93935700
H	-1.17514100	-2.35373600	1.54520300
H	-0.60094500	-0.67846800	-0.24398300
O	0.46769600	2.45098200	2.69367000
O	0.27114800	1.90807000	0.46882700
B	0.67440100	2.87997200	1.38967400
O	1.03546100	4.14851500	1.05952400
As	2.22674200	4.58407300	-0.21583000
C	2.77535700	6.34483900	0.56619200
C	1.15099800	4.59374600	-1.92009400
C	-0.30788400	4.89604200	-1.55985200
H	-0.42848100	5.87096200	-1.06632400
H	-0.73546800	4.12073200	-0.91114300
H	-0.89292000	4.91834700	-2.49457300
C	1.72495800	5.65076300	-2.86884300
H	2.79248800	5.47807300	-3.06407100
H	1.59287500	6.67181700	- 2.48158400

H	1.18347900	5.58848700	-3.82783800
C	1.28309200	3.18851200	-2.52004400
H	2.32325200	2.96675700	-2.79521200
H	0.66482200	3.14266600	-3.43232500
H	0.92693600	2.41582900	-1.82459700
C	1.51397400	7.20108500	0.72916900
H	1.78476400	8.12745500	1.26288100
H	0.74215400	6.68372700	1.31581100
H	1.08699600	7.49419400	-0.24158400
C	3.81532100	7.04245400	-0.31418100
H	4.69928600	6.41095100	-0.47369100
H	4.13104100	7.96845900	0.19551900
H	3.41269500	7.32180800	-1.29709100
C	3.37942200	5.98714600	1.93192700
H	4.27209600	5.35352400	1.82640000
H	2.65703200	5.46499500	2.57407900
H	3.68126500	6.92043200	2.43561600
C	3.67793200	3.26149000	-0.17232500
S	3.60712100	2.07050800	0.96803300
S	4.74233200	3.72703700	-1.38587600

Table S22
B/Sb-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-5.02872300	-1.54296200	2.02852100
C	-4.87221400	-0.78649600	1.25737800
C	-4.41258400	1.19470300	-0.74358200
C	-5.89843200	0.08764400	0.84965200
C	-3.63237300	-0.64571000	0.65275900
C	-3.40405500	0.33780300	-0.32952700
C	-5.67446200	1.05607000	-0.13248900
H	-6.88362600	0.00735100	1.31526500
H	-6.48801200	1.72138200	-0.43090600
H	-4.22538100	1.95125900	-1.50854900
O	-2.49140500	-1.34837600	0.88805000
O	-2.10663400	0.29198600	-0.73439700
B	-1.45369200	-0.70088800	0.12892500
O	-0.42504700	-0.12722500	0.97760700
Sb	1.28813100	0.13890600	0.10194700
C	2.66820000	-0.21960300	1.78265400
C	1.29855300	2.13932200	-0.85278200
C	0.80129600	3.13979800	0.19062800
H	1.49475800	3.24008100	1.03991700
H	-0.19204300	2.86524500	0.57798900
H	0.71375000	4.13321200	-0.28495900
C	2.73287900	2.41422700	-1.30808300
H	3.10637500	1.62960000	-1.98558100
H	3.43090000	2.50830300	- 0.46134500

H	2.75635300	3.36861700	-1.86403000
C	0.33193400	2.02051900	-2.03257300
H	0.69792100	1.31008200	-2.78989700
H	0.24185200	3.01116400	-2.51388800
H	-0.67151900	1.69855900	-1.71399400
C	2.49531500	0.92111500	2.78663800
H	3.09957900	0.70258400	3.68532600
H	1.44819300	1.02902500	3.10975600
H	2.84107000	1.88617000	2.38544800
C	4.08969200	-0.30382000	1.22332700
H	4.17104400	-1.04906800	0.41574400
H	4.78016900	-0.60574200	2.03165200
H	4.43865800	0.66669800	0.83578400
C	2.19320100	-1.55472800	2.36269200
H	2.30650600	-2.37864900	1.64141400
H	1.13817800	-1.50919400	2.67086900
H	2.80439700	-1.79589500	3.24984100
C	1.02509000	-1.54915900	-1.27448900
S	-0.57655400	-2.09902700	-1.11282900
S	2.28441700	-2.05527200	-2.19476900

Table S23
B/Bi-Prod

Atomic	Coordinates (Angstroms) X	Y	Z
H	-5.06444600	-1.82158900	1.74011200
C	-4.94463300	-0.95730000	1.08450300
C	-4.55031600	1.29264300	-0.63346300
C	-5.98495700	-0.04514200	0.83392500
C	-3.73926900	-0.74025600	0.44060400
C	-3.52433800	0.39171200	-0.37449700
C	-5.79733900	1.04787000	-0.01828500
H	-6.95793900	-0.21578400	1.29935900
H	-6.63572700	1.71961700	-0.21741200
H	-4.40882900	2.14534400	-1.30209700
O	-2.64867500	-1.54191300	0.45891000
O	-2.24179200	0.37415600	-0.84653100
B	-1.60791100	-0.78237800	-0.17743800
O	-0.70227500	-0.42566900	0.88546900
Bi	1.03062800	0.18427800	0.23498700
C	2.36181800	-0.58916200	1.68471800
C	1.23476800	2.09581000	-0.62873100
C	0.86377100	3.01890700	0.53143900
H	1.59120000	2.95160800	1.35639800
H	-0.12807100	2.76000000	0.94231800
H	0.83091900	4.04873700	0.15855800
C	2.69812900	2.12203100	-1.08025800
H	2.96348600	1.23927800	-1.68778700
H	3.39641100	2.17312600	- 0.23065400

H	2.81868100	3.02158500	-1.69806200
C	0.22710900	2.05320500	-1.77411300
H	0.57205200	1.38978400	-2.58104900
H	0.13260700	3.07983100	-2.14934500
H	-0.76691700	1.69540400	-1.45658900
C	2.21404500	0.37947100	2.85862100
H	2.77366600	-0.01974900	3.71334800
H	1.15668200	0.49520600	3.15585300
H	2.60395700	1.38011400	2.61068500
C	3.72978700	-0.60639600	1.00165400
H	3.67698400	-1.02716900	-0.01751400
H	4.39474800	-1.23660500	1.60589000
H	4.15954600	0.40352500	0.92282300
C	1.78217600	-1.97888200	1.94639700
H	1.83428300	-2.61913900	1.05165000
H	0.72644600	-1.93203500	2.25579600
H	2.38178700	-2.42993200	2.74790800
C	1.01603100	-1.21855400	-1.41626000
S	-0.56266900	-1.83854500	-1.60072800
S	2.41686600	-1.50099700	-2.24659700

Table S24
B/N-TS

Atomic	X	Coordinates (Angstroms) Y	Z
H	-4.39090000	-2.40467400	0.12709100
C	-4.36947900	-1.31482400	0.17525500
C	-4.27597900	1.53954000	0.30262900
C	-5.54760700	-0.54678000	0.21204200
C	-3.16621600	-0.62759700	0.20291800
C	-3.12027200	0.77544100	0.26561100
C	-5.50185700	0.84987700	0.27433400
H	-6.51504000	-1.05338600	0.18973100
H	-6.43407100	1.41855400	0.29995400
H	-4.22603600	2.62841600	0.35166000
O	-1.89491300	-1.12281900	0.18363200
O	-1.81927700	1.18627900	0.28712000
B	-1.02841200	0.00896700	0.13491300
O	0.18121200	-0.06482000	0.86035700
N	1.48126000	-0.07888300	0.40571400
C	2.02811300	-1.47377100	0.77873700
C	2.10355700	1.24330300	0.90388900
C	1.89068200	1.42530100	2.41714300
H	2.51337500	0.74571000	3.01057900
H	0.83900400	1.28315800	2.69268400
H	2.18276700	2.45173700	2.68398500
C	3.59986100	1.36209000	0.58953700
H	3.83365900	1.10160900	-0.44777000
H	4.22245700	0.76231200	1.26158800

H	3.88360900	2.41359100	0.74270700
C	1.36827600	2.38544000	0.17779700
H	1.56936700	2.37738500	-0.90113400
H	1.74042200	3.34035300	0.57565400
H	0.28460000	2.35463000	0.34147800
C	1.81019800	-1.77790800	2.27146800
H	2.03801500	-2.84042600	2.44244100
H	0.77075700	-1.59556700	2.56894400
H	2.47736300	-1.19492500	2.91722900
C	3.51393400	-1.65109000	0.44224100
H	3.75964100	-1.31163700	-0.56910400
H	3.73503500	-2.72708600	0.49698900
H	4.17364100	-1.15302100	1.16030100
C	1.22511100	-2.50130000	-0.04088600
H	1.42250300	-2.40693300	-1.11646100
H	0.14568600	-2.42237300	0.13420800
H	1.54237200	-3.50823500	0.26579600
C	1.29915300	0.02660600	-1.76677800
S	-0.31061500	0.07831500	-1.92916900
S	2.68624000	0.02457900	-2.54279200

Table S25
B/As-TS

Atomic	Coordinates (Angstroms) X	Y	Z
H	-5.22295500	-1.91613400	0.79054400
C	-4.89977400	-0.91064600	0.51776000
C	-4.01500700	1.71837900	-0.19774600
C	-5.80538600	0.07623600	0.09123800
C	-3.56371600	-0.54908400	0.57301400
C	-3.13249900	0.73858900	0.22460500
C	-5.37322000	1.36109000	-0.25890300
H	-6.86815200	-0.16767800	0.03022100
H	-6.10420300	2.10235000	-0.58877300
H	-3.66481200	2.71472800	-0.47089400
O	-2.47782900	-1.30376700	0.94407200
O	-1.76934500	0.80777800	0.38240700
B	-1.37625000	-0.46990300	0.79023100
O	-0.10875700	-0.83685000	1.07326600
As	1.35250900	-0.26167300	0.15434300
C	2.52576600	-1.82372100	0.64059900
C	1.85278300	1.44447300	1.13427600
C	1.37298400	1.39525500	2.58581200
H	1.84975100	0.58943400	3.16051400
H	0.28409000	1.26449300	2.64848100
H	1.62563900	2.35287200	3.07412200
C	3.37077600	1.63563300	1.04588300
H	3.72839100	1.59489900	0.00591900
H	3.92162400	0.89059700	1.63765200

H	3.62765500	2.63112700	1.44752100
C	1.13298100	2.56073200	0.36272100
H	1.47483600	2.61252100	-0.68162500
H	1.35199600	3.52954400	0.84388000
H	0.04344900	2.41607800	0.36217800
C	2.70720400	-1.93375000	2.15571900
H	3.25112900	-2.86618700	2.38791800
H	1.73873600	-1.97076000	2.67539200
H	3.29602300	-1.10009700	2.56495800
C	3.86813500	-1.67061200	-0.08615000
H	3.73237700	-1.53726200	-1.16970900
H	4.46518700	-2.58518400	0.07088700
H	4.45664300	-0.82280700	0.29024400
C	1.77414500	-3.04985600	0.09932800
H	1.60223000	-2.97908000	-0.98534300
H	0.80053600	-3.17774900	0.59209500
H	2.38023000	-3.95212100	0.28851100

Table S26
B/Sb-TS

Atomic	Coordinates (Angstroms) X	Y	Z
H	-5.34677500	-0.84669900	-2.26677700
C	-5.06074100	-0.55010700	-1.25674300
C	-4.27361400	0.22681200	1.38515600
C	-5.99748600	-0.06931100	-0.32511200
C	-3.74377800	-0.62745000	-0.83470500
C	-3.36025900	-0.24905500	0.45980700
C	-5.61285200	0.31128100	0.96596400
H	-7.04650400	0.01059500	-0.61821800
H	-6.36631600	0.68402700	1.66311800
H	-3.95950500	0.52480900	2.38641600
O	-2.63596800	-1.04710500	-1.53079000
O	-2.00739900	-0.44016100	0.59426800
B	-1.56435500	-0.91119500	-0.65180700
O	-0.27997300	-1.16877900	-0.93885200
Sb	1.17417800	-0.07368400	-0.02727800
C	2.60972700	-0.26322300	-1.70621200
C	1.68331000	-1.39649500	1.70187100
C	1.44229900	-2.84457300	1.28009600
H	2.16053500	-3.18221800	0.51944400
H	0.42819800	-2.99980200	0.88485600
H	1.56163500	-3.49611800	2.16484900
C	3.14324600	-1.14329200	2.08093000
H	3.33343200	-0.08203300	2.29545300
H	3.83844600	-1.47098800	1.29248600

H	3.38272400	-1.72375100	2.99068100
C	0.72859400	-0.96859000	2.81863900
H	0.89446500	0.07994400	3.10971300
H	0.90776800	-1.60058000	3.70711300
H	-0.32587800	-1.08164100	2.52575700
C	2.91885000	-1.74370200	-1.92734300
H	3.51781500	-1.85423900	-2.84962300
H	2.00237500	-2.33947700	-2.05409200
H	3.50848100	-2.17140400	-1.10242000
C	3.86462000	0.53997000	-1.35955400
H	3.63459500	1.59051300	-1.12746800
H	4.55248800	0.52672400	-2.22422500
H	4.40412800	0.11530100	-0.49911400
C	1.87642800	0.33389000	-2.91111100
H	1.58775000	1.38280700	-2.74198200
H	0.96832900	-0.23636900	-3.15576600
H	2.54576500	0.30639600	-3.78962200

Table S27
B/Bi-TS

Atomic	Coordinates (Angstroms) X	Y	Z
H	-5.25418800	0.00235500	-2.52002600
C	-5.08159700	-0.13695700	-1.45185600
C	-4.59002500	-0.49706600	1.34473700
C	-6.11076100	0.00369000	-0.50423000
C	-3.82336600	-0.45782800	-0.96822000
C	-3.58368600	-0.63624100	0.40305000
C	-5.87065000	-0.17223300	0.86346600
H	-7.11682600	0.25857500	-0.84453700
H	-6.69209900	-0.05243600	1.57323000
H	-4.38929800	-0.63348100	2.40847000
O	-2.65477200	-0.64124700	-1.65917600
O	-2.26081500	-0.94208700	0.58709100
B	-1.67374800	-0.91010600	-0.69716500
O	-0.38089900	-1.12800600	-0.93202400
Bi	1.11827600	0.00701700	-0.02432600
C	2.64987500	-0.45111500	-1.64236800
C	1.52484100	-1.37105500	1.76121400
C	1.08064900	-2.79464500	1.43802600
H	1.59368300	-3.20961100	0.55848900
H	-0.00247500	-2.84406500	1.25514700
H	1.30925600	-3.45498700	2.29701600
C	3.01344600	-1.30088000	2.09846000
H	3.36262400	-0.26705600	2.25826100
H	3.63822300	-1.75722200	1.31511900

H	3.21058700	-1.85639200	3.03522000
C	0.66646000	-0.77175400	2.87693500
H	0.98982500	0.24724300	3.14619800
H	0.74616800	-1.39611600	3.78672400
H	-0.39797400	-0.73183100	2.59495100
C	2.79167500	-1.95551500	-1.85079400
H	3.50468500	-2.15449100	-2.67438200
H	1.82978500	-2.41664500	-2.12158900
H	3.18145900	-2.46436100	-0.95594600
C	3.96805500	0.20010500	-1.22002700
H	3.84370300	1.26459900	-0.96015700
H	4.69291000	0.15002300	-2.05407500
H	4.42625800	-0.31052100	-0.35898700
C	2.07160300	0.22228600	-2.88790200
H	1.98762100	1.31491600	-2.76248400
H	1.07514000	-0.17389600	-3.13850100
H	2.73479100	0.04166300	-3.75452200
C	0.28056700	2.50903500	0.40721600
S	-1.23179600	2.56031500	-0.07343500
S	1.58975400	3.17491300	1.03892600
