Supporting Information

Probing the Origins of Activation Barriers in Nitrous Oxide Capture Reactions by Analyzing Lewis Acid-Base Pairs with Dimethylxanthene-Linked Group-13 (P) and Group-15 (B) Elements

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

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

*E-mail: midesu@mail.ncyu.edu.tw

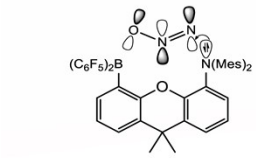
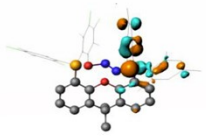
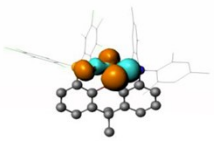
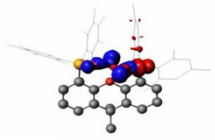
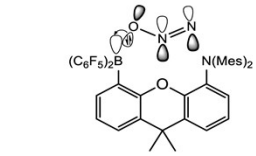
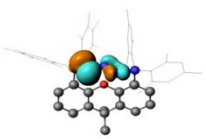
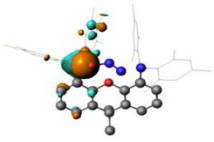
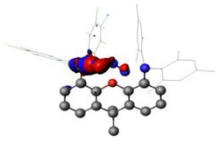
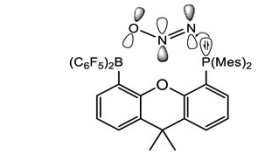
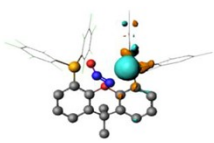
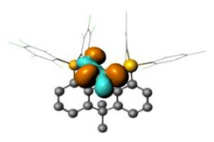
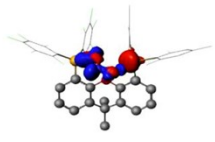
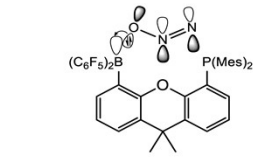
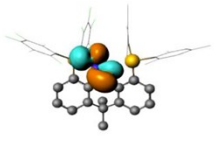
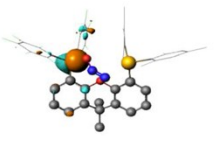
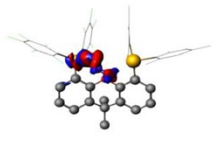
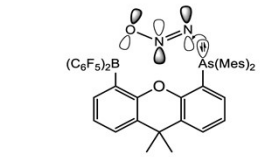
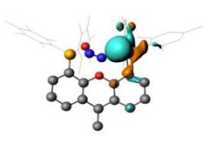
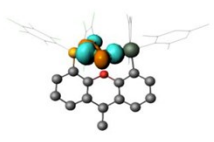
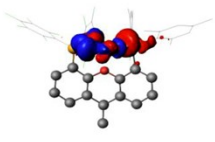
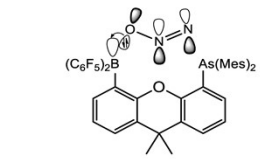
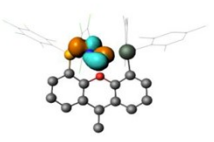
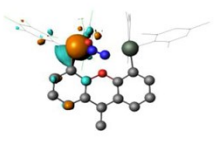
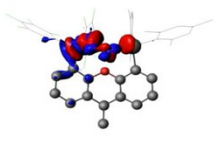
Table S1. The bonding energy between intramolecular dimethylxanthene-based **B/G15-Rea** and N_2O in **B/G15-TS** was analyzed using energy decomposition analysis at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level. The EDA-NOCV analysis considered both singlet and triplet spin states, and the energy values are presented in kcal/mol.

Molecules	**B/N-TS**		**B/P-TS**		**B/As-TS**		**B/Sb-TS**		**B/Bi-TS**	
	B/N-Rea(S) + N_2O(S)	**B/N-Rea(T) + N_2O(T)**	**B/P-Rea(S) + N_2O(S)**	**B/P-Rea(T) + N_2O(T)**	**B/As-Rea(S) + N_2O(S)**	**B/As-Rea(T) + N_2O(T)**	**B/Sb-Rea(S) + N_2O(S)**	**B/Sb-Rea(T) + N_2O(T)**	**B/Bi-Rea(S) + N_2O(S)**	**B/Bi-Rea(T) + N_2O(T)**
ΔE_{INT}[a]	-58.3	-94.5	-27.7	-142.5	-26.1	-142.6	-23.3	-138.6	-24.9	-134.4
ΔE_{Pauli}	336.1	430.6	139.4	225.3	139.8	224.1	124.7	193.3	150.5	237.0
ΔE_{Elstat}[b]	-167.6 (42.5 %)	-199.0 (37.9 %)	-65.9 (39.4 %)	-109.8 (29.9 %)	-65.8 (39.7 %)	-109.2 (29.8 %)	-59.2 (40.0 %)	-94.3 (28.4 %)	-70.4 (40.5 %)	-115.3 (31.0%)
ΔE_{Orb}[b]	-213.8 (54.2 %)	-313.1 (59.6 %)	-89.6 (53.6 %)	-246.4 (67.0 %)	-89.1 (53.7 %)	-246.5 (67.2 %)	-78.9 (53.3 %)	-227.7 (68.6 %)	-95.7 (54.2 %)	-246.7 (66.4 %)
$\Delta E_{Orb(1)}$[c]	-100.1 (46.8 %)	-219.9 (70.2 %)	-52.8 (58.9 %)	-210.4 (85.4 %)	-47.7 (53.5 %)	-67.2 (85.2 %)	-46.6 (59.1 %)	-196.1 (86.1 %)	-58.8 (61.4 %)	-66.4 (84.0 %)
$\Delta E_{Orb(2)}$[c]	-73.9 (34.6 %)	-57.1 (18.2 %)	-21.2 (23.7 %)	-18.5 (7.5 %)	-33.0 (37.0 %)	-209.9 (7.7 %)	-29.0 (36.8 %)	-16.3 (7.2 %)	-33.5 (35.0 %)	-207.3 (8.5 %)
ΔE_{Rest}[c]	-39.8 (18.6 %)	-36.2 (11.5 %)	-15.6 (17.4 %)	-17.5 (7.1 %)	-8.4 (9.4 %)	-17.5 (7.1 %)	-3.3 (4.1 %)	-15.3 (6.7 %)	-3.4 (3.6 %)	-18.4 (7.5 %)
ΔE_{Disper}[b]	-13.0 (3.3 %)	-13.0 (2.5 %)	-11.6 (7.0 %)	-11.6 (3.2 %)	-11.0 (6.6 %)	-11.0 (3.0 %)	-9.9 (6.7 %)	-9.9 (3.0 %)	-9.4 (5.3 %)	-9.4 (2.5 %)

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

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

(c) The values presented in parentheses indicate the percentage contribution to the overall orbital interactions, ΔE_{Or}

(a) Donor- Acceptor Interaction	(b) Donor Orbital	Acceptor Orbital	(c) Deformation Densities Δρ
			 Δρ₁
HOMO of B/N-FLP to LUMO of N_2O	HOMO of B/N-FLP	LUMO of N_2O	ΔE_1 = -100.1 kcal/mol; ν = ±1.26
			 Δρ₂
HOMO of N_2O to LUMO of B/N-FLP	HOMO of N_2O	LUMO of B/N-FLP	ΔE_2 = -73.9 kcal/mol; ν = ±0.68
			 Δρ₁
HOMO of B/P-FLP to LUMO of N_2O	HOMO of B/P-FLP	LUMO of N_2O	ΔE_1 = -52.8 kcal/mol; ν = ±0.71
			 Δρ₂
HOMO of N_2O to LUMO of B/P-FLP	HOMO of N_2O	LUMO of B/P-FLP	ΔE_2 = -21.2 kcal/mol; ν = ±0.51
			 Δρ₁
HOMO of B/As-FLP to LUMO of N_2O	HOMO of B/As-FLP	LUMO of N_2O	ΔE_1 = -47.7 kcal/mol; ν = ±0.71
			 Δρ₂
HOMO of N_2O to LUMO of B/As-FLP	HOMO of N_2O	LUMO of B/As-FLP	ΔE_2 = -33.0 kcal/mol; ν = ±0.50

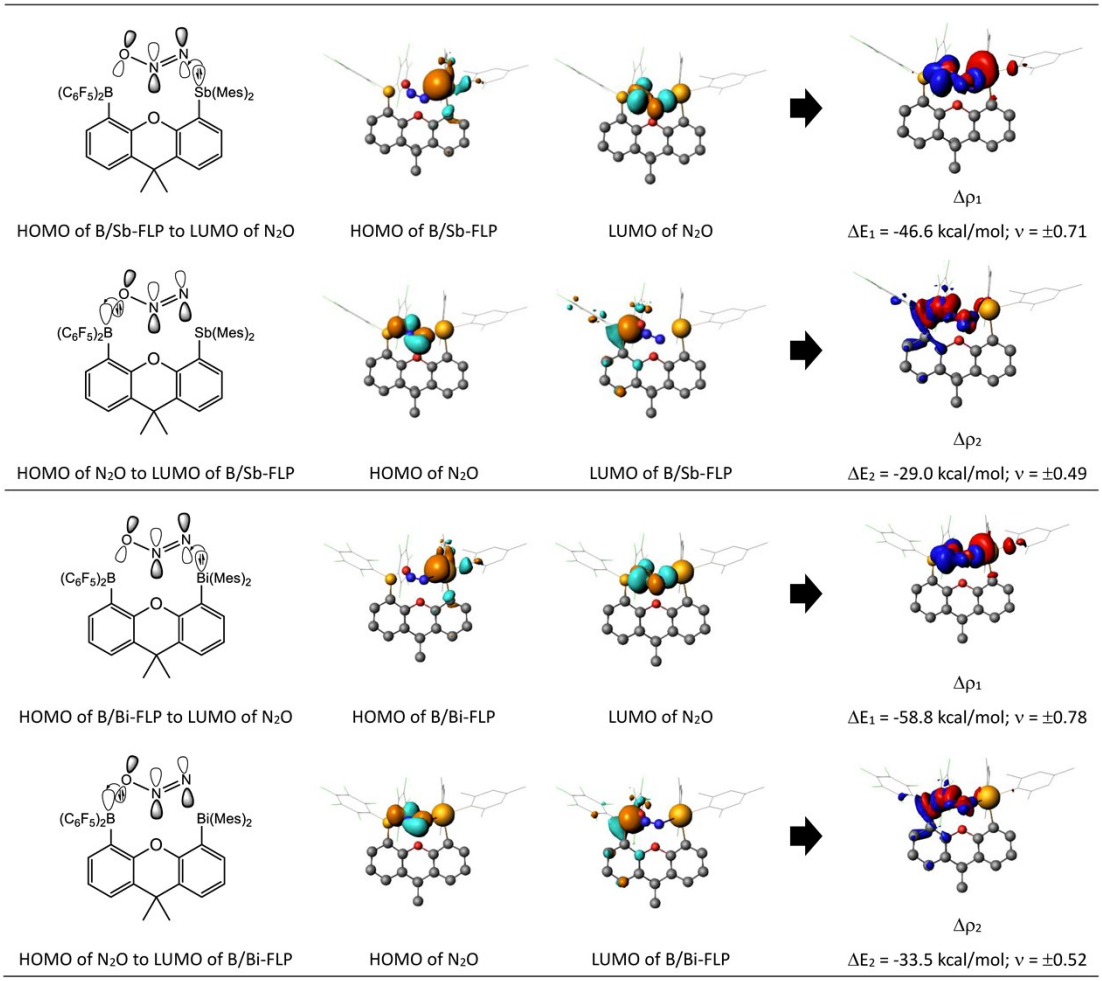


Figure S1: The EDA-NOCV analysis of **B/G15-TS** includes the following: (a) A qualitative depiction of the orbital interactions between **B/G15-Rea** and N_2O. (b) The shape of the most important interaction between the occupied and empty orbitals of **B/G15-Rea** and N_2O fragments. Hydrogen atoms have been omitted for clarity. (c) A plot showing the deformation densities ($\Delta\rho_1$ and $\Delta\rho_2$) resulting from the pairwise orbital interactions between the two fragments in their closed-shell state, accompanied by the respective associated interaction energies $\Delta E_{\mathrm{Orb}(1)}$ and $\Delta E_{\mathrm{Orb}(2)}$ measured in kcal/mol. The direction of charge flow in the deformation densities is denoted by the color gradient from red to blue.

(All calculations were based on B3LYP-D3(BJ)/def2-TZVP level.)

Table S2
B/P-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	8.03539600	2.54702100	0.73624900
C	6.57933800	1.86431400	-0.17885100
C	5.44283400	1.30753100	0.42739700
C	4.30580700	1.01220000	-0.32848300
C	4.27603900	1.26953900	-1.70153600
C	5.38608800	1.83029900	-2.34503400
C	6.50417000	2.12034200	-1.55608000
O	7.61099700	2.69007500	-2.13227600
C	7.39593300	3.56702900	-3.16831700
C	8.26743900	4.65886000	-3.23982100
C	8.01788600	5.60812300	-4.24440000
C	6.96539900	5.43466800	-5.14599900
C	6.11920200	4.32713500	-5.03534100
C	6.31802000	3.36715300	-4.03458300
C	5.49080300	2.09190200	-3.85191400
C	4.11333100	2.19886600	-4.51345200
C	6.27389500	0.91692300	-4.49499500
B	9.37940200	4.85846800	-2.15934500
C	10.50314100	3.81551300	-1.85999300
C	11.39127000	3.93993600	-0.77198000
F	11.27321900	4.94093000	0.10269000
C	12.42333000	3.04180100	-0.51864100
F	13.23506100	3.21485400	0.52062600
C	12.57746900	1.92839900	-1.34263200
F	13.55213500	1.06140900	-1.11608900
C	11.70066500	1.73072400	-2.40811300
C	10.70040900	2.66731000	-2.65582200
F	9.92820300	2.41799300	-3.71282000
F	11.81607500	0.64309800	-3.16449100

C	9.28664900	6.21884500	-1.36570000
C	10.32789300	7.14409900	-1.27035800
F	11.48210700	6.90279500	-1.90308700
C	10.22244500	8.32002100	-0.53004800
F	11.23191900	9.18377100	-0.46453400
C	9.03361600	8.58552200	0.15725800
F	8.92070000	9.69178900	0.88168100
C	7.96687300	7.68761900	0.08199600
C	8.09972400	6.53891500	-0.69831600
F	7.05281500	5.71075000	-0.75534500
F	6.84336800	7.92812600	0.75411100
C	7.42367400	2.41318700	2.48321800
C	7.01328000	3.63084400	3.08745000
C	7.01815300	4.93964700	2.33374300
C	6.59101200	3.62880700	4.41991400
C	6.55681500	2.45704400	5.18502200
C	6.10701100	2.49136700	6.62296100
C	6.94430700	1.26582400	4.56919000
C	7.37373400	1.21427700	3.23345700
C	7.75398600	-0.13760200	2.67856700
C	9.46779800	1.36345100	0.71570300
C	9.64886800	0.23758000	-0.12613300
C	8.66750400	-0.19213000	-1.18749000
C	10.80785800	-0.54016500	0.01251200
C	11.80192100	-0.25639100	0.95086300
C	13.02729900	-1.11961700	1.09237000
C	11.63111500	0.88261700	1.74063800
C	10.50680700	1.70690400	1.62642200
C	10.46461500	2.94458800	2.49198400
H	5.43901000	1.12665200	1.50188300
H	3.42955300	0.58104400	0.16081400
H	3.37852100	1.02901700	-2.27197600
H	8.65432000	6.49368700	-4.31853000
H	6.78990800	6.17384800	-5.93056400
H	5.29185900	4.21643900	-5.73718100
H	4.21348200	2.37007700	-5.59469300
H	3.51982500	3.01963900	-4.08378100
H	3.55018600	1.26242200	-4.39407900

H	6.38754700	1.08282100	-5.57756500
H	7.27890900	0.82450700	-4.05949600
H	5.73873800	-0.03200400	-4.33497400
H	6.64529200	5.75761400	2.96623800
H	8.03195000	5.20445000	1.99414400
H	6.39412000	4.89884100	1.43033600
H	6.27878200	4.57345800	4.87471000
H	6.09297900	1.48555700	7.06758300
H	6.77593900	3.12153100	7.23274600
H	5.09457700	2.91836000	6.71381300
H	6.90675400	0.33493700	5.14239200
H	7.28681300	-0.93635000	3.27318000
H	8.84341000	-0.29302200	2.70439000
H	7.44284800	-0.26276800	1.63443800
H	9.00282900	-1.12708100	-1.65689100
H	8.58185500	0.56596200	-1.97804600
H	7.65930800	-0.35713700	-0.78436700
H	10.93360300	-1.40320200	-0.64660300
H	13.02520100	-1.65766300	2.05539300
H	13.94339800	-0.50968300	1.06018500
H	13.08878500	-1.86730500	0.28849600
H	12.41288800	1.16314800	2.45152400
H	11.48479600	3.24871900	2.76471500
H	9.99118100	3.78965800	1.97204700
H	9.89453400	2.77710800	3.41861900

Table S3
Al/P-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z

P	8.16535900	2.64918500	0.71925900
C	6.61860600	2.19218600	-0.17994000
C	5.49448800	1.64225100	0.44717300
C	4.34694400	1.34238400	-0.28765500
C	4.31661500	1.57948300	-1.65931400

C	5.39876600	2.17136600	-2.33050100
C	6.51159200	2.50208300	-1.54710900
O	7.60805100	3.12003900	-2.12563600
C	7.54567700	3.56151600	-3.46730600
C	8.62405300	4.39898900	-3.72595100
C	8.71153100	4.89464600	-5.02851500
C	7.73667200	4.54072900	-5.97491300
C	6.65595900	3.72457900	-5.62570100
C	6.51836000	3.21021200	-4.32375900
C	5.36290200	2.33202400	-3.85959900
C	4.02692300	2.96431900	-4.30191200
C	5.51665500	0.92831000	-4.49494600
Al	9.22837700	4.50005700	-1.85174200
C	10.90159400	3.62338500	-1.29970000
C	11.72196600	4.08907300	-0.27345700
F	11.35813900	5.16248100	0.44767400
C	12.90755400	3.45530600	0.09529600
F	13.63360400	3.89144400	1.12617400
C	13.28581500	2.29016700	-0.57180900
F	14.37370900	1.62772600	-0.18632000
C	12.49491600	1.78458700	-1.60311600
C	11.31918500	2.45403900	-1.93479300
F	10.55645500	1.91158100	-2.90013900
F	12.83896100	0.64529800	-2.20329800
C	8.59697700	6.15233800	-0.97098800
C	9.46717200	7.23387500	-0.85480600
F	10.71229900	7.12981800	-1.35363300
C	9.10986900	8.44082100	-0.25279100
F	9.97281100	9.44938100	-0.15091900
C	7.80811900	8.58724400	0.23602400
F	7.44023700	9.72456500	0.81714600
C	6.89344700	7.53900200	0.11030600
C	7.30440000	6.35594700	-0.50311700
F	6.38975400	5.37122400	-0.60335100
F	5.65686200	7.67149500	0.58990100
C	7.61451900	2.51126800	2.48368000
C	7.37730500	3.72875300	3.17294600
C	7.45486600	5.06609000	2.48154200

C	7.04093700	3.69812200	4.52896500
C	6.92232100	2.49679100	5.23646100
C	6.57014100	2.49849000	6.70134800
C	7.13489400	1.30782200	4.53721400
C	7.47742000	1.28256300	3.17599000
C	7.67803500	-0.07631600	2.54779000
C	9.43523000	1.30159000	0.57124100
C	9.43688300	0.21459600	-0.33847500
C	8.34066000	-0.06375100	-1.33700400
C	10.52341400	-0.67106800	-0.33753900
C	11.61403200	-0.53172900	0.52258100
C	12.80179900	-1.45317600	0.44489700
C	11.59934900	0.54981300	1.40495800
C	10.55006800	1.47480100	1.43669700
C	10.67127300	2.62270600	2.41181800
H	5.52121000	1.44447300	1.51778100
H	3.47962100	0.90415900	0.21032200
H	3.42880400	1.29882800	-2.22718200
H	9.52538500	5.56457800	-5.31945500
H	7.80776200	4.91991700	-6.99722700
H	5.90297500	3.48788600	-6.38011500
H	3.99668600	3.08436500	-5.39403400
H	3.89234000	3.95419000	-3.84179400
H	3.17151200	2.33258300	-4.02415400
H	5.50856100	0.99956200	-5.59345100
H	6.46695300	0.46641800	-4.18863800
H	4.69533800	0.26487400	-4.18313300
H	7.35934200	5.88784200	3.20506800
H	8.39794600	5.19508000	1.93073500
H	6.64356700	5.17159400	1.74743200
H	6.86565600	4.64459800	5.04825600
H	6.47173800	1.47686100	7.09616700
H	7.34263600	3.01755200	7.29308400
H	5.61965800	3.02730100	6.88148500
H	7.02903800	0.35576100	5.06490800
H	7.13634900	-0.83997300	3.12492000
H	8.74147300	-0.35959600	2.53194900
H	7.32585700	-0.12025500	1.51111200

H	8.53821800	-1.01193900	-1.85530600
H	8.29498900	0.72178500	-2.10368900
H	7.34873800	-0.13352300	-0.87166600
H	10.51683800	-1.49828700	-1.05190400
H	13.21788600	-1.66240600	1.44235800
H	13.60171500	-0.98688800	-0.15359500
H	12.54294900	-2.40981600	-0.03216400
H	12.45216500	0.70660300	2.07161900
H	11.72754400	2.81224900	2.64778100
H	10.25099900	3.55640700	2.01314700
H	10.14353600	2.41289400	3.35489900

Table S4
Ga/P-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	8.08422400	2.61560300	0.62794800
C	6.53792200	2.07452700	-0.22668400
C	5.38647800	1.61956000	0.43200800
C	4.21560200	1.36204000	-0.28394100
C	4.17583700	1.54109400	-1.66865100
C	5.29815200	2.00442300	-2.36753000
C	6.44138700	2.28911400	-1.61042400
O	7.56557800	2.77737000	-2.22355800
C	7.40767000	3.49591000	-3.39642400
C	8.35729100	4.49745600	-3.57839900
C	8.25885200	5.26890800	-4.74128500
C	7.22553100	5.02689100	-5.65579500
C	6.27087100	4.03535300	-5.40667300
C	6.33869300	3.23891700	-4.25373900
C	5.37550300	2.10460400	-3.89843000
C	3.99311600	2.32179700	-4.52655200
C	5.97345500	0.77628600	-4.43123900
Ga	9.43859600	4.73978500	-1.94877700
C	11.01698800	3.66740900	-1.46879200

C	11.89090100	4.02306200	-0.44050200
F	11.66797000	5.12361700	0.28922500
C	12.99249000	3.24589000	-0.09094200
F	13.77117400	3.57780000	0.93910300
C	13.22206500	2.05086500	-0.77231600
F	14.23366100	1.26938500	-0.41051100
C	12.36298700	1.64871000	-1.79434200
C	11.27544300	2.45839500	-2.11791200
F	10.45543700	2.02378600	-3.08416100
F	12.56289800	0.48202700	-2.40427600
C	8.96253600	6.38512000	-0.94939500
C	9.85837600	7.41519700	-0.67839500
F	11.11778100	7.34181300	-1.13293100
C	9.49317900	8.55302500	0.04386900
F	10.36968400	9.52241000	0.29514400
C	8.17428400	8.67674200	0.49165900
F	7.80792500	9.74840900	1.18578900
C	7.24102900	7.67570400	0.21000400
C	7.65086700	6.56248900	-0.52218700
F	6.73319600	5.61420400	-0.78041800
F	5.99085100	7.78568600	0.65532500
C	7.55233500	2.50837800	2.40437200
C	7.28438800	3.73573100	3.06323800
C	7.33987900	5.05578400	2.33727800
C	6.94721200	3.73257800	4.41947200
C	6.85850100	2.54702800	5.15758100
C	6.51237700	2.57705700	6.62374400
C	7.09753500	1.34610900	4.48776700
C	7.43900800	1.29539800	3.12690400
C	7.65457400	-0.07180900	2.52372800
C	9.41043400	1.31534800	0.53689300
C	9.44445100	0.16910800	-0.30040900
C	8.36593300	-0.18872600	-1.29048800
C	10.54079400	-0.69734900	-0.22320900
C	11.61703300	-0.48492200	0.64314000
C	12.79788000	-1.41880900	0.64921300
C	11.57937100	0.65805500	1.44084900
C	10.51514700	1.56901800	1.39260400

C	10.61110900	2.78929200	2.27839800
H	5.40364800	1.47877400	1.51234100
H	3.32615200	1.00980700	0.24288700
H	3.25805900	1.30900600	-2.20936900
H	8.96897700	6.07758900	-4.93470900
H	7.14926100	5.63003500	-6.56349200
H	5.46229800	3.88530100	-6.12310100
H	4.06777300	2.37108900	-5.62193000
H	3.52863600	3.25184900	-4.16661700
H	3.32065300	1.48342200	-4.29680500
H	6.07419800	0.81533900	-5.52699600
H	6.96957400	0.59201800	-4.00421700
H	5.32352300	-0.07138700	-4.16338900
H	7.11174100	5.88835600	3.01765600
H	8.33091300	5.23498000	1.89384800
H	6.61498600	5.08810400	1.51237600
H	6.74588000	4.68734300	4.91367000
H	6.36383200	1.56422700	7.02611500
H	7.31477600	3.05774600	7.20910300
H	5.59225300	3.15645200	6.80514200
H	7.00998800	0.40498600	5.03810700
H	7.13921900	-0.83422900	3.12599100
H	8.72253000	-0.33546700	2.49080000
H	7.27923200	-0.14015500	1.49607900
H	8.58588100	-1.15974600	-1.75472100
H	8.31335900	0.56009100	-2.09168500
H	7.37154100	-0.25135300	-0.82896100
H	10.55453500	-1.57326700	-0.87721200
H	13.45049500	-1.24132100	1.51623900
H	13.40389900	-1.27226500	-0.25985700
H	12.47770100	-2.47257400	0.66502800
H	12.42195200	0.87590600	2.10317700
H	11.66280200	3.01944700	2.49861100
H	10.16885200	3.67880200	1.80779700
H	10.08696500	2.64062100	3.23503100

Table S5

In/P-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	8.01648100	2.47792700	0.50914000
C	6.60144500	1.62711400	-0.33504900
C	5.53283000	0.99432400	0.32294300
C	4.40167200	0.59788300	-0.39283100
C	4.28905800	0.85483800	-1.76499900
C	5.32452400	1.49216500	-2.45428000
C	6.46325600	1.83175700	-1.71225900
O	7.49396700	2.46050000	-2.34776600
C	7.09372000	3.47159800	-3.21859400
C	7.78218800	4.66869800	-3.09190600
C	7.36752900	5.71667900	-3.92362500
C	6.29675200	5.52994000	-4.80884400
C	5.60538900	4.31177300	-4.86077300
C	5.99408200	3.24107300	-4.04531000
C	5.33016400	1.86051900	-3.94742200
C	3.91931400	1.85869600	-4.54074600
C	6.20902600	0.83380700	-4.70795600
In	9.22308300	4.55421100	-1.45334700
C	10.92729300	3.19875800	-1.72895900
C	11.98491300	3.11435000	-0.82941700
F	12.03421500	3.92572700	0.23633500
C	13.01054100	2.17817000	-0.95445900
F	13.98877000	2.10210700	-0.05098800
C	12.97255400	1.26758500	-2.00944700
F	13.91071200	0.32685800	-2.10815100
C	11.93207100	1.32000000	-2.93718100
C	10.93859400	2.28918200	-2.78443400
F	9.95793400	2.29150200	-3.70271400
F	11.88477600	0.43505700	-3.93350900
C	9.39597600	6.49394100	-0.42077200
C	10.59395800	7.09825200	-0.04802100
F	11.76469000	6.49611000	-0.28838200
C	10.64210600	8.35047300	0.57244800

F	11.80296600	8.89888000	0.92640500
C	9.45124600	9.04369700	0.80160100
F	9.47808700	10.23659100	1.38632000
C	8.23148200	8.48181500	0.41562700
C	8.23482500	7.23205900	-0.20479700
F	7.04244800	6.73778000	-0.58409900
F	7.09592000	9.14474200	0.63109800
C	7.34205500	2.54503000	2.23364000
C	6.79259800	3.77394200	2.67274000
C	6.75215800	4.98283300	1.77821400
C	6.28764200	3.87730800	3.97138700
C	6.30217000	2.79556000	4.85863400
C	5.77101200	2.94216100	6.26065200
C	6.82115800	1.58430800	4.39764300
C	7.33947600	1.42595600	3.10277700
C	7.85504100	0.05293000	2.73772400
C	9.52000300	1.41462800	0.68069500
C	9.81463500	0.27893900	-0.11455700
C	8.92898600	-0.21974900	-1.22833200
C	11.00433200	-0.41698300	0.12268600
C	11.92585500	-0.03006900	1.10121400
C	13.22287700	-0.77511200	1.27014200
C	11.63501300	1.11411200	1.84289300
C	10.46358300	1.85637100	1.64294600
C	10.29417300	3.11281600	2.46529000
H	5.56441100	0.84358600	1.40055300
H	3.58072700	0.10553400	0.13286400
H	3.37939800	0.56283300	-2.29110200
H	7.85627100	6.69358100	-3.87169100
H	5.97645800	6.35309500	-5.45232900
H	4.75357000	4.20856400	-5.53463900
H	3.95004500	2.12971500	-5.60584200
H	3.25922200	2.56966200	-4.02168500
H	3.47010200	0.85666100	-4.47901100
H	6.24428400	1.08866100	-5.77827200
H	7.23981000	0.83161200	-4.32669900
H	5.79389800	-0.18045000	-4.59999500
H	6.20481700	5.81055700	2.24999200

H	7.76916600	5.33895000	1.55771500
H	6.27204200	4.77249500	0.81241600
H	5.86825400	4.83327000	4.29724900
H	5.71582500	1.97298500	6.77714000
H	6.41790600	3.60585600	6.85899700
H	4.76422600	3.38990600	6.26135100
H	6.81927800	0.71829300	5.06538100
H	7.38401600	-0.70523500	3.38013200
H	8.94431400	-0.01905800	2.87698500
H	7.65492000	-0.21512000	1.69404800
H	9.39418600	-1.08461400	-1.72076800
H	8.77398000	0.55285100	-1.99322700
H	7.93767900	-0.52983700	-0.86777200
H	11.22875400	-1.28705600	-0.50062400
H	13.75285200	-0.46419400	2.18177000
H	13.88784500	-0.57943000	0.41328900
H	13.05916800	-1.86337400	1.31636100
H	12.35906900	1.47198900	2.57902700
H	11.27749400	3.48502800	2.78149200
H	9.80870300	3.92040500	1.89827000
H	9.68450700	2.93834100	3.36426200

Table S6
Tl/P-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	8.05907500	2.55053400	0.52094600
C	6.49345000	1.97752700	-0.27685800
C	5.34661600	1.56560200	0.41915600
C	4.15509900	1.31908100	-0.26664300
C	4.08137900	1.47858500	-1.65388100
C	5.19932900	1.89548700	-2.38615700
C	6.37124200	2.14606600	-1.66307400
O	7.49091900	2.57897500	-2.31938200
C	7.29144800	3.39926000	-3.41547900

C	8.19852900	4.44110200	-3.55771200
C	8.03608100	5.30631500	-4.64146200
C	6.96754500	5.11228500	-5.52811700
C	6.04553200	4.08020000	-5.32253700
C	6.18743600	3.19364000	-4.24583300
C	5.25626600	2.02201800	-3.91615000
C	3.86363800	2.21366800	-4.52599300
C	5.88532700	0.72208400	-4.48159600
Tl	9.49260500	4.65539600	-1.76357600
C	11.31024400	3.47411300	-1.32938800
C	12.24533400	3.85399300	-0.37466300
F	12.07574300	4.97558500	0.33659400
C	13.35858300	3.06717800	-0.07893700
F	14.20487300	3.41144100	0.89207100
C	13.54093600	1.86553400	-0.76329700
F	14.56859500	1.07839900	-0.45664000
C	12.61463000	1.45517700	-1.72280300
C	11.50824900	2.26246500	-1.98411100
F	10.61686500	1.82420600	-2.88384900
F	12.77161400	0.27934200	-2.33022300
C	8.97840000	6.58464400	-0.74148200
C	9.90436200	7.54527200	-0.35667200
F	11.20734000	7.37758200	-0.61955300
C	9.52131900	8.71840900	0.30059400
F	10.42136600	9.62819500	0.66865000
C	8.16606600	8.94106700	0.56052400
F	7.78456800	10.04911100	1.18772500
C	7.21072800	8.00139800	0.16228500
C	7.63750100	6.84998400	-0.49867800
F	6.69809100	5.95885500	-0.86622800
F	5.92171000	8.21123900	0.42489000
C	7.55734300	2.53610000	2.30793800
C	7.30219900	3.78919700	2.91977700
C	7.37127900	5.07922500	2.14532000
C	6.97722800	3.84034800	4.27796500
C	6.88907200	2.68491900	5.06228700
C	6.55467900	2.77373200	6.52862000
C	7.11590700	1.45758800	4.43753000

C	7.44468300	1.35158900	3.07685700
C	7.64884900	-0.04003400	2.52752800
C	9.39320000	1.25986000	0.47482000
C	9.42310700	0.08635800	-0.32142300
C	8.33633200	-0.31080800	-1.28702100
C	10.52405200	-0.77301900	-0.22196800
C	11.60491800	-0.52632400	0.62834000
C	12.79057100	-1.45357300	0.66194100
C	11.57059000	0.64619100	1.38308200
C	10.50324400	1.55044300	1.31276600
C	10.60200400	2.79778700	2.15951800
H	5.38010000	1.45736600	1.50281500
H	3.27017100	1.00086100	0.28867200
H	3.14087700	1.27214300	-2.16554700
H	8.71545200	6.14957300	-4.79192200
H	6.83685400	5.78904600	-6.37591100
H	5.20527600	3.97312400	-6.00950800
H	3.92660400	2.28341600	-5.62117400
H	3.37774400	3.12484500	-4.14649000
H	3.21666700	1.35356900	-4.30196500
H	5.97645800	0.78841200	-5.57677000
H	6.88886000	0.55317500	-4.06591900
H	5.25845600	-0.14739500	-4.22926800
H	7.09341600	5.93280100	2.77966500
H	8.38321700	5.26337800	1.75410500
H	6.69662100	5.06824700	1.27879700
H	6.78568900	4.81478300	4.73621100
H	6.42353100	1.77769200	6.97586100
H	7.35453300	3.29084200	7.08509400
H	5.62798000	3.34760500	6.69230700
H	7.02866000	0.53907100	5.02470600
H	7.13507100	-0.77428900	3.16496600
H	8.71529300	-0.30982800	2.49711600
H	7.26458600	-0.15002500	1.50685700
H	8.55828800	-1.29505000	-1.72135100
H	8.26808700	0.41150200	-2.11107600
H	7.34813200	-0.36670800	-0.81099400
H	10.53545800	-1.67236700	-0.84328700

H	12.47629400	-2.50884500	0.66109300
H	13.41723500	-1.27800500	1.54830700
H	13.42219800	-1.29765200	-0.22759300
H	12.41629800	0.88811300	2.03302700
H	11.65396300	3.02793700	2.37790200
H	10.17160200	3.67715000	1.66002400
H	10.07296100	2.68310000	3.11781000

Table S7
B/N-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
N	7.40872000	1.53764700	0.99649400
C	6.38050400	1.34949200	0.05343800
C	5.19643000	0.69393000	0.42675500
C	4.15266400	0.53033900	-0.47736300
C	4.27892900	0.99790400	-1.78760500
C	5.44468400	1.65586800	-2.19347800
C	6.47217600	1.84964800	-1.25837700
O	7.58772800	2.59163700	-1.58795000
C	7.43149000	3.58860300	-2.51810500
C	8.31115500	4.68557700	-2.44866000
C	8.03839300	5.77560600	-3.30178200
C	6.99797500	5.73652100	-4.22813200
C	6.20693900	4.59134500	-4.32523700
C	6.41878200	3.49336600	-3.48255100
C	5.69283700	2.15674000	-3.61300200
C	4.40175200	2.26960000	-4.42836500
C	6.64777200	1.15811100	-4.32086500
B	9.64421500	4.77112000	-1.65280600
C	10.76710400	3.68031000	-1.71001500
C	11.93120300	3.75848500	-0.92002700
F	12.02963800	4.65300400	0.06686600
C	13.02929300	2.92290600	-1.08452400
F	14.08783900	3.02755400	-0.28318000

C	12.98094500	1.91225400	-2.04330500
F	14.00561200	1.08622300	-2.19365100
C	11.83502600	1.75223600	-2.81915400
C	10.76335600	2.62818800	-2.64811700
F	9.73578400	2.43785800	-3.47304300
F	11.77446000	0.77462000	-3.71773100
C	9.92937600	6.16413000	-0.95719200
C	11.04797300	6.94983200	-1.25088700
F	11.95571800	6.50954900	-2.13061500
C	11.26619400	8.19859400	-0.67169000
F	12.33780300	8.92131300	-0.98357600
C	10.33379800	8.69525600	0.24403800
F	10.52641300	9.88006400	0.80858000
C	9.20152300	7.94371900	0.56532700
C	9.01332000	6.70583400	-0.05090700
F	7.91421700	6.01872900	0.27949400
F	8.31678900	8.41422900	1.43906800
C	7.01060700	1.86434100	2.33182900
C	6.25182900	3.03775100	2.55151700
C	5.83216800	3.93218000	1.41531700
C	5.88972700	3.37049900	3.86064500
C	6.26185800	2.58845600	4.95937200
C	5.90446900	2.99669700	6.36596200
C	6.99707600	1.42485000	4.71029300
C	7.36955900	1.03477400	3.41777200
C	8.11379200	-0.26247400	3.22868600
C	8.76744000	1.20692000	0.73046000
C	9.11866100	0.01777500	0.04275400
C	8.10368000	-0.93099500	-0.54444800
C	10.47023700	-0.33455900	-0.04315400
C	11.48575900	0.41452500	0.55868700
C	12.91384700	-0.06767000	0.55373600
C	11.11637700	1.60666400	1.18684900
C	9.78665400	2.03918500	1.25167300
C	9.49249800	3.38526500	1.86160000
H	5.11323700	0.32060100	1.44807000
H	3.23902600	0.01958100	-0.16563200
H	3.46350000	0.84708300	-2.49374200

H	8.67772100	6.65959200	-3.25223100
H	6.81226800	6.58909800	-4.88449700
H	5.41486600	4.55204200	-5.07320700
H	4.61677600	2.61570300	-5.44927500
H	3.68613100	2.96618600	-3.96665900
H	3.91781500	1.28764300	-4.52472000
H	6.88044600	1.50894600	-5.33840800
H	7.59546000	1.05595800	-3.77426600
H	6.17519000	0.16574100	-4.38675200
H	5.62401700	4.94936100	1.77561500
H	6.60592400	3.99446400	0.64100100
H	4.92268600	3.55155700	0.92191100
H	5.31014900	4.28348800	4.02514000
H	5.74193200	2.11948400	7.01190200
H	6.71408400	3.59243400	6.82447300
H	4.99276800	3.61345400	6.38869300
H	7.27716000	0.78075100	5.54906000
H	8.03261200	-0.88427000	4.13172700
H	9.18317100	-0.10149300	3.02123900
H	7.71374600	-0.83515100	2.38020700
H	8.58824900	-1.87791400	-0.82099900
H	7.61988900	-0.52467200	-1.44594200
H	7.29327800	-1.15574800	0.16311600
H	10.73076000	-1.26154100	-0.56203500
H	13.09378900	-0.76711000	1.38870900
H	13.62697200	0.76095400	0.66604900
H	13.15827800	-0.60291700	-0.37555700
H	11.89130200	2.24390800	1.62186200
H	10.39471800	4.01107100	1.84538400
H	8.70106900	3.90797100	1.30997700
H	9.14877100	3.30979700	2.90496900

Table S8
B/As-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z

As	8.11259600	2.67245900	0.71069400
C	6.55611700	1.89119800	-0.22226600
C	5.42261000	1.35097100	0.39782600
C	4.28387300	1.04696100	-0.35504000
C	4.25320600	1.28577600	-1.73208400
C	5.36540000	1.83059000	-2.38619100
C	6.48489200	2.12100000	-1.60009600
O	7.59770100	2.67591500	-2.18561800
C	7.38287500	3.55667500	-3.21746900
C	8.24950400	4.65305600	-3.28181300
C	7.99611000	5.60500700	-4.28354200
C	6.94534500	5.42956100	-5.18661200
C	6.10150800	4.31930300	-5.07951000
C	6.30314100	3.35680200	-4.08210300
C	5.47382500	2.08223800	-3.89480400
C	4.09799800	2.18716300	-4.55959000
C	6.25746800	0.90263000	-4.52852700
B	9.35204800	4.85805700	-2.19211300
C	10.48534600	3.82745300	-1.88110700
C	11.35774900	3.96183600	-0.78136400
F	11.21152500	4.95772500	0.09550000
C	12.39716000	3.07645500	-0.51367000
F	13.19212300	3.26019800	0.53588700
C	12.57962500	1.96880400	-1.33992300
F	13.56559000	1.11758700	-1.10393000
C	11.71869800	1.76040700	-2.41657300
C	10.70799500	2.68323800	-2.67568200
F	9.94911100	2.42494500	-3.73991200
F	11.85992000	0.67655000	-3.17379100
C	9.24084000	6.21406900	-1.39200300
C	10.26787500	7.15562400	-1.30895600
F	11.41822900	6.93113800	-1.95561500
C	10.15357700	8.32874600	-0.56553700
F	11.14978800	9.20841600	-0.51207300
C	8.97005800	8.57353000	0.13827700
F	8.84809800	9.67719100	0.86524000
C	7.91784500	7.65745900	0.07698200

C	8.05950400	6.51117100	-0.70537600
F	7.02749500	5.66169700	-0.74423200
F	6.80015200	7.87906700	0.76516300
C	7.42801400	2.48051200	2.55849200
C	7.03776000	3.68796200	3.19021500
C	7.09519000	5.02246700	2.48159800
C	6.58302600	3.65331700	4.51220200
C	6.49710300	2.45717800	5.23472600
C	5.99744900	2.45355400	6.65680800
C	6.87239400	1.27768400	4.58972100
C	7.33642200	1.26013300	3.26372000
C	7.71513400	-0.07858200	2.67641200
C	9.59048600	1.34632000	0.73273300
C	9.74678100	0.23080700	-0.12637200
C	8.75925200	-0.14302600	-1.20210300
C	10.88089400	-0.57897100	0.01031300
C	11.87587200	-0.32997200	0.96174700
C	13.08293400	-1.22416000	1.06452800
C	11.72391900	0.79448200	1.77219400
C	10.61364400	1.64506800	1.66579700
C	10.57433400	2.85570900	2.56939600
H	5.41810200	1.19036100	1.47621600
H	3.40541600	0.62729800	0.14042700
H	3.35234600	1.04377400	-2.29690800
H	8.62760500	6.49441600	-4.35372800
H	6.76766200	6.17067500	-5.96885800
H	5.27348300	4.20974300	-5.78078000
H	4.20009000	2.34991900	-5.64204200
H	3.50538600	3.01229500	-4.13706800
H	3.53288700	1.25277000	-4.43316100
H	6.37643300	1.06267100	-5.61143300
H	7.25995700	0.80995900	-4.08713900
H	5.71923700	-0.04415600	-4.36627900
H	6.72174200	5.82697800	3.13064500
H	8.12450900	5.27991500	2.18359600
H	6.49412900	5.02944200	1.56116100
H	6.28483700	4.59021300	4.99211300
H	6.05842900	1.44749400	7.10463400

H	6.58484400	3.14656700	7.28784100
H	4.94298200	2.78596500	6.70843000
H	6.80101200	0.32995500	5.13143000
H	7.21766600	-0.89064700	3.22685000
H	8.80096200	-0.24978000	2.73409300
H	7.43970100	-0.16400800	1.61839700
H	9.07851900	-1.06305400	-1.71084900
H	8.67830600	0.64821300	-1.95959200
H	7.75045200	-0.30913000	-0.79961500
H	10.99069200	-1.43664900	-0.65942700
H	13.72163500	-0.94459400	1.91484400
H	13.69271600	-1.15892600	0.14888700
H	12.79004800	-2.27934000	1.18786300
H	12.50204100	1.03866400	2.50007000
H	11.58205700	3.08650600	2.94123500
H	10.20468400	3.74909500	2.04438700
H	9.91482500	2.69642600	3.43608700

Table S9
B/Sb-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Sb	8.19101300	2.83108600	0.71779400
C	6.48291000	1.88647500	-0.25979100
C	5.34971100	1.35095800	0.36244900
C	4.22056000	1.02497100	-0.39831200
C	4.20019200	1.24555700	-1.77964600
C	5.31571500	1.78480500	-2.43376400
C	6.42688700	2.08187500	-1.63996000
O	7.54787400	2.63471400	-2.22493200
C	7.32934900	3.53238400	-3.24081200
C	8.18399500	4.64030800	-3.28862300
C	7.91143900	5.60702100	-4.27279700
C	6.85986500	5.43484100	-5.17482400
C	6.03197600	4.31080000	-5.08643700

C	6.24982400	3.33342900	-4.10756600
C	5.43607100	2.04446700	-3.93977100
C	4.06585000	2.13424800	-4.61748800
C	6.24363300	0.88110500	-4.57332200
B	9.31773100	4.84911900	-2.23258100
C	10.46475400	3.81892600	-1.95352800
C	11.36389300	3.94936900	-0.87419500
F	11.22722200	4.93579800	0.01654000
C	12.40855000	3.06385200	-0.62997200
F	13.22075000	3.24290500	0.40646500
C	12.58023200	1.96454300	-1.47024800
F	13.57383900	1.11511600	-1.26295800
C	11.69824200	1.76242000	-2.53080900
C	10.67694100	2.68226700	-2.76120800
F	9.89609400	2.42736000	-3.81015900
F	11.82899600	0.68725100	-3.30168400
C	9.25343600	6.21949900	-1.44968500
C	10.30668800	7.13532600	-1.40923900
F	11.43040100	6.87372200	-2.08799500
C	10.24888000	8.31788400	-0.67428500
F	11.26943300	9.17050700	-0.66307200
C	9.09632100	8.60173000	0.06516000
F	9.02799900	9.71466200	0.78451500
C	8.01964400	7.71261900	0.04880500
C	8.10303900	6.55776700	-0.72928600
F	7.04416500	5.73980700	-0.72163000
F	6.93188000	7.96845700	0.77224100
C	7.37612600	2.58247600	2.73395800
C	6.95590500	3.77033200	3.38071700
C	7.07189500	5.13078600	2.72591100
C	6.41344000	3.69348600	4.66833600
C	6.27173800	2.47257400	5.33936600
C	5.68743900	2.42415000	6.72819000
C	6.68694500	1.31284100	4.68215200
C	7.23985500	1.34083500	3.39058600
C	7.67558800	0.03083000	2.77888000
C	9.77957400	1.31462400	0.76792400
C	9.90644700	0.21660500	-0.11304300

C	8.88615600	-0.11363600	-1.17250600
C	11.03376900	-0.61033100	-0.01282900
C	12.04559000	-0.38742000	0.92671200
C	13.26264600	-1.27265500	0.97764900
C	11.91127200	0.71253600	1.77623800
C	10.80566400	1.57185700	1.70703900
C	10.76323600	2.75538000	2.64592900
H	5.33496600	1.21263300	1.44523600
H	3.33859800	0.60816300	0.09374000
H	3.30298800	0.99562100	-2.34716500
H	8.53200500	6.50489800	-4.33065100
H	6.66948900	6.18816800	-5.94225600
H	5.20355100	4.20255800	-5.78745600
H	4.17572200	2.30339600	-5.69829300
H	3.45762900	2.94891000	-4.19678300
H	3.51277100	1.19149500	-4.49960500
H	6.37045700	1.04996000	-5.65401700
H	7.24294100	0.80019100	-4.12250800
H	5.71756700	-0.07434900	-4.42265600
H	6.66548900	5.91720500	3.37748000
H	8.12184400	5.38926400	2.50926600
H	6.53038300	5.18458900	1.76886600
H	6.08746900	4.61441700	5.16135500
H	5.58584500	1.39024000	7.08893800
H	6.32225400	2.97086000	7.44560200
H	4.69106500	2.89492500	6.75896400
H	6.57840400	0.34800300	5.18643400
H	7.20495000	-0.81609500	3.29919000
H	8.76693000	-0.09692300	2.84544700
H	7.41916800	-0.03733300	1.71352100
H	9.17753600	-1.01884900	-1.72320700
H	8.78340600	0.70292800	-1.90034500
H	7.88901000	-0.28243200	-0.74111200
H	11.12485900	-1.45592600	-0.70067100
H	13.76574200	-1.21376400	1.95419500
H	13.99135100	-0.96627300	0.20840700
H	13.00466900	-2.32526900	0.78412300
H	12.69700600	0.92354800	2.50675900

H	11.70395100	2.84352400	3.20645900
H	10.62201100	3.70212000	2.09950200
H	9.93922000	2.67255600	3.37154700

Table S10
B/Bi-Rea

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Bi	8.22316400	2.91964800	0.75425600
C	6.43914600	1.90767900	-0.26273300
C	5.30878600	1.35981900	0.34984200
C	4.19181000	1.01802300	-0.42378500
C	4.18597400	1.23462800	-1.80588100
C	5.30286500	1.78516400	-2.44929900
C	6.40000200	2.09900600	-1.64219500
O	7.52461200	2.66662000	-2.21457400
C	7.31667300	3.54108800	-3.25063800
C	8.17567300	4.64618700	-3.31556400
C	7.90986900	5.59843700	-4.31580800
C	6.86338600	5.41349000	-5.22085900
C	6.03659600	4.28955500	-5.12128700
C	6.24634500	3.32709200	-4.12596300
C	5.43782000	2.03539400	-3.95536700
C	4.07467800	2.11114800	-4.64909100
C	6.26005500	0.87268000	-4.57124000
B	9.31523100	4.86522400	-2.27052700
C	10.45632100	3.83305200	-1.97593100
C	11.35994700	3.97503300	-0.90090700
F	11.21957300	4.96642000	-0.01436800
C	12.41057900	3.09726600	-0.65526400
F	13.22578700	3.28734100	0.37617500
C	12.58509200	1.99390900	-1.49009300
F	13.58623900	1.15464100	-1.28438400
C	11.69754300	1.77806300	-2.54357700
C	10.66879000	2.68936900	-2.77455200

F	9.88239800	2.42202100	-3.81534800
F	11.83093200	0.69891500	-3.30730000
C	9.26114400	6.24297000	-1.49855400
C	10.31156300	7.16256100	-1.48697000
F	11.42337100	6.89670600	-2.18328500
C	10.26245400	8.35220100	-0.76271900
F	11.27886100	9.20903700	-0.77967800
C	9.12336100	8.63839700	-0.00319100
F	9.06457900	9.75778500	0.70626800
C	8.05128700	7.74346000	0.01267400
C	8.12573200	6.58182900	-0.75597100
F	7.07417400	5.75294500	-0.71364400
F	6.97815100	7.99925700	0.75687100
C	7.34159000	2.61058900	2.85052600
C	6.90280000	3.78436400	3.50521700
C	7.04559700	5.15611200	2.87830100
C	6.31868400	3.68140400	4.77334800
C	6.15525400	2.44541600	5.41188700
C	5.52062500	2.36655100	6.77736100
C	6.59470100	1.29946000	4.74528000
C	7.18946600	1.35599200	3.47274500
C	7.65512200	0.06683300	2.83969900
C	9.86507800	1.29901200	0.78660800
C	9.96651700	0.21514600	-0.11137600
C	8.92052200	-0.08730700	-1.15421400
C	11.09109100	-0.62012500	-0.04320300
C	12.11938300	-0.41502600	0.88301700
C	13.33379800	-1.30569400	0.89722800
C	12.00341500	0.66928800	1.75597200
C	10.89925900	1.53361500	1.71824900
C	10.86644300	2.70414500	2.67444800
H	5.28503600	1.22192900	1.43322800
H	3.30873200	0.59135300	0.05803400
H	3.29891100	0.97164500	-2.38337700
H	8.53366200	6.49325900	-4.38552400
H	6.67787700	6.15481800	-6.00101700
H	5.21466000	4.16898300	-5.82788000
H	4.19498200	2.27183000	-5.73010500

H	3.45673600	2.92519100	-4.24154200
H	3.52631900	1.16596300	-4.52929900
H	6.39809800	1.03380000	-5.65180400
H	7.25462600	0.80177300	-4.10827900
H	5.73863600	-0.08497700	-4.41862400
H	6.62349000	5.93501200	3.52900600
H	8.10369000	5.41468200	2.70195300
H	6.53280300	5.23156100	1.90589400
H	5.97702700	4.59155200	5.27621000
H	5.44493800	1.32722800	7.12891100
H	6.10465900	2.93325000	7.52170200
H	4.50559200	2.79731400	6.77148200
H	6.47302900	0.32445400	5.22677900
H	7.21643800	-0.80216700	3.35146400
H	8.75070200	-0.02841100	2.88944000
H	7.38717100	0.00888900	1.77571200
H	9.18301400	-0.99179100	-1.72073900
H	8.81515300	0.73886200	-1.87128900
H	7.92966000	-0.24086400	-0.70283000
H	11.16666600	-1.45644300	-0.74445700
H	13.87193100	-1.24203000	1.85455500
H	14.03608100	-1.00967200	0.09977300
H	13.06438000	-2.35870400	0.72167100
H	12.80021600	0.86111100	2.48009700
H	11.75618400	2.71269300	3.31906200
H	10.85251400	3.66566800	2.13454500
H	9.97700300	2.67658300	3.32351600

Table S11
N_2O

Atomic Coordinates (Angstroms)

Number	X	Y	Z

N	2.90387200	-0.43652600	0.12566500
N	2.13052300	-0.96440800	-0.50754100
O	1.32173300	-1.51562300	-1.16967000

Table S12
B/P-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	2.31460300	-0.10841100	-0.76228700
N	0.63217000	-1.39062100	-2.37617100
N	-0.34751600	-0.91405500	-2.04325600
O	-0.86339900	0.00625300	-1.38430200
B	-2.13680800	-0.36260000	-0.31245400
C	-2.05276600	-1.93633400	-0.01910500
C	-0.89635700	-2.57866000	0.45968200
O	0.26138200	-1.81324500	0.52926700
C	1.47655500	-2.44652400	0.54179100
C	2.58433900	-1.71764100	0.06418100
C	3.83650300	-2.35017700	0.05317400
C	3.97412400	-3.65823000	0.51627300
C	2.86340900	-4.34984800	1.00020500
C	1.59636900	-3.75371900	1.02998100
C	0.36294800	-4.41154100	1.64383400
C	-0.86802000	-3.91090800	0.88795000
C	-2.03647200	-4.66731400	0.72733600
C	-3.19075900	-4.09245500	0.19968500
C	-3.19611800	-2.74018300	-0.14619700
C	0.46790000	-5.94133400	1.63663600
C	0.23823300	-3.92114400	3.11214200
C	-1.73227100	0.65584400	0.88051400
C	-1.57355100	0.30365500	2.22242000
F	-1.67659500	-0.97012600	2.62952600
C	-1.30140900	1.23434200	3.22642500
F	-1.08921200	0.83680000	4.48233400
C	-1.20538700	2.58373900	2.90205900
F	-0.91415900	3.47898900	3.84431600
C	-1.36130900	2.98470000	1.57718100
C	-1.59680800	2.02060600	0.60119000

F	-1.71473100	2.46011400	-0.66118800
F	-1.24319600	4.27404700	1.25396800
C	-3.49156600	0.08652600	-1.08129400
C	-4.57172200	0.64700700	-0.39242700
F	-4.51436100	0.81973000	0.93582800
C	-5.76033600	1.03406900	-1.01614000
F	-6.75735700	1.56584800	-0.31188300
C	-5.90059300	0.85209500	-2.39202500
F	-7.02316000	1.21387300	-3.00533800
C	-4.85764500	0.27579200	-3.11791700
C	-3.69022000	-0.10036800	-2.45151000
F	-2.74004000	-0.68399700	-3.20191700
F	-4.98740500	0.08273100	-4.42942200
C	3.97580300	0.33195400	-1.45997200
C	4.16294100	0.22254200	-2.86316000
C	3.09774600	-0.29822900	-3.79544700
C	5.38705200	0.60350700	-3.42453300
C	6.44398200	1.08853500	-2.64952500
C	7.73714900	1.52589400	-3.28578100
C	6.25073300	1.16798600	-1.26919300
C	5.04498500	0.80362400	-0.65392700
C	4.97887400	0.92801100	0.84699200
C	1.96214600	1.27071400	0.41177900
C	1.92608700	1.20639100	1.82674000
C	1.95633900	-0.06948000	2.62882900
C	1.84977900	2.40632100	2.54863600
C	1.77771100	3.65860200	1.93573400
C	1.71928400	3.69002200	0.53944900
C	1.78731800	2.52780700	-0.23229800
C	1.65225600	2.65938200	-1.72988100
C	1.68022400	4.92705800	2.73955200
H	4.70344300	-1.81732800	-0.33704000
H	4.95378500	-4.14030600	0.50036700
H	2.98905500	-5.36789100	1.36813500
H	-2.05251300	-5.71254300	1.03612600
H	-4.09457500	-4.69374200	0.07991100
H	-4.11814200	-2.29099400	-0.51913700
H	-0.41740500	-6.39392000	2.10354800

H	1.33346800	-6.27725100	2.22455200
H	0.56416200	-6.33677200	0.61437200
H	-0.64605500	-4.37356100	3.58680300
H	1.13443900	-4.20126000	3.68778600
H	0.11788400	-2.82993800	3.15901700
H	3.44283400	-0.24741700	-4.83749300
H	2.83843900	-1.34346700	-3.57545000
H	2.16733500	0.28303200	-3.71735800
H	5.51599600	0.51442100	-4.50661200
H	8.57182400	1.49297400	-2.57006200
H	7.99555000	0.89420000	-4.14931000
H	7.65953900	2.56363300	-3.65393100
H	7.06994800	1.52179300	-0.63710100
H	5.99391500	0.95944200	1.26782200
H	4.44827300	0.08923100	1.31206400
H	4.45952800	1.84818500	1.15241700
H	1.94812000	0.16074300	3.70257200
H	1.07296900	-0.68428300	2.41530900
H	2.83990500	-0.68776900	2.42018400
H	1.83312600	2.35178900	3.64005300
H	1.59468700	4.64946000	0.03103500
H	1.36263900	3.68474400	-1.99765300
H	0.87504900	1.98078400	-2.11271000
H	2.59019900	2.42717000	-2.25752500
H	0.66016000	5.33796800	2.67966200
H	1.90890900	4.75273100	3.80036400
H	2.36913600	5.69606500	2.35587900

Table S13
Al/P-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.68640900
N	1.11778300	0.00000000	2.89277900

O	2.27311500	0.08390600	2.44854800
Al	3.44338400	-1.49659300	2.60799600
C	2.21330700	-2.90225100	3.19749600
C	1.12929800	-3.34506800	2.42791900
O	0.79186000	-2.55869400	1.32551100
C	-0.46694200	-2.66337900	0.79267400
C	-0.95001400	-1.56536100	0.05008800
C	-2.24791400	-1.64401700	-0.47769300
C	-3.02586600	-2.78492900	-0.28926900
C	-2.51139700	-3.86924100	0.42046000
C	-1.22133400	-3.83366700	0.96382400
C	-0.56359500	-5.03518400	1.63960200
C	0.40358100	-4.51111300	2.69832200
C	0.72037000	-5.20280400	3.87587400
C	1.74726800	-4.76619200	4.71313200
C	2.49986400	-3.64394900	4.35721100
C	-1.59801400	-6.00421500	2.22454800
C	0.27872300	-5.78216400	0.56942300
C	4.19875500	-1.62914400	0.78513000
C	4.17165500	-2.78567700	0.01095300
F	3.51321800	-3.87770000	0.44249900
C	4.79599500	-2.87979900	-1.23259100
F	4.68877200	-3.97961000	-1.98129600
C	5.49173800	-1.77533200	-1.72242600
F	6.05088600	-1.82730600	-2.93008400
C	5.54077200	-0.59365300	-0.98244400
C	4.87812900	-0.54335600	0.24061700
F	4.90897800	0.62021500	0.91669800
F	6.16141100	0.47774400	-1.48096000
C	4.73767600	-0.89743300	3.98945300
C	6.12110700	-0.99890200	3.85702200
F	6.65132300	-1.55948400	2.75788700
C	7.01323400	-0.54286600	4.83049600
F	8.33047900	-0.65613200	4.67020400
C	6.50425500	0.04044000	5.99381100
F	7.33439400	0.47955300	6.93418800
C	5.12307700	0.15970800	6.17196400
C	4.27786800	-0.31031500	5.16628500

F	2.95040100	-0.18134600	5.36667100
F	4.64217500	0.71533900	7.28326000
C	-1.15507300	1.19906700	-0.82494300
C	-1.77087700	2.19637400	-0.02367400
C	-1.57968500	2.28268500	1.46987800
C	-2.59818200	3.15035200	-0.62662800
C	-2.84727300	3.15837100	-2.00178100
C	-3.71355700	4.21960800	-2.62763800
C	-2.25231800	2.15776800	-2.77171900
C	-1.41295900	1.17892400	-2.22086200
C	-0.85122100	0.15241000	-3.17172900
C	1.43432000	-0.04973500	-1.16436100
C	1.83143800	-1.13323700	-1.98676700
C	1.29098700	-2.53540600	-1.87351900
C	2.79047400	-0.90093500	-2.98250600
C	3.39840000	0.34076800	-3.17761300
C	3.07528300	1.36256200	-2.28010100
C	2.12362200	1.19107600	-1.27096000
C	1.87751100	2.34234800	-0.32637300
C	4.41602800	0.55960800	-4.26509800
H	-2.65530900	-0.79641900	-1.02772000
H	-4.03539200	-2.82991000	-0.70296100
H	-3.12300900	-4.76255200	0.54429400
H	0.17000800	-6.10742400	4.13538700
H	1.97586700	-5.31834300	5.62763800
H	3.33334300	-3.33836800	4.99669900
H	-1.10148900	-6.86749900	2.68813400
H	-2.24831100	-6.40826700	1.43618600
H	-2.22841500	-5.51585100	2.98267200
H	0.77504300	-6.65480900	1.02138400
H	-0.36534000	-6.12598100	-0.25525800
H	1.06148400	-5.13205400	0.15358900
H	-2.12340600	3.14671400	1.87653600
H	-1.94551800	1.38180500	1.98223500
H	-0.51849100	2.39582900	1.73672000
H	-3.06406200	3.91207000	0.00444900
H	-4.10544100	3.89863000	-3.60396100
H	-4.56555000	4.47758300	-1.98003600

H	-3.13809700	5.14715600	-2.79134500
H	-2.44965900	2.12648800	-3.84683800
H	-1.46698900	0.10598500	-4.08126300
H	-0.82177300	-0.85184100	-2.73453500
H	0.17570700	0.40435500	-3.47440900
H	1.79069800	-3.19068100	-2.59960100
H	1.47748000	-2.94707300	-0.87466400
H	0.20816300	-2.59158900	-2.05355100
H	3.07720300	-1.73570800	-3.62722400
H	3.58662400	2.32547900	-2.35918400
H	2.63149000	3.12690300	-0.47811900
H	1.94339700	2.01119000	0.72080100
H	0.88590600	2.79795700	-0.47147800
H	5.42256400	0.67502700	-3.83465900
H	4.44657100	-0.28661700	-4.96557200
H	4.19491200	1.47573200	-4.83542700

Table S14
Ga/P-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	2.40126800	0.09313700	0.89199000
N	0.86297900	1.52901100	2.26515000
N	-0.17290900	1.04580400	2.13703900
O	-0.73054000	0.04225200	1.64110800
Ga	-2.07557100	0.46621200	0.09580100
C	-1.70050500	2.36104800	-0.28179800
C	-0.45509900	2.80959300	-0.73488900
O	0.60309300	1.90720800	-0.65463100
C	1.88449200	2.38979600	-0.64870700
C	2.87709600	1.58697700	-0.04921700
C	4.19297200	2.07358300	-0.01740500
C	4.50774800	3.30936100	-0.57950100
C	3.51112800	4.07393500	-1.18545000
C	2.18600400	3.62555700	-1.23976800

C	1.07706400	4.36452100	-1.98610100
C	-0.24065500	4.08751300	-1.26516100
C	-1.31307000	4.98903000	-1.22106200
C	-2.55371300	4.60667800	-0.70993800
C	-2.74791400	3.29412200	-0.27147000
C	1.36838200	5.86446800	-2.11155200
C	0.96730500	3.75061600	-3.40868300
C	-1.53571000	-0.89667700	-1.24887800
C	-1.22186800	-0.56904000	-2.56373800
F	-1.13988500	0.71878800	-2.94558800
C	-0.97053600	-1.53161900	-3.54144200
F	-0.61163200	-1.18458900	-4.77894700
C	-1.05353200	-2.87909500	-3.19502500
F	-0.77676300	-3.81407800	-4.10506500
C	-1.35261500	-3.24975400	-1.88362100
C	-1.57181900	-2.25207900	-0.93668800
F	-1.83160400	-2.63774000	0.32263900
F	-1.36743700	-4.54009100	-1.54790600
C	-3.79437900	0.08193100	1.03308500
C	-4.75765700	-0.79194700	0.53610000
F	-4.57769700	-1.39127600	-0.65153900
C	-5.93805500	-1.08355200	1.22380800
F	-6.84024400	-1.92507900	0.72203100
C	-6.17056900	-0.47298100	2.45883400
F	-7.28858300	-0.73420200	3.12862100
C	-5.23057400	0.41448400	2.98969100
C	-4.06560600	0.67176100	2.26492400
F	-3.18161500	1.53086600	2.80224500
F	-5.45798700	0.99568400	4.16670600
C	3.96636400	-0.43361600	1.73972000
C	4.09377500	-0.22798600	3.13853200
C	3.03574000	0.44555900	3.97521500
C	5.24987000	-0.66794000	3.79390000
C	6.29403300	-1.30592100	3.11991000
C	7.50915000	-1.80147200	3.85872800
C	6.15997500	-1.48314500	1.74177100
C	5.02439900	-1.06656300	1.03376100
C	5.02270100	-1.31723000	-0.45321700

C	1.98301100	-1.36196000	-0.16087000
C	2.01989400	-1.42143000	-1.57925100
C	2.17475600	-0.22389500	-2.48110500
C	1.90768500	-2.67227700	-2.19584200
C	1.72436800	-3.86060300	-1.48056900
C	1.57788200	-3.76112300	-0.09702100
C	1.69059700	-2.53980000	0.57801100
C	1.48234400	-2.53836100	2.07203600
C	1.65252900	-5.18617000	-2.19004500
H	4.97127200	1.48655300	0.46883600
H	5.53534200	3.67683400	-0.54479100
H	3.77340200	5.03317500	-1.63105700
H	-1.18519300	6.00038400	-1.60741500
H	-3.37545500	5.32577100	-0.68004800
H	-3.73625300	2.98858900	0.08327100
H	0.56597300	6.36945200	-2.66647100
H	2.29387500	6.03914500	-2.67789300
H	1.46522800	6.34305100	-1.12554900
H	0.16923100	4.25382900	-3.97602800
H	1.91842900	3.86752300	-3.95165500
H	0.71992600	2.68053000	-3.36326800
H	3.33567700	0.45825800	5.03214100
H	2.86051100	1.48334500	3.65986600
H	2.07028300	-0.07659900	3.90574500
H	5.33290100	-0.50297700	4.87144600
H	8.38259500	-1.87967900	3.19459800
H	7.76921400	-1.13847800	4.69778500
H	7.32616700	-2.80472300	4.28118500
H	6.97169900	-1.95997600	1.18548900
H	6.05209900	-1.46142300	-0.81083500
H	4.58491800	-0.48746300	-1.01930800
H	4.44930200	-2.22076600	-0.70704800
H	2.13504300	-0.53821800	-3.53277900
H	1.36330300	0.49533700	-2.32053200
H	3.12189800	0.31083900	-2.32233200
H	1.95710700	-2.71579700	-3.28709200
H	1.36207500	-4.66115000	0.48380300
H	1.11121900	-3.51734800	2.40477000

H	0.73974900	-1.78026000	2.36098800
H	2.41204400	-2.32913900	2.62291500
H	1.33182200	-5.98833600	-1.51097900
H	0.94609800	-5.14761000	-3.03133300
H	2.63796100	-5.46204200	-2.60205000

Table S15
In/P-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	2.41351000	0.09362500	0.96129100
N	1.01687400	1.60427500	2.20462400
N	-0.05932400	1.17222800	2.19944700
O	-0.64801900	0.13456000	1.80909800
In	-2.02391400	0.51893400	-0.00816900
C	-1.49800800	2.57008100	-0.42259500
C	-0.21381400	2.92986200	-0.83918800
O	0.78989000	1.97168000	-0.70128200
C	2.09179600	2.39133300	-0.62906000
C	3.01092300	1.55565300	0.03793900
C	4.34141000	1.98755300	0.14623400
C	4.74452500	3.19791600	-0.41439500
C	3.82252100	3.99158100	-1.09605900
C	2.48509900	3.59949300	-1.22406500
C	1.45587200	4.36851700	-2.04963700
C	0.09418000	4.18354400	-1.38357200
C	-0.92238200	5.14798000	-1.39419000
C	-2.20036800	4.85052300	-0.91913700
C	-2.48949400	3.56084600	-0.46400100
C	1.83128400	5.84594000	-2.20955000
C	1.38277100	3.71191500	-3.45537500
C	-1.38584700	-1.05033700	-1.37818200
C	-1.00152200	-0.77456800	-2.68343700
F	-0.87591400	0.50185000	-3.09708900
C	-0.71579100	-1.77957300	-3.60756600

F	-0.27509400	-1.49112900	-4.83434400
C	-0.84167300	-3.11173700	-3.21244600
F	-0.52334300	-4.08770600	-4.06158600
C	-1.22580900	-3.42325300	-1.90740300
C	-1.46938300	-2.38619500	-1.00967700
F	-1.78946000	-2.71398900	0.25211500
F	-1.29008900	-4.70005300	-1.52209700
C	-3.94358900	0.12124000	0.96165600
C	-4.80045000	-0.89365400	0.54987600
F	-4.49825700	-1.64154100	-0.52388500
C	-5.99697700	-1.17779900	1.21280400
F	-6.80176200	-2.15616600	0.80079100
C	-6.35219800	-0.41116600	2.32621200
F	-7.48815600	-0.66290200	2.96927000
C	-5.51738900	0.62090400	2.76443100
C	-4.33140600	0.86611700	2.06950100
F	-3.54743300	1.86617000	2.51033800
F	-5.86526100	1.34872500	3.82493400
C	3.89241600	-0.48354200	1.92359700
C	3.92265900	-0.32149200	3.33221500
C	2.81335900	0.32087400	4.12585500
C	5.02993100	-0.79221300	4.05215200
C	6.11238300	-1.41905000	3.43524400
C	7.28668300	-1.92971400	4.22771500
C	6.06714100	-1.56661100	2.04636200
C	4.98703300	-1.12255800	1.27519500
C	5.07631400	-1.36397800	-0.21149300
C	2.03165900	-1.36057200	-0.10930400
C	2.15275900	-1.41508600	-1.52159000
C	2.34556300	-0.21924200	-2.41767800
C	2.09936300	-2.66766700	-2.14669000
C	1.89315700	-3.85889200	-1.44842600
C	1.65642500	-3.76536900	-0.07428900
C	1.70629500	-2.54651000	0.60851900
C	1.40155600	-2.55347100	2.08535300
C	1.86201600	-5.18864900	-2.15296800
H	5.06204100	1.37996300	0.69175200
H	5.78267800	3.52228700	-0.31895600

H	4.15373800	4.92936600	-1.54142400
H	-0.72034900	6.14230300	-1.79274000
H	-2.97734800	5.61839000	-0.92850800
H	-3.50404900	3.32686300	-0.12992600
H	1.08359000	6.37084200	-2.81974800
H	2.79084500	5.95269000	-2.73468900
H	1.90582200	6.35379600	-1.23636800
H	0.63896500	4.23349200	-4.07720100
H	2.36322800	3.76361000	-3.95449400
H	1.08155400	2.65669500	-3.38830100
H	3.02787600	0.25384100	5.20122200
H	2.68571700	1.38184600	3.87107000
H	1.84736500	-0.17213200	3.94576600
H	5.03780000	-0.66224900	5.13730800
H	8.23771800	-1.55526600	3.81611600
H	7.22677900	-1.62640100	5.28274100
H	7.33398500	-3.03116400	4.19517900
H	6.90687100	-2.04553900	1.53487300
H	6.12551100	-1.51134500	-0.50439500
H	4.67828000	-0.53275500	-0.80316700
H	4.51744700	-2.26561700	-0.50204000
H	2.32763300	-0.53468000	-3.46950400
H	1.53904800	0.50888500	-2.27846300
H	3.29684000	0.30137400	-2.23639200
H	2.21831900	-2.70673700	-3.23239800
H	1.41705900	-4.67016500	0.49037300
H	0.95737800	-3.51570500	2.37457700
H	0.68562200	-1.75943000	2.34174100
H	2.30579700	-2.40612500	2.69542900
H	0.84339400	-5.60506500	-2.15156400
H	2.18595500	-5.09847800	-3.19915200
H	2.51517300	-5.91814600	-1.64819200

Table S16
Tl/P-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.29226600
N	1.11019800	0.00000000	2.66616900
O	2.22861800	0.08090300	2.10436300
Tl	3.41693700	-2.08349300	2.22327600
C	1.77394300	-3.26630900	3.07036300
C	0.59815200	-3.48631200	2.35015100
O	0.36935500	-2.69317200	1.23264700
C	-0.92025800	-2.53351400	0.79653300
C	-1.22684300	-1.35557500	0.08609000
C	-2.54801300	-1.16837700	-0.34594800
C	-3.52139100	-2.13449900	-0.09798200
C	-3.18669500	-3.30188500	0.58713200
C	-1.88107400	-3.52578200	1.03890300
C	-1.42850000	-4.82344200	1.70465500
C	-0.33151800	-4.47259400	2.70810300
C	-0.11260300	-5.16444500	3.90655500
C	1.01543200	-4.91179000	4.68815500
C	1.96981500	-3.98705600	4.25362600
C	-2.59453600	-5.57603500	2.35504100
C	-0.79156600	-5.72603100	0.61266400
C	4.01374100	-2.37970800	0.09323300
C	3.67339700	-3.54660300	-0.57518300
F	2.84116000	-4.43968500	-0.00408900
C	4.15447500	-3.84025900	-1.85103800
F	3.76516100	-4.93624800	-2.50573400
C	5.02958700	-2.94095400	-2.46093900
F	5.46888100	-3.18134700	-3.69748500
C	5.38418400	-1.75509900	-1.81590200
C	4.85697700	-1.48715400	-0.55317200
F	5.18328000	-0.32369300	0.02612000
F	6.17078200	-0.87587200	-2.43753700
C	5.06734700	-1.22849800	3.45592600
C	6.39330300	-1.27935400	3.04501200
F	6.73452700	-1.94593600	1.93094000
C	7.41601600	-0.65595800	3.76391800

F	8.68293500	-0.71330600	3.35611600
C	7.09562400	0.03392200	4.93660900
F	8.05521700	0.63013700	5.63756900
C	5.77067000	0.09512300	5.37780100
C	4.77842900	-0.54114900	4.62804600
F	3.51624600	-0.47153300	5.07711500
F	5.47733900	0.75070700	6.50008200
C	-0.94489700	1.43702700	-0.69760600
C	-1.25327600	2.55755700	0.12097700
C	-0.85974000	2.67361800	1.57157300
C	-1.94272000	3.63996700	-0.43728400
C	-2.34269800	3.66735200	-1.77574000
C	-3.08380800	4.85261200	-2.33573500
C	-2.02867800	2.56079800	-2.56421800
C	-1.33538400	1.44923000	-2.06426000
C	-1.05438600	0.33915300	-3.04702800
C	1.32827300	-0.26925400	-1.25373500
C	1.46438800	-1.40770400	-2.09427300
C	0.70497900	-2.69867100	-1.92786800
C	2.35934500	-1.34005300	-3.16668500
C	3.15823300	-0.22134500	-3.42376900
C	3.08966600	0.83674700	-2.51832600
C	2.19960900	0.83926400	-1.43703500
C	2.22113900	2.03560300	-0.52023000
C	4.06783300	-0.17990600	-4.62227300
H	-2.82165300	-0.24833200	-0.86020900
H	-4.54616800	-1.97315400	-0.43833500
H	-3.95549700	-4.05286500	0.76733300
H	-0.82348500	-5.92528100	4.22886100
H	1.16473600	-5.45689700	5.62289300
H	2.87351300	-3.82734700	4.84763700
H	-2.24412300	-6.51172200	2.81187400
H	-3.34564000	-5.85943200	1.60448600
H	-3.08596400	-4.97109600	3.13161100
H	-0.44037700	-6.66883600	1.05962300
H	-1.52975900	-5.95719200	-0.17129300
H	0.07311800	-5.23601500	0.14257600
H	-1.13411500	3.66405700	1.95962500

H	-1.35097600	1.91424500	2.19460200
H	0.22362000	2.54841600	1.70938100
H	-2.17024000	4.49611100	0.20342900
H	-3.32191000	4.71639400	-3.40038100
H	-4.02890000	5.02067100	-1.79364000
H	-2.48793100	5.77458500	-2.23532800
H	-2.33262500	2.55244100	-3.61434100
H	-1.75532400	0.40093400	-3.89151600
H	-1.15129600	-0.65833000	-2.60593300
H	-0.03431700	0.41641200	-3.45130900
H	1.05127200	-3.43268800	-2.66784000
H	0.87318400	-3.12868800	-0.93466000
H	-0.37987800	-2.57558900	-2.05643000
H	2.43995100	-2.20852400	-3.82543400
H	3.75025300	1.69708700	-2.65019100
H	3.10825000	2.65068200	-0.72409400
H	2.25834800	1.72167700	0.53247100
H	1.33498700	2.67413600	-0.65580100
H	4.80635700	0.62925800	-4.53873600
H	4.61150000	-1.12717000	-4.74559500
H	3.48554500	-0.01437600	-5.54482700

Table S17
B/N-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
N	2.58738500	-0.08562100	0.44732200
N	1.19134500	0.21518000	1.60727500
N	0.24760800	-0.17857500	0.96276700
O	-1.01595000	0.11383000	1.54695200
B	-2.05592800	0.40594400	0.40443800
C	-1.93240200	1.95888600	-0.03098600
C	-0.72154300	2.53834600	-0.43679000
O	0.39297700	1.66030300	-0.45837900
C	1.68060600	2.12579900	-0.52390700

C	2.75146600	1.26352500	-0.19350700
C	4.06144200	1.69225400	-0.42078300
C	4.31644800	2.94411500	-0.96272000
C	3.25740800	3.80704200	-1.22928600
C	1.93797300	3.42045100	-1.00063900
C	0.78913400	4.38665400	-1.32754700
C	-0.55952200	3.85917400	-0.82860100
C	-1.70279600	4.66978900	-0.83630500
C	-2.93318000	4.15175900	-0.44678800
C	-3.03883500	2.81775200	-0.04399800
C	1.08512500	5.75679400	-0.66340000
C	0.70499100	4.53011200	-2.87234300
C	-1.78002800	-0.65134000	-0.79217300
C	-1.41004600	-0.33731600	-2.09164700
F	-1.20642500	0.95695300	-2.51130100
C	-1.14161100	-1.31351300	-3.03835700
F	-0.62690400	-0.98421200	-4.26838600
C	-1.27888300	-2.64417200	-2.70645200
F	-0.95726700	-3.60288100	-3.63079800
C	-1.62496500	-3.00310900	-1.41725200
C	-1.86209300	-2.00659700	-0.48177600
F	-2.15905000	-2.39338600	0.79909800
F	-1.65581800	-4.33206100	-1.07588100
C	-3.47039100	0.10236200	1.12145700
C	-4.59669200	0.01104200	0.31677200
F	-4.46430200	0.22866200	-1.03577300
C	-5.86123100	-0.25738900	0.81907600
F	-6.94946600	-0.33349100	-0.00295500
C	-6.01183300	-0.44659700	2.18516600
F	-7.24428900	-0.71833500	2.70635500
C	-4.91206800	-0.34889300	3.02060300
C	-3.65930700	-0.06677000	2.48621000
F	-2.62910600	0.04044600	3.37876700
F	-5.06632200	-0.52608900	4.36688800
C	3.78434300	-0.35379800	1.32508800
C	3.92254100	0.31189500	2.56545000
C	3.00399300	1.38393400	3.14260000
C	5.05155300	0.02000400	3.33887300

C	6.05555800	-0.84790300	2.91449300
C	7.26608700	-1.10741900	3.78707200
C	5.93361400	-1.41083000	1.64801700
C	4.82314800	-1.17150200	0.82835600
C	4.87733800	-1.77537900	-0.56851100
C	2.15464400	-1.25944600	-0.34990000
C	1.91046500	-1.21862900	-1.74012800
C	1.90446600	0.01632900	-2.62880400
C	1.62686300	-2.42791900	-2.39400600
C	1.54130100	-3.64392700	-1.72440400
C	1.70436800	-3.63750000	-0.33874200
C	1.99883800	-2.47599700	0.36990400
C	2.15560500	-2.63107700	1.87602900
C	1.17891600	-4.93073500	-2.43435500
H	4.88071500	1.04129000	-0.16281000
H	5.33669100	3.24760700	-1.15662500
H	3.46119300	4.79000400	-1.63217500
H	-1.63161400	5.70034500	-1.16045000
H	-3.81302800	4.78391700	-0.46196500
H	-4.00087700	2.43180000	0.26101200
H	0.29347600	6.47132000	-0.90055200
H	2.02982600	6.17263800	-1.02474500
H	1.13928800	5.63737500	0.42250500
H	-0.09240600	5.23212700	-3.13515000
H	1.65414500	4.90044700	-3.27609000
H	0.47678600	3.55797100	-3.32011000
H	3.57194500	1.96738900	3.87508400
H	2.62874700	2.05620800	2.36985800
H	2.14015500	0.94091100	3.64182900
H	5.15214600	0.51736000	4.29721500
H	7.98886800	-1.74818200	3.27489700
H	7.76182100	-0.16414200	4.04455400
H	6.97020000	-1.59809100	4.72148200
H	6.72985900	-2.03743500	1.26333000
H	5.91420600	-2.04583500	-0.78847200
H	4.53939800	-1.07321000	-1.33254800
H	4.26062700	-2.67339800	-0.64683400
H	1.72815800	-0.30175000	-3.65895000

H	1.07485500	0.66810600	-2.35595000
H	2.83969400	0.57785200	-2.58401800
H	1.40695800	-2.39250600	-3.45435900
H	1.58146100	-4.56265800	0.21288000
H	1.64177900	-3.54829600	2.18574500
H	1.71760600	-1.79109800	2.41813300
H	3.21115600	-2.70821000	2.16044500
H	1.87273400	-5.73127100	-2.15716000
H	0.16729900	-5.21761600	-2.13533300
H	1.19089100	-4.80264100	-3.51748700

Table S18
B/As-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
As	2.82758000	0.29579600	0.72184700
N	1.36250600	0.88522700	2.91777600
N	0.38877400	0.40334700	2.57050700
O	-0.10955500	-0.34577200	1.71107800
B	-1.57242800	0.09651200	0.96387700
C	-1.71462600	1.68414900	1.14010100
C	-0.73676400	2.60339900	0.71768900
O	0.46208200	2.07378300	0.26071500
C	1.58337700	2.86416500	0.26718500
C	2.82303200	2.20846600	0.34709600
C	3.98885600	2.98192400	0.37857600
C	3.90908000	4.37419200	0.31234900
C	2.66593300	5.00121400	0.21495600
C	1.47883700	4.25785700	0.18278100
C	0.09370600	4.86446100	-0.02691300
C	-0.92385700	3.99091800	0.70901100
C	-2.11717500	4.48496500	1.25207400
C	-3.09174300	3.61673500	1.74033300
C	-2.89430400	2.23711200	1.66214300
C	0.03742700	6.32912400	0.42296600

C	-0.23810900	4.78727800	-1.54216600
C	-1.25605700	-0.48811000	-0.51473100
C	-1.37088900	0.23236100	-1.70552000
F	-1.68879100	1.53492100	-1.70687400
C	-1.17125800	-0.33934400	-2.96272900
F	-1.22722500	0.40820200	-4.06648400
C	-0.86572100	-1.69328400	-3.05930400
F	-0.65228200	-2.24597700	-4.25195900
C	-0.74248600	-2.45547900	-1.89996100
C	-0.91877300	-1.83850200	-0.66373200
F	-0.76801600	-2.61447900	0.42150900
F	-0.42698300	-3.74880700	-1.98558800
C	-2.73172000	-0.75094000	1.71691000
C	-3.86776400	-1.17762200	1.02163000
F	-4.01760300	-0.87866600	-0.27686700
C	-4.90514500	-1.89926100	1.61635900
F	-5.96408500	-2.28213000	0.90594300
C	-4.82696700	-2.21336200	2.97341500
F	-5.80246100	-2.90002200	3.56002400
C	-3.72272600	-1.78954600	3.71317200
C	-2.71215900	-1.06530600	3.07763000
F	-1.69640100	-0.65719300	3.85763700
F	-3.64594900	-2.07008400	5.01297400
C	4.74841300	-0.05592300	1.02166700
C	5.15667700	-0.36754000	2.34285800
C	4.20194400	-0.38541000	3.51247100
C	6.50082500	-0.66841700	2.58751900
C	7.46042100	-0.66880900	1.56948400
C	8.89707200	-1.01197100	1.86608900
C	7.03803400	-0.34855800	0.27872400
C	5.70112400	-0.04527500	-0.02401700
C	5.37378500	0.27335900	-1.46108700
C	2.48662600	-0.76139600	-0.90434900
C	2.20906200	-0.26250100	-2.19608900
C	1.94388400	1.18769300	-2.50851300
C	2.16091900	-1.17249800	-3.26306400
C	2.34124700	-2.54691700	-3.09346700
C	2.53978900	-3.01960300	-1.79274100

C	2.59771100	-2.15927900	-0.69318500
C	2.75257000	-2.76050600	0.68321900
C	2.23916500	-3.50519900	-4.24940000
H	4.95983600	2.49451600	0.47344700
H	4.82170600	4.97337600	0.33855500
H	2.62232700	6.08867400	0.15612600
H	-2.29766100	5.55969700	1.27648600
H	-4.01711900	4.01605400	2.16103600
H	-3.68235800	1.56728800	2.01042100
H	-0.95837700	6.75493600	0.23907200
H	0.74709600	6.94174700	-0.15050600
H	0.26992500	6.43404600	1.49330000
H	-1.23624900	5.21124600	-1.73187000
H	0.50573100	5.35095600	-2.12694800
H	-0.24644100	3.74660500	-1.89527200
H	4.71882500	-0.71133800	4.42578700
H	3.77346200	0.60896000	3.70525100
H	3.35624500	-1.06895500	3.34181000
H	6.80683500	-0.90800000	3.60981800
H	9.54543700	-0.82829700	0.99725200
H	9.28218900	-0.42141600	2.71281100
H	8.99884900	-2.07491400	2.14286600
H	7.77171600	-0.33043700	-0.53199200
H	6.28505200	0.56380800	-2.00303500
H	4.65185900	1.09311500	-1.55392300
H	4.93969800	-0.59730200	-1.97469800
H	1.71636000	1.30969100	-3.57603200
H	1.08217100	1.55957100	-1.94077800
H	2.79679800	1.83740400	-2.26587800
H	1.94891600	-0.78629500	-4.26335300
H	2.62730400	-4.09569900	-1.62224900
H	2.69516400	-3.85636400	0.63292500
H	1.94976000	-2.41572200	1.35342600
H	3.71642800	-2.49745800	1.14631500
H	1.29470500	-4.06941400	-4.18990400
H	2.25385300	-2.97963100	-5.21467000
H	3.06275100	-4.23639600	-4.23752100

Table S19
B/Sb-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Sb	2.66739100	0.15063600	0.78461300
N	1.31698200	1.01449000	3.09629500
N	0.31514200	0.55822300	2.78194300
O	-0.19423800	-0.22554200	1.96686300
B	-1.67057800	0.18375100	1.07470900
C	-1.80687900	1.77466600	1.15159700
C	-0.82136200	2.67629300	0.70616000
O	0.38368700	2.13315100	0.29146500
C	1.50854500	2.92604900	0.28544600
C	2.73959900	2.26679600	0.38735000
C	3.91011100	3.02960000	0.42381700
C	3.83749700	4.42271800	0.33488000
C	2.59867000	5.05359300	0.20314800
C	1.40707400	4.31648500	0.16615100
C	0.02797100	4.91695100	-0.09186800
C	-1.00784400	4.06403500	0.64390200
C	-2.21286800	4.57768500	1.13986800
C	-3.20028900	3.72942900	1.63693100
C	-2.99931400	2.34896000	1.62211500
C	-0.03712900	6.39385800	0.31458700
C	-0.26750400	4.79561700	-1.61174500
C	-1.24733500	-0.51699000	-0.31930100
C	-1.31149100	0.09728200	-1.57259100
F	-1.64924600	1.38845200	-1.69866000
C	-1.04662800	-0.57949700	-2.76417700
F	-1.07473600	0.06490700	-3.93147200
C	-0.71419100	-1.93095700	-2.73046400
F	-0.47642100	-2.58746200	-3.86278300
C	-0.61483500	-2.58202900	-1.50323600
C	-0.87817000	-1.86737500	-0.33710400
F	-0.77877700	-2.55136700	0.81538400

F	-0.26178000	-3.86627800	-1.45314000
C	-2.83250800	-0.62334800	1.85852400
C	-3.86737300	-1.27343900	1.17831400
F	-3.93077600	-1.23807500	-0.15994900
C	-4.89145900	-1.96767000	1.82738700
F	-5.85200600	-2.57125800	1.13088400
C	-4.90631500	-2.01875200	3.22117700
F	-5.87166500	-2.67387900	3.85750700
C	-3.90597000	-1.36654400	3.94331500
C	-2.90573200	-0.68024700	3.25336000
F	-1.99534400	-0.04042800	4.00498200
F	-3.92017300	-1.39586000	5.27455500
C	4.79630500	-0.20876600	1.10523300
C	5.20108100	-0.61379800	2.40023900
C	4.22518300	-0.77474200	3.54366800
C	6.55430000	-0.87579300	2.63980400
C	7.52291300	-0.74767000	1.63701900
C	8.97342500	-1.03058800	1.93161300
C	7.10020100	-0.34932800	0.36801100
C	5.75261800	-0.08215100	0.07400500
C	5.40821900	0.30272800	-1.34386900
C	2.43883900	-0.88019400	-1.12366500
C	2.20330400	-0.26514800	-2.37033900
C	1.89238500	1.19993600	-2.53579500
C	2.25110800	-1.06128900	-3.52466200
C	2.49488600	-2.43604200	-3.47855700
C	2.66360800	-3.02859500	-2.22294500
C	2.62606200	-2.27908700	-1.04257200
C	2.75350900	-2.99803400	0.27987000
C	2.50439000	-3.27440000	-4.72858700
H	4.87861600	2.53858400	0.53711500
H	4.75153800	5.01980600	0.36660400
H	2.56260200	6.13992100	0.12021000
H	-2.39218200	5.65266800	1.11987100
H	-4.13587100	4.14429900	2.01803800
H	-3.79534700	1.69408700	1.97981700
H	-1.02529200	6.81814300	0.09009800
H	0.69172800	6.98720100	-0.25507700

H	0.16537200	6.52822700	1.38771000
H	-1.26126400	5.21200900	-1.83811600
H	0.48977300	5.34288200	-2.19483100
H	-0.26421900	3.74458500	-1.93371400
H	4.73610700	-1.15076600	4.44106400
H	3.74248100	0.17838100	3.80980800
H	3.41885400	-1.48495100	3.29843700
H	6.86172500	-1.18736700	3.64239400
H	9.59930000	-0.91434900	1.03512700
H	9.36112600	-0.34889400	2.70679100
H	9.10890500	-2.05691500	2.31050800
H	7.84013400	-0.24363100	-0.43052200
H	6.30142500	0.66383900	-1.87345500
H	4.64784100	1.09205800	-1.39213000
H	5.01042700	-0.55824700	-1.90228700
H	1.62288100	1.41908600	-3.57769300
H	1.04898200	1.50187300	-1.90281100
H	2.74556200	1.83919900	-2.26369100
H	2.06694400	-0.58684600	-4.49209900
H	2.80682100	-4.11034200	-2.15574600
H	2.82670700	-4.08360700	0.12886300
H	1.87070300	-2.81459300	0.91393300
H	3.64964500	-2.68168800	0.83861800
H	1.59098600	-3.88885800	-4.78128900
H	2.54043700	-2.65129000	-5.63374300
H	3.36571000	-3.96063900	-4.74539100

Table S20
B/Bi-TS

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Bi	2.64352100	0.11997400	0.86418100
N	1.27558000	1.00608500	3.20688800
N	0.26289900	0.61691300	2.83632600
O	-0.19662200	-0.13446700	1.94532800

B	-1.61981100	0.21035300	1.13931000
C	-1.80098800	1.80527900	1.17595900
C	-0.82756000	2.70967200	0.71150200
O	0.38246900	2.17004900	0.30564100
C	1.50040100	2.97416200	0.28760900
C	2.73554900	2.33120400	0.40986000
C	3.90154700	3.09767600	0.42980400
C	3.81711300	4.48920600	0.30870700
C	2.57305500	5.10748000	0.16267800
C	1.38640600	4.36097600	0.13891600
C	0.00078100	4.94182800	-0.13179200
C	-1.02649700	4.09425200	0.62313500
C	-2.23483800	4.60448200	1.11451700
C	-3.20987600	3.75457900	1.63377800
C	-2.99587600	2.37559300	1.64301300
C	-0.07920300	6.42637500	0.24242100
C	-0.29354600	4.78372900	-1.64847100
C	-1.24318100	-0.51557500	-0.26715600
C	-1.33111900	0.07287400	-1.53090300
F	-1.66326500	1.36259400	-1.67472300
C	-1.08979900	-0.62954900	-2.71274400
F	-1.13881600	-0.01024600	-3.89272600
C	-0.75790200	-1.98111400	-2.65753000
F	-0.53960600	-2.66025600	-3.78062300
C	-0.63692900	-2.60711500	-1.41957700
C	-0.87586600	-1.86621000	-0.26364200
F	-0.73747800	-2.52221400	0.90290100
F	-0.27809800	-3.88891600	-1.34756100
C	-2.80810200	-0.59889200	1.89217600
C	-3.97095500	-0.90604100	1.17848900
F	-4.09743600	-0.50348100	-0.09497100
C	-5.04992400	-1.60018100	1.72799900
F	-6.13444900	-1.86429300	1.00236600
C	-4.98316700	-2.01548900	3.05884900
F	-5.99723300	-2.67938600	3.60514300
C	-3.84990700	-1.71681900	3.81509200
C	-2.79660100	-1.01395800	3.22441900
F	-1.75016600	-0.73854700	4.02170100

F	-3.78314100	-2.09710100	5.08984800
C	4.88667500	-0.22627100	1.16888900
C	5.30891100	-0.61515600	2.45916500
C	4.34214900	-0.78438800	3.60915900
C	6.67068300	-0.84936700	2.68213900
C	7.62179200	-0.70652600	1.66389300
C	9.08209000	-0.95807800	1.93961100
C	7.17471000	-0.32333900	0.39797100
C	5.81731700	-0.08380700	0.12131300
C	5.43266500	0.28524700	-1.29052100
C	2.41224400	-0.96012500	-1.14385700
C	2.16937600	-0.32725100	-2.37625900
C	1.86040600	1.14060200	-2.51649900
C	2.21131400	-1.11398000	-3.53822300
C	2.45780100	-2.48915700	-3.50371300
C	2.64367100	-3.09249900	-2.25533600
C	2.61367400	-2.35286200	-1.06696400
C	2.76073100	-3.07439900	0.25191800
C	2.45030300	-3.31588500	-4.76178200
H	4.87409200	2.61573800	0.55392000
H	4.72607300	5.09479600	0.32760600
H	2.52910700	6.19166300	0.05730200
H	-2.42624500	5.67689900	1.07506500
H	-4.14703900	4.16699300	2.01379800
H	-3.78100500	1.72090000	2.02431400
H	-1.07176800	6.83554900	0.00921700
H	0.64392800	7.01433700	-0.34008400
H	0.12200000	6.58608500	1.31232500
H	-1.29183500	5.18404400	-1.88371500
H	0.45771100	5.32602900	-2.24387500
H	-0.27888100	3.72578100	-1.94675100
H	4.86295400	-1.13280300	4.51197600
H	3.83532700	0.16031400	3.86278000
H	3.55542800	-1.52191700	3.37838900
H	6.99861600	-1.14918600	3.68201900
H	9.69177300	-0.84067600	1.03216500
H	9.46867600	-0.25940700	2.70014300
H	9.24371100	-1.97685800	2.32842600

H	7.90161200	-0.20819100	-0.41133300
H	6.31017700	0.63329500	-1.85393100
H	4.67636300	1.08064000	-1.32271500
H	5.00957700	-0.57926000	-1.82454100
H	1.55626100	1.37305800	-3.54601500
H	1.04283700	1.44127400	-1.85003900
H	2.72829400	1.77016100	-2.26752300
H	2.02085300	-0.63141600	-4.50062400
H	2.79601500	-4.17375200	-2.19933400
H	2.88294900	-4.15498700	0.09712000
H	1.86373900	-2.93512900	0.87758200
H	3.63843900	-2.72241600	0.81935800
H	1.48918300	-3.84671000	-4.86036600
H	2.57832600	-2.69107300	-5.65763200
H	3.24810800	-4.07448500	-4.75044300

Table S21
B/P-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	4.93232800	4.22651800	-1.02283400
N	5.95229800	3.84846400	-2.34987000
N	6.90955800	3.19107200	-1.84667400
O	7.93021300	3.06315000	-2.60762300
B	9.22076800	2.80564800	-1.76518600
C	9.82945800	4.30532900	-1.54872800
C	9.14679400	5.33468400	-0.87879200
O	7.85221000	5.05795700	-0.41037100
C	6.96807500	6.06942200	-0.25996100
C	5.58300300	5.80724200	-0.40882700
C	4.67101200	6.86086000	-0.21015400
C	5.11985500	8.13335300	0.12263300
C	6.49022600	8.37287200	0.25860000
C	7.42875500	7.35401000	0.08292600
C	8.92382100	7.51730400	0.34776800

C	9.67915600	6.60172500	-0.61641600
C	10.94006000	6.89847800	-1.14622200
C	11.63559400	5.93546200	-1.87549600
C	11.09041100	4.66276100	-2.05239900
C	9.36765400	8.97974400	0.23471600
C	9.20669600	7.01405500	1.79036400
C	8.79026400	2.00783400	-0.39226800
C	9.09257500	2.38781600	0.91481800
F	9.77565700	3.51267100	1.17997000
C	8.69009700	1.65930400	2.03823300
F	8.94156700	2.11192300	3.27083000
C	7.98214800	0.47503400	1.86914000
F	7.56526900	-0.21755600	2.93324800
C	7.66323200	0.04721000	0.58188500
C	8.06278600	0.81788400	-0.50698200
F	7.68744800	0.37989100	-1.71907200
F	6.94455400	-1.06901100	0.41245700
C	10.21539600	1.83789300	-2.62011600
C	11.38161900	1.37272600	-2.00354100
F	11.67778900	1.77392000	-0.75567500
C	12.29363900	0.51365200	-2.61686900
F	13.39301500	0.10792600	-1.97954600
C	12.03942200	0.07642200	-3.91750600
F	12.89097200	-0.74640300	-4.52763100
C	10.89140300	0.51529100	-4.57491800
C	10.00548900	1.38114900	-3.92346000
F	8.93237100	1.75575200	-4.62741100
F	10.64556400	0.10450700	-5.82041300
C	3.25182000	4.57112200	-1.62939600
C	3.04091200	5.01171600	-2.96448000
C	4.14129900	5.36608200	-3.93537800
C	1.72228100	5.16874000	-3.40772000
C	0.61590900	4.93927900	-2.58569500
C	-0.78623600	5.07089300	-3.11641800
C	0.85661600	4.59654100	-1.25261200
C	2.14872600	4.41824300	-0.74639000
C	2.26890300	4.11656800	0.73087600
C	4.89173300	2.81305500	0.12415600

C	5.34417200	2.86107300	1.46454200
C	6.03894700	4.04186900	2.09360600
C	5.16486600	1.72554900	2.26424500
C	4.59126200	0.54660500	1.78392000
C	4.19885800	0.51314600	0.44240400
C	4.33172100	1.61573400	-0.40389400
C	3.84800300	1.46277200	-1.82783400
C	4.46846900	-0.67684500	2.64875900
H	3.60427900	6.68258000	-0.34336500
H	4.40309600	8.94310400	0.27053500
H	6.82919500	9.37452800	0.52265900
H	11.39107300	7.87615400	-0.97629600
H	12.61767900	6.17224200	-2.29143300
H	11.66440800	3.91930300	-2.60731900
H	10.44125800	9.07266700	0.44628500
H	8.85001200	9.60755800	0.97408800
H	9.17541400	9.38680300	-0.76934600
H	10.27911700	7.11586800	2.01544500
H	8.63121300	7.60014200	2.52459100
H	8.94639000	5.95225800	1.90175500
H	3.72366500	5.95125900	-4.76640100
H	4.93915200	5.95303500	-3.46117600
H	4.63348400	4.47363700	-4.34386300
H	1.56018600	5.49987100	-4.43662600
H	-1.50150500	5.31294400	-2.31675800
H	-0.85284400	5.84833600	-3.89200400
H	-1.11475800	4.12290300	-3.57627500
H	0.01019100	4.47670500	-0.57144200
H	1.35651800	4.44687100	1.24709200
H	3.11771100	4.62952100	1.20191200
H	2.39472400	3.04179000	0.92671000
H	6.27447700	3.82030800	3.14262000
H	6.98756000	4.24982300	1.58185800
H	5.43576200	4.96081800	2.06795700
H	5.52200400	1.75734600	3.29580200
H	3.78416900	-0.41078300	0.03222100
H	3.74082500	0.39719200	-2.07136600
H	4.53924600	1.90118500	-2.55861800

H	2.86697200	1.94077700	-1.97501600
H	3.50826700	-1.18928300	2.48380900
H	5.27286500	-1.38677800	2.39988600
H	4.55909400	-0.43084300	3.71592300

Table S22
Al/P-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	4.90315500	4.26102800	-1.05031300
N	5.82419200	3.79640400	-2.42339900
N	6.79288900	3.10595400	-2.00226300
O	7.66397200	2.78811100	-2.89399900
Al	9.25659700	2.61751700	-1.90830600
C	9.87031100	4.48466900	-1.64273900
C	9.15520600	5.46811200	-0.94965600
O	7.84067100	5.14290700	-0.56206100
C	6.94766000	6.12792500	-0.33093300
C	5.56483900	5.84751000	-0.46699200
C	4.63528400	6.87337600	-0.20911100
C	5.06246600	8.13787000	0.17545300
C	6.42896800	8.39160300	0.31798900
C	7.38522700	7.40097500	0.08614200
C	8.87216500	7.58459800	0.38202700
C	9.66263600	6.72439000	-0.60153800
C	10.94078800	7.05275200	-1.07221800
C	11.67858100	6.13443500	-1.81919300
C	11.15439200	4.86439500	-2.07425600
C	9.28892700	9.05910400	0.33636500
C	9.13915700	7.02811300	1.80825600
C	8.74960800	1.69935400	-0.19427200
C	8.95011900	2.22023000	1.08013600
F	9.55293000	3.41335800	1.24906900
C	8.51791100	1.58243100	2.24400000
F	8.65858100	2.15493200	3.44517200

C	7.86668900	0.35551100	2.13946800
F	7.40793600	-0.24887400	3.23889200
C	7.63256900	-0.20275600	0.88342300
C	8.07716000	0.48150900	-0.24763600
F	7.80556100	-0.07351900	-1.44347100
F	6.94895100	-1.34908000	0.78510000
C	10.55353000	1.52497700	-2.95464800
C	11.75122700	1.17101200	-2.33856100
F	11.99906100	1.60662300	-1.08644900
C	12.73058300	0.38612900	-2.94852400
F	13.86560700	0.07164100	-2.32244400
C	12.50170800	-0.07293300	-4.24826300
F	13.41595800	-0.82347700	-4.85894700
C	11.31600300	0.25813000	-4.90847300
C	10.36953400	1.04839600	-4.25006000
F	9.24804800	1.34239800	-4.92369600
F	11.10737500	-0.18259500	-6.15021500
C	3.21179100	4.61551400	-1.62608000
C	2.99686700	5.09339700	-2.94806700
C	4.09441400	5.50190600	-3.90177900
C	1.67741900	5.24642800	-3.38930500
C	0.57319300	4.98244400	-2.57456300
C	-0.82971600	5.10952500	-3.10430700
C	0.81741600	4.61591600	-1.24858000
C	2.11123800	4.43970200	-0.74485300
C	2.23149700	4.12414600	0.72983300
C	4.86483600	2.86494200	0.11842700
C	5.35466300	2.92545700	1.44582000
C	6.10999800	4.09358600	2.02668500
C	5.15036300	1.81791400	2.27767000
C	4.52064700	0.65027300	1.84019900
C	4.10238900	0.59774200	0.50738800
C	4.24904300	1.67705600	-0.36750600
C	3.69174400	1.50908500	-1.76339300
C	4.35175300	-0.53998000	2.74354100
H	3.57056100	6.67933600	-0.33275500
H	4.33264800	8.92671600	0.36571800
H	6.75236200	9.38288700	0.63496500

H	11.37517000	8.02476700	-0.83763600
H	12.67441200	6.40305800	-2.17994300
H	11.76529700	4.14380000	-2.62517900
H	10.35732400	9.16316700	0.56790500
H	8.74996200	9.64685900	1.09307900
H	9.10348900	9.50345900	-0.65306100
H	10.20484000	7.14206000	2.05848000
H	8.53780600	7.57125000	2.55474800
H	8.89824800	5.95750700	1.87130400
H	3.67579800	6.14624100	-4.68751800
H	4.89840800	6.05329000	-3.39548500
H	4.57568800	4.63455100	-4.37191700
H	1.51259400	5.60500700	-4.40862200
H	-1.55364500	5.29212000	-2.29671300
H	-0.91136200	5.92565400	-3.83786300
H	-1.13374600	4.18037200	-3.61656600
H	-0.02788000	4.47667400	-0.56969300
H	1.32027800	4.45445100	1.24817500
H	3.08263400	4.62953200	1.20434100
H	2.35213900	3.04763800	0.91913900
H	6.40806200	3.86884300	3.05869800
H	7.02844800	4.28456700	1.45764200
H	5.52125600	5.02245700	2.03666000
H	5.53047500	1.86184300	3.30048000
H	3.64059300	-0.31824700	0.13029400
H	3.65582300	0.44153400	-2.02073200
H	4.28466500	2.01483900	-2.53441900
H	2.66514100	1.90335800	-1.82926500
H	3.35949100	-0.99916500	2.61508900
H	5.10632300	-1.30372100	2.49957400
H	4.48179100	-0.26897600	3.80025500

Table S23
Ga/P-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z

P	4.93456100	4.21534000	-1.04249900
N	5.86381400	3.72353000	-2.38862200
N	6.84499700	3.05320300	-1.94101300
O	7.71695200	2.72918900	-2.81496000
Ga	9.40249100	2.59967500	-1.75112300
C	9.93527200	4.50604700	-1.56638700
C	9.17821300	5.48825300	-0.91780100
O	7.86841500	5.15032900	-0.53860700
C	6.95380000	6.12774100	-0.34473200
C	5.57628400	5.82270100	-0.48524200
C	4.63061800	6.84144300	-0.26202000
C	5.03319700	8.12294400	0.09195200
C	6.39345800	8.40164600	0.23788600
C	7.36595900	7.41901300	0.04075600
C	8.84613400	7.63818600	0.34311200
C	9.65909500	6.76680600	-0.61092400
C	10.93085000	7.11172700	-1.08619700
C	11.69740700	6.18946600	-1.79795900
C	11.20960200	4.89738800	-2.00728800
C	9.23751600	9.11809800	0.26207100
C	9.11199600	7.12461400	1.78561500
C	8.81381800	1.71926000	-0.04104300
C	8.96250100	2.29415800	1.21532100
F	9.54417000	3.50128900	1.35733700
C	8.50281100	1.68943000	2.38637300
F	8.59730300	2.30576800	3.57010000
C	7.87617800	0.44886200	2.30371100
F	7.39408700	-0.12605900	3.40843800
C	7.69255500	-0.15731300	1.06105700
C	8.16455400	0.48896200	-0.08072100
F	7.95431400	-0.11690500	-1.25994400
F	7.03238500	-1.31805800	0.98421600
C	10.61031000	1.49692200	-2.90354800
C	11.19760100	0.30795900	-2.47860700
F	11.01081800	-0.13221100	-1.22379400
C	12.00367900	-0.47563500	-3.30823300
F	12.55062300	-1.61010800	-2.87015400

C	12.23901900	-0.05412100	-4.61883500
F	13.00562200	-0.78431700	-5.42499300
C	11.67351000	1.13627600	-5.08209300
C	10.87343000	1.88379700	-4.21537800
F	10.35071600	3.02457500	-4.69315100
F	11.90543500	1.53722900	-6.33256800
C	3.24529000	4.54769100	-1.64190900
C	3.04321500	4.99406800	-2.97713300
C	4.14949200	5.39054100	-3.92584800
C	1.72842000	5.12741500	-3.43831300
C	0.61568800	4.87359600	-2.63197100
C	-0.78111500	4.97878900	-3.18250900
C	0.84571500	4.53907900	-1.29524600
C	2.13451300	4.38432800	-0.77138400
C	2.23671100	4.10435300	0.71187900
C	4.88546300	2.85385300	0.16838400
C	5.35203100	2.95627700	1.50112300
C	6.08559400	4.14887300	2.06032700
C	5.14454800	1.87126100	2.36167800
C	4.53459700	0.68489500	1.94740800
C	4.13716600	0.59137600	0.61054400
C	4.28709200	1.64712200	-0.29225100
C	3.75130600	1.43574700	-1.69058500
C	4.36446200	-0.48266600	2.87993600
H	3.57024300	6.62820000	-0.39017400
H	4.28904900	8.90457800	0.25452900
H	6.69963400	9.40594200	0.52964800
H	11.33754300	8.10247800	-0.88325400
H	12.68657000	6.47199000	-2.16592100
H	11.83890500	4.17154900	-2.52893500
H	10.30196600	9.24720700	0.49922200
H	8.68231400	9.71528200	0.99924900
H	9.05202400	9.53361800	-0.73976400
H	10.17390900	7.26193800	2.04038400
H	8.49681800	7.67877100	2.51239300
H	8.88580700	6.05281300	1.87674600
H	3.73477100	6.00815600	-4.73485000
H	4.93892100	5.96525000	-3.42241600

H	4.64990100	4.51701200	-4.36300500
H	1.57414400	5.46182000	-4.46749100
H	-1.51890100	5.15718900	-2.38656000
H	-0.86269800	5.78937700	-3.92241100
H	-1.06580400	4.04279300	-3.69354100
H	-0.00711400	4.40872100	-0.62402300
H	1.31605300	4.44001900	1.20977200
H	3.07764900	4.62699500	1.18568900
H	2.36242100	3.03360500	0.92843300
H	6.37255900	3.95582200	3.10184800
H	7.00899100	4.33699100	1.49835600
H	5.48546800	5.07022400	2.03755100
H	5.50659600	1.94878800	3.38903200
H	3.68899800	-0.33901100	0.25263100
H	3.70889700	0.36039400	-1.91191100
H	4.36251400	1.91163500	-2.46637700
H	2.72986600	1.83693600	-1.78733300
H	3.37784500	-0.95391500	2.75143800
H	5.12859400	-1.24602800	2.66585800
H	4.47866500	-0.18291000	3.93071100

Table S24
In/P-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z

P	4.93490200	4.29627200	-1.10276800
N	5.82189700	3.86006100	-2.48446800
N	6.81513400	3.14971000	-2.11685500
O	7.61225200	2.82392400	-3.05026400
In	9.47024200	2.59356100	-1.84406900
C	9.98427400	4.69415500	-1.58137300
C	9.18718700	5.61699200	-0.89363100
O	7.87406900	5.23695100	-0.56919100
C	6.94519500	6.18860000	-0.30756000
C	5.57101400	5.87842100	-0.46856800

C	4.61382400	6.87035800	-0.18354200
C	4.99831600	8.13142600	0.25354500
C	6.35373100	8.41267600	0.42722900
C	7.33768000	7.45499000	0.17111100
C	8.80968600	7.67219500	0.50660900
C	9.64385800	6.88115600	-0.49629900
C	10.91414800	7.28132300	-0.92963700
C	11.71256700	6.42176500	-1.68225200
C	11.26025600	5.13204700	-1.97199500
C	9.18271300	9.15889500	0.53637500
C	9.06676400	7.06178000	1.91267400
C	8.78700600	1.60376600	0.00656200
C	8.88644700	2.20251900	1.25534900
F	9.41969600	3.43419500	1.38432700
C	8.42393100	1.59415400	2.42233000
F	8.46315000	2.22491200	3.60145200
C	7.84737700	0.32778800	2.33902400
F	7.35537300	-0.24878300	3.43763900
C	7.72073100	-0.30243700	1.10132700
C	8.19258000	0.34904100	-0.03971600
F	8.04126100	-0.27906300	-1.21627600
F	7.11690600	-1.49318000	1.02552900
C	10.73324000	1.29487400	-3.08430100
C	12.11537400	1.32398100	-2.95611500
F	12.68877800	2.19273900	-2.09611200
C	12.96429300	0.48485300	-3.67990900
F	14.28879300	0.54107900	-3.53593900
C	12.39876400	-0.43490300	-4.56685800
F	13.18260200	-1.24916200	-5.26910200
C	11.01111900	-0.49994100	-4.71749200
C	10.20339500	0.36347000	-3.97154500
F	8.87895800	0.26322000	-4.13875200
F	10.48134500	-1.38273700	-5.56437300
C	3.23542800	4.65173900	-1.66637500
C	3.02035900	5.16177900	-2.97665200
C	4.11563400	5.62026900	-3.91036700
C	1.70153800	5.30364700	-3.42405900
C	0.59615600	4.99885200	-2.62564600

C	-0.80505000	5.11360700	-3.16304800
C	0.83769100	4.60448500	-1.30743300
C	2.13108800	4.43821000	-0.79846100
C	2.24282200	4.09434900	0.67070100
C	4.89107600	2.88640100	0.05405600
C	5.35272000	2.93913100	1.39191900
C	6.08270600	4.11047300	1.99879400
C	5.13679400	1.82634000	2.21377500
C	4.52140500	0.65842000	1.75703200
C	4.12834800	0.61393400	0.41654600
C	4.28637100	1.69992800	-0.44916200
C	3.74266600	1.54013100	-1.85143400
C	4.33477700	-0.53611200	2.65211900
H	3.55661300	6.65270100	-0.32751700
H	4.24423900	8.89244400	0.46172200
H	6.64812700	9.39750400	0.78866600
H	11.29655200	8.26480300	-0.65682700
H	12.70277800	6.74481700	-2.01210600
H	11.92744100	4.44559500	-2.49707900
H	10.24222000	9.28384400	0.79657900
H	8.61097000	9.69473500	1.30711600
H	9.00392100	9.64316400	-0.43535400
H	10.12426900	7.19258300	2.18846600
H	8.43759600	7.55762200	2.66896700
H	8.85097900	5.98411500	1.92773600
H	3.68918100	6.28176200	-4.67770600
H	4.90575700	6.17010500	-3.38084800
H	4.61716700	4.77639700	-4.40103700
H	1.53807500	5.68662500	-4.43475800
H	-1.53789900	5.26489900	-2.35686100
H	-0.89597000	5.94506100	-3.87824900
H	-1.08934700	4.19137600	-3.69882800
H	-0.00972800	4.43468000	-0.63811400
H	1.32333300	4.40434100	1.18716000
H	3.08381100	4.60002200	1.16214400
H	2.37363000	3.01589800	0.84067000
H	6.37334900	3.87550200	3.03053900
H	7.00339100	4.32763500	1.44366300

H	5.47738100	5.02846800	2.01649200
H	5.49011800	1.86896000	3.24625200
H	3.67173800	-0.29917900	0.02598500
H	3.70533100	0.47399500	-2.11452200
H	4.34257000	2.05159800	-2.61272100
H	2.71733200	1.93712900	-1.92247500
H	3.35058700	-1.00259100	2.49206000
H	5.10117700	-1.29557300	2.43258300
H	4.42933200	-0.26632700	3.71294000

Table S25
Tl/P-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	4.97982400	4.24584300	-1.08054300
N	5.85922600	3.81177500	-2.45299200
N	6.83121600	3.03984700	-2.11695200
O	7.60035400	2.72193800	-3.06243100
Tl	9.60526100	2.58667700	-1.75786800
C	9.98043600	4.76195200	-1.68472600
C	9.17972700	5.66267800	-0.97663700
O	7.90198300	5.25057200	-0.57959700
C	6.95304800	6.19325600	-0.33299600
C	5.58549800	5.85262300	-0.47012700
C	4.61486700	6.83340700	-0.19531700
C	4.98064300	8.11158000	0.20884400
C	6.33197500	8.42479100	0.35290200
C	7.32920700	7.47894800	0.10283900
C	8.80562000	7.73552100	0.38612400
C	9.61459800	6.95404400	-0.64414900
C	10.83430600	7.39273700	-1.17360000
C	11.61208700	6.55008100	-1.96712000
C	11.19948500	5.23408500	-2.19015500
C	9.14575500	9.22973900	0.38891200
C	9.13070100	7.14406000	1.78599200

C	8.78729100	1.63604300	0.10018800
C	8.94451400	2.23724100	1.33904000
F	9.55748300	3.43441500	1.44495800
C	8.46399400	1.66132100	2.51545300
F	8.56248200	2.28996000	3.69199700
C	7.80882000	0.43328500	2.44263300
F	7.30199200	-0.11234300	3.55043200
C	7.61569900	-0.18686300	1.20780900
C	8.10384900	0.42866000	0.05464500
F	7.88079300	-0.18128700	-1.11610900
F	6.92890300	-1.33216800	1.14624100
C	10.83887000	1.23626000	-3.04252300
C	11.12590500	-0.07154000	-2.66948400
F	10.71672900	-0.55023400	-1.48573000
C	11.85117500	-0.93503000	-3.49512100
F	12.11586300	-2.18697400	-3.12281600
C	12.31219400	-0.46769100	-4.72866200
F	13.00797200	-1.27377000	-5.52550800
C	12.04723700	0.84586200	-5.12565400
C	11.31751800	1.67451900	-4.27040000
F	11.08727600	2.93549700	-4.67425000
F	12.49690200	1.28524900	-6.30085800
C	3.26651800	4.56788800	-1.63354900
C	3.02842600	5.02709400	-2.95883800
C	4.10335300	5.47110900	-3.92300300
C	1.70244800	5.13234500	-3.39595200
C	0.61037200	4.84007700	-2.57527600
C	-0.79819600	4.91287600	-3.10088000
C	0.87248000	4.49945100	-1.24633100
C	2.17392500	4.37187800	-0.74636700
C	2.30298100	4.08816800	0.73444200
C	4.94366200	2.87319600	0.12402600
C	5.39307200	2.97702000	1.46321700
C	6.15319700	4.15358600	2.02190900
C	5.13323100	1.91399800	2.33632500
C	4.49230000	0.74143700	1.92908800
C	4.12943100	0.63562200	0.58387000
C	4.32651200	1.67427900	-0.33102400

C	3.80525900	1.45514400	-1.73368000
C	4.25559800	-0.39826800	2.88189600
H	3.56038100	6.59432500	-0.32341300
H	4.21436600	8.86218800	0.41039300
H	6.61305200	9.42453500	0.68262200
H	11.19149900	8.39826100	-0.95199400
H	12.55551200	6.90899300	-2.38487100
H	11.83427700	4.56700400	-2.77782400
H	10.21195900	9.37999300	0.60571900
H	8.59211500	9.75856400	1.17751700
H	8.91750900	9.70204500	-0.57830700
H	10.19472400	7.30080300	2.02022700
H	8.52018000	7.63406900	2.56092200
H	8.93833400	6.06234100	1.82039500
H	3.65346200	6.09250600	-4.71037800
H	4.88781300	6.05657300	-3.42455600
H	4.61958700	4.61998900	-4.38468900
H	1.52239700	5.47568200	-4.41801700
H	-1.52417300	5.08814300	-2.29325600
H	-0.90877300	5.71222800	-3.84916900
H	-1.07582500	3.96519300	-3.59408400
H	0.03522500	4.34259700	-0.56115500
H	1.38747700	4.41587500	1.24721800
H	3.14665000	4.61615300	1.19627800
H	2.43897100	3.01804400	0.94702700
H	6.47267600	3.93666100	3.04931400
H	7.05814600	4.35094600	1.43484400
H	5.55671200	5.07765800	2.04060000
H	5.47310100	1.99826400	3.37083200
H	3.66314700	-0.28727300	0.22944400
H	3.78125800	0.37892300	-1.95452000
H	4.41170900	1.94231900	-2.50478400
H	2.77729800	1.83896400	-1.83388000
H	3.26600000	-0.85290800	2.72020700
H	5.01181400	-1.18313300	2.72500400
H	4.32695000	-0.07206400	3.92893900

Table S26
B/N-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
N	2.66816900	-0.09747800	0.39094700
N	1.10837800	0.21179600	1.71416600
N	0.19514200	-0.14558500	1.08966400
O	-1.06995000	0.10025600	1.54538400
B	-2.06579500	0.40993100	0.39856200
C	-1.91689900	1.96425100	-0.03013700
C	-0.69543300	2.53364500	-0.42973500
O	0.40985700	1.66171100	-0.44125200
C	1.69279400	2.11495100	-0.52236200
C	2.77377000	1.24696400	-0.20199300
C	4.07991600	1.69920700	-0.42863400
C	4.33236600	2.95114500	-0.96588100
C	3.26752500	3.80476700	-1.23418100
C	1.94807100	3.41184200	-1.00411100
C	0.80440300	4.38047600	-1.33443400
C	-0.53942800	3.85489600	-0.83344100
C	-1.68388100	4.66626700	-0.84565700
C	-2.91727700	4.15612600	-0.45661700
C	-3.02231900	2.82421600	-0.04998200
C	1.09875100	5.74973900	-0.67558800
C	0.71902700	4.52399400	-2.87597300
C	-1.77857500	-0.65125200	-0.79497600
C	-1.41165200	-0.34062800	-2.10064100
F	-1.22176300	0.93674400	-2.51803500
C	-1.14765300	-1.31884400	-3.05119800
F	-0.64741800	-0.99299900	-4.26625400
C	-1.28892900	-2.65477500	-2.71708800
F	-0.97773100	-3.60014300	-3.62913800
C	-1.62933300	-3.01249800	-1.42034600
C	-1.86070900	-2.00977800	-0.48500200
F	-2.15631100	-2.39703400	0.77817800
F	-1.66690700	-4.31991300	-1.07431200

C	-3.48479500	0.11410100	1.11464100
C	-4.61284500	0.01659700	0.30880100
F	-4.48601800	0.22211600	-1.02917100
C	-5.88149100	-0.25076500	0.81043500
F	-6.95293100	-0.32673300	-0.00397700
C	-6.03443900	-0.43743900	2.18173600
F	-7.25043300	-0.70339800	2.69594000
C	-4.93179800	-0.33665700	3.02128200
C	-3.67773100	-0.05362000	2.48392700
F	-2.66639600	0.05393300	3.37425700
F	-5.08152300	-0.50869300	4.35044000
C	3.80808700	-0.35468600	1.29655400
C	3.93738300	0.31273800	2.54491800
C	3.02454800	1.38342500	3.12494100
C	5.05925400	0.01594600	3.32738100
C	6.06832100	-0.85580300	2.91708200
C	7.26775700	-1.11558800	3.79488900
C	5.95036800	-1.42730800	1.65356300
C	4.84856600	-1.18608600	0.82520400
C	4.89664500	-1.78877000	-0.56490300
C	2.16883300	-1.23675000	-0.34169700
C	1.91018000	-1.21604700	-1.74008000
C	1.91434100	0.00592500	-2.63409400
C	1.62610000	-2.42784400	-2.38430500
C	1.53921300	-3.64556300	-1.71337100
C	1.69700100	-3.62561000	-0.32663500
C	1.99756200	-2.46221400	0.37958600
C	2.15922200	-2.62528400	1.87823200
C	1.18643300	-4.93064900	-2.42006800
H	4.90456300	1.04546800	-0.17833200
H	5.35556300	3.25794900	-1.16118600
H	3.46684900	4.79191800	-1.63944000
H	-1.61123600	5.69984400	-1.17362700
H	-3.79962900	4.79228800	-0.47412300
H	-3.99169000	2.44170200	0.25335100
H	0.30761900	6.46939900	-0.91201700
H	2.04475700	6.17101900	-1.03460900
H	1.15310700	5.63846000	0.41438300

H	-0.07914700	5.22733600	-3.14486200
H	1.66833600	4.89318900	-3.28697400
H	0.48869600	3.55192700	-3.32987400
H	3.59409700	1.97739400	3.85080900
H	2.62913600	2.05397400	2.35715100
H	2.16704100	0.94629500	3.64592800
H	5.15500400	0.51698400	4.28966400
H	8.03169300	-1.69434000	3.25831800
H	7.71981500	-0.16781900	4.12750200
H	6.97768900	-1.68008900	4.69558700
H	6.74969600	-2.05945900	1.27412900
H	5.93062700	-2.06706300	-0.79535900
H	4.55446100	-1.08624700	-1.33106100
H	4.27377400	-2.68630800	-0.64683200
H	1.74210200	-0.31077000	-3.66693100
H	1.08923100	0.67062400	-2.36764800
H	2.84984000	0.57162300	-2.58904400
H	1.41901500	-2.39994600	-3.45138200
H	1.57429500	-4.55304800	0.22974700
H	1.63948800	-3.53934700	2.19261400
H	1.73896900	-1.78396800	2.43318700
H	3.21499200	-2.71408700	2.16472200
H	1.87720900	-5.73626100	-2.13944800
H	0.17281100	-5.23106100	-2.12800300
H	1.19850700	-4.80959000	-3.50724500

Table S27
B/As-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
As	2.82475300	0.45686400	0.65674500
N	1.82538000	0.67958600	2.33948800
N	0.63109600	0.42165100	2.30820900
O	0.17333400	-0.17354700	1.23156800
B	-1.29584400	0.09618000	0.81865000

C	-1.59045200	1.68671800	1.00813100
C	-0.68011900	2.65932500	0.57178500
O	0.52573000	2.19251500	0.03617600
C	1.61852100	2.98704100	0.12854300
C	2.85920200	2.34972300	0.27668500
C	4.02337400	3.11805800	0.38418800
C	3.92829200	4.50958000	0.33337700
C	2.68042900	5.12911000	0.20073200
C	1.50179100	4.38228500	0.09357100
C	0.10135000	4.95743700	-0.11207500
C	-0.89134200	4.04132900	0.61468100
C	-2.07279100	4.48651200	1.22040200
C	-2.99072400	3.56576300	1.72510400
C	-2.75403000	2.19385800	1.60519800
C	0.01151000	6.41105300	0.36382700
C	-0.22597400	4.89735400	-1.62859700
C	-1.25413700	-0.44765700	-0.73551100
C	-1.47468800	0.30324200	-1.89098600
F	-1.72262100	1.62099200	-1.83502000
C	-1.43208000	-0.23913300	-3.17927300
F	-1.59496600	0.53987400	-4.25124000
C	-1.18959100	-1.59978700	-3.34172100
F	-1.10936700	-2.13072400	-4.56498800
C	-0.97702400	-2.39432600	-2.21784100
C	-0.98403500	-1.80319900	-0.95678500
F	-0.70646800	-2.61644600	0.07563400
F	-0.71249300	-3.69576600	-2.36421500
C	-2.34142400	-0.84784700	1.65067800
C	-3.66827300	-0.92158700	1.21736800
F	-4.06319200	-0.18873500	0.16121200
C	-4.63943600	-1.72129600	1.82115100
F	-5.89349500	-1.74085700	1.36807000
C	-4.27864600	-2.51459100	2.91073000
F	-5.18282500	-3.29008000	3.50644500
C	-2.96245800	-2.48771200	3.37002500
C	-2.02433200	-1.66837600	2.73477500
F	-0.77537700	-1.72886700	3.22431400
F	-2.60716900	-3.25260000	4.40397400

C	4.65683200	0.00031100	1.15951900
C	5.03347100	-0.33960800	2.48588800
C	4.09253400	-0.41065600	3.66287900
C	6.37739100	-0.64771500	2.73153800
C	7.35491300	-0.63488800	1.73256700
C	8.78554700	-0.97793100	2.05278100
C	6.95386100	-0.30404900	0.43835300
C	5.62415600	0.00648600	0.12231900
C	5.31876100	0.31103800	-1.32444200
C	2.37222500	-0.73999400	-0.81202200
C	2.13437200	-0.31003600	-2.13854900
C	1.95740700	1.12508900	-2.56043300
C	2.01985200	-1.29717000	-3.12368100
C	2.10365200	-2.66535900	-2.84239600
C	2.25908600	-3.04959600	-1.50910900
C	2.38332100	-2.11243900	-0.47731900
C	2.46600600	-2.59812600	0.94663000
C	1.96385900	-3.67741800	-3.94693600
H	4.99051100	2.63620600	0.53368400
H	4.83131300	5.11746400	0.41643400
H	2.63048800	6.21810700	0.18015800
H	-2.28630800	5.55344700	1.28915200
H	-3.90652300	3.92029900	2.20373400
H	-3.49776400	1.49964300	1.99721400
H	-0.99575300	6.81304500	0.18932000
H	0.70620500	7.05137600	-0.19896000
H	0.24056300	6.50176200	1.43618100
H	-1.23455600	5.29929400	-1.80865500
H	0.50184300	5.48960700	-2.20583700
H	-0.21241400	3.86255600	-1.99846000
H	4.62781100	-0.78513200	4.54575900
H	3.65986300	0.56921700	3.90320500
H	3.24207000	-1.08060500	3.47464000
H	6.66669800	-0.90978700	3.75256500
H	9.43847500	-0.85592400	1.17676200
H	9.17424700	-0.33959100	2.86268500
H	8.87111900	-2.02192900	2.39736800
H	7.69622100	-0.28678400	-0.36366300

H	6.24465700	0.55893600	-1.86122300
H	4.63343700	1.15833300	-1.45084900
H	4.86029200	-0.55448300	-1.82527600
H	1.82482900	1.18384400	-3.64874100
H	1.06449500	1.55551500	-2.08864400
H	2.81031700	1.76315700	-2.29075100
H	1.83426400	-0.97972900	-4.15307300
H	2.25843100	-4.11150000	-1.25359100
H	2.39731900	-3.69317700	0.98440800
H	1.63041300	-2.19636000	1.53999500
H	3.41219700	-2.31169700	1.42979000
H	1.00212300	-3.54842400	-4.46581300
H	2.76206200	-3.55477100	-4.69741600
H	2.00764800	-4.70524600	-3.56124500

Table S28
B/Sb-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Sb	2.12903400	0.29722700	0.38273700
N	1.07912700	0.64020500	2.32597200
N	-0.09356500	0.39518900	2.19209300
O	-0.47136900	-0.17615000	1.05666500
B	-1.92333900	0.07665800	0.54805300
C	-2.22981700	1.66709100	0.70118900
C	-1.33179700	2.63948500	0.23874900
O	-0.12350800	2.17677700	-0.29264600
C	0.96089200	2.99598100	-0.22048200
C	2.20546500	2.37849000	-0.06086500
C	3.36011100	3.15969400	0.03916900
C	3.24633700	4.55070000	-0.03236700
C	1.99107100	5.15144500	-0.18130200
C	0.82176900	4.38753400	-0.28112800
C	-0.58686600	4.93617500	-0.49703100
C	-1.56093200	4.02027300	0.25501700

C	-2.74171100	4.46339500	0.86329700
C	-3.64428100	3.54365200	1.39642200
C	-3.39332700	2.17284300	1.30010800
C	-0.69899300	6.39886200	-0.05525500
C	-0.91744500	4.83474300	-2.01055300
C	-1.80527400	-0.50359500	-0.98748700
C	-2.00937700	0.21469300	-2.16699600
F	-2.27866400	1.52818900	-2.15161400
C	-1.93094600	-0.36029800	-3.43901300
F	-2.06257600	0.39165600	-4.53447400
C	-1.67260300	-1.72166600	-3.56086100
F	-1.55656600	-2.28144700	-4.76669700
C	-1.48640600	-2.48764300	-2.41272700
C	-1.52072300	-1.86299600	-1.16840500
F	-1.26409700	-2.64793900	-0.10856700
F	-1.22421900	-3.79315800	-2.52188700
C	-3.00705400	-0.86057300	1.33759800
C	-4.31660900	-0.91265400	0.85031300
F	-4.65727300	-0.16818600	-0.21599400
C	-5.32214800	-1.70269400	1.40845300
F	-6.55694600	-1.70103500	0.90535900
C	-5.01586500	-2.51057500	2.50414900
F	-5.95371800	-3.27777700	3.05638300
C	-3.71856200	-2.50721900	3.01477300
C	-2.74391500	-1.69692600	2.42408800
F	-1.51549500	-1.78360600	2.95782600
F	-3.41477200	-3.28709000	4.05364100
C	4.17886600	-0.16740400	0.88042600
C	4.54890400	-0.57942900	2.18209300
C	3.56379000	-0.73958900	3.31301900
C	5.89705800	-0.86387500	2.43040000
C	6.88033300	-0.75623700	1.44038900
C	8.32300100	-1.05071600	1.75781000
C	6.48091900	-0.36611500	0.16046800
C	5.14353900	-0.07757600	-0.14893000
C	4.80742900	0.27970900	-1.57675500
C	1.74646900	-1.00140700	-1.28972700
C	1.53515300	-0.53599000	-2.60202100

C	1.34575100	0.91653600	-2.95351600
C	1.47116500	-1.49469100	-3.62201300
C	1.58150200	-2.86706400	-3.37254600
C	1.73856800	-3.28741300	-2.04775300
C	1.81116800	-2.37665800	-0.98854100
C	1.91897400	-2.88190400	0.42855000
C	1.43017000	-3.86384700	-4.48935500
H	4.33437100	2.69295900	0.19823700
H	4.14029800	5.17287500	0.04575900
H	1.92720200	6.23928100	-0.21957200
H	-2.96656900	5.52906000	0.91211000
H	-4.55888800	3.89761000	1.87767200
H	-4.12443900	1.47758000	1.71368800
H	-1.71200000	6.78214600	-0.23887100
H	-0.01325300	7.03524900	-0.63324100
H	-0.47082700	6.51847600	1.01445900
H	-1.93366600	5.21409800	-2.19705600
H	-0.20201300	5.42695700	-2.60303000
H	-0.88468200	3.79207900	-2.35637700
H	4.05888600	-1.15946400	4.19903100
H	3.10265300	0.21663400	3.59811200
H	2.73658100	-1.41515300	3.04475400
H	6.18602500	-1.18218000	3.43586100
H	8.94560400	-1.05436500	0.85176400
H	8.73527300	-0.29544400	2.44778500
H	8.42978100	-2.02943600	2.25212900
H	7.22957200	-0.28777900	-0.63245900
H	5.71953300	0.51806600	-2.14073000
H	4.14286900	1.15210200	-1.65116200
H	4.30514200	-0.55601500	-2.08769600
H	1.08037600	1.02228600	-4.01395700
H	0.53578500	1.36155900	-2.36131500
H	2.25353000	1.51276400	-2.77285100
H	1.29635400	-1.15333100	-4.64572000
H	1.77551000	-4.35661100	-1.82567600
H	1.82196100	-3.97514800	0.46273900
H	1.11257100	-2.46780600	1.05535800
H	2.89038400	-2.62469200	0.88199900

H	0.36091500	-4.06437800	-4.66467300
H	1.85333700	-3.48351400	-5.43109900
H	1.91538600	-4.82061300	-4.24733700

Table S29
B/Bi-Prod

Atomic Coordinates (Angstroms)

Number	X	Y	Z
Bi	1.93305100	0.20035800	0.40838000
N	0.77195400	0.65281700	2.51479100
N	-0.36587100	0.41215400	2.29191300
O	-0.74462600	-0.17771200	1.17977900
B	-2.17548000	0.10792900	0.59641400
C	-2.44758400	1.70340900	0.70834900
C	-1.53049400	2.65632500	0.23764200
O	-0.31953500	2.17197000	-0.25834200
C	0.76960700	2.99610100	-0.22299700
C	2.01806600	2.38762800	-0.07296200
C	3.17209300	3.16816900	-0.00525800
C	3.05657500	4.55907500	-0.10408000
C	1.79968800	5.15393900	-0.25391600
C	0.62979800	4.38582500	-0.32168200
C	-0.77675200	4.93277000	-0.55309400
C	-1.75728200	4.03820800	0.21428300
C	-2.94579100	4.50180100	0.79183500
C	-3.86434200	3.60285100	1.33208700
C	-3.62018900	2.22920000	1.27155800
C	-0.88724000	6.40609900	-0.14670600
C	-1.10254000	4.79650000	-2.06506600
C	-1.97725300	-0.51453400	-0.91148800
C	-2.15398900	0.16670600	-2.11728500
F	-2.44672500	1.47405000	-2.14672400
C	-2.02842600	-0.44596400	-3.36679200
F	-2.13514900	0.26937800	-4.48905700
C	-1.74253300	-1.80568000	-3.43917400

F	-1.59212500	-2.39782400	-4.62445000
C	-1.57194800	-2.53394100	-2.26447000
C	-1.66288600	-1.87324000	-1.04105700
F	-1.43574300	-2.62114200	0.05276700
F	-1.28126700	-3.83569800	-2.32627100
C	-3.31513900	-0.78792900	1.35002700
C	-4.58735100	-0.85476300	0.77290400
F	-4.84645000	-0.15219300	-0.34273900
C	-5.63601900	-1.61313300	1.29400300
F	-6.83100900	-1.63067300	0.70375100
C	-5.41663600	-2.36633600	2.44831200
F	-6.39776100	-3.10164200	2.96662300
C	-4.16198400	-2.33842900	3.05554000
C	-3.14183300	-1.56025200	2.49934300
F	-1.96167900	-1.60318800	3.13669100
F	-3.94298400	-3.05890500	4.15616200
C	4.12289400	-0.23338700	0.85513200
C	4.50035800	-0.64177800	2.15040500
C	3.50834800	-0.80169500	3.27659500
C	5.85310000	-0.91410700	2.38946100
C	6.82444700	-0.79256100	1.38780200
C	8.27385500	-1.07325700	1.68959200
C	6.41055100	-0.39867400	0.11299700
C	5.06611000	-0.12131600	-0.18439900
C	4.70035700	0.24734900	-1.60176400
C	1.60838700	-1.09436600	-1.43353100
C	1.37551400	-0.56403700	-2.71135100
C	1.15068500	0.90082500	-2.98174000
C	1.33432500	-1.47245500	-3.78123200
C	1.48662200	-2.85046700	-3.60095400
C	1.68569100	-3.33170200	-2.30149900
C	1.73730300	-2.47482300	-1.19672600
C	1.88990300	-3.04561600	0.19183200
C	1.34277300	-3.80604100	-4.75455000
H	4.14982800	2.70492100	0.14624500
H	3.95088200	5.18380700	-0.05133400
H	1.73378800	6.24018500	-0.32088600
H	-3.16500100	5.56957600	0.80843700

H	-4.78534600	3.97430400	1.78709600
H	-4.36413800	1.54606800	1.68306100
H	-1.89792600	6.78856200	-0.34445000
H	-0.19695700	7.02636700	-0.73636400
H	-0.66314100	6.55059400	0.92079900
H	-2.11733400	5.17305600	-2.26516200
H	-0.38322100	5.37300200	-2.66812800
H	-1.06920700	3.74581100	-2.38584100
H	4.00010300	-1.18937700	4.17919100
H	3.02436000	0.15093900	3.53897600
H	2.70183500	-1.50579300	3.01353000
H	6.15548500	-1.23135700	3.39165100
H	8.88410700	-1.08287000	0.77510600
H	8.69097200	-0.30696900	2.36455200
H	8.39524800	-2.04548700	2.19328500
H	7.15234900	-0.30730700	-0.68539400
H	5.59845200	0.49745300	-2.18331800
H	4.02619700	1.11480100	-1.64875200
H	4.19118600	-0.58613800	-2.10991000
H	0.82350000	1.05402300	-4.01897700
H	0.37429300	1.31135900	-2.32385500
H	2.06481200	1.49463900	-2.82358500
H	1.13891000	-1.08440200	-4.78438400
H	1.76887900	-4.40885200	-2.13566700
H	1.89771600	-4.14352200	0.16649700
H	1.04582000	-2.74216800	0.83228600
H	2.83016200	-2.72078900	0.66771400
H	0.32378900	-4.22631800	-4.76150800
H	1.50161300	-3.30482900	-5.72012800
H	2.04938300	-4.64611700	-4.67479300
