

Supporting Information

Understanding the Influence of Group 13 Elements on the Reactivity of G13– As–Ge Imine Analogues in 1,3- Addition with Methyl Iodide

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(All were calculated at the M06-2X-D3/def2-TZVP level)

Table S1

B=As-Rea

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.23491600	-0.04484000	-0.07318100
As	0.62654000	0.07027300	2.35604900
B	2.54542100	0.10659300	2.64186500
N	-1.13055800	-1.61274000	0.02088600
N	3.01293100	0.08419700	4.09336200
N	3.75276400	0.15898000	1.71943300
N	-1.40098400	1.28065000	-0.08775900
C	4.24729300	-0.28288100	4.44802000
C	5.24156000	-0.43394000	3.47802600
H	6.25214900	-0.68550300	3.78797300
C	3.58712500	0.45967300	0.31250200
C	-0.62937400	-2.84601100	-0.49992500
C	5.00021400	-0.08671900	2.14971800
C	3.75167900	-0.56627300	-0.63537400
C	4.04107000	-2.01177000	-0.26106600
H	4.39249100	-2.04709800	0.78046000
C	-0.22264400	-3.90545400	0.34069200
C	-1.06933900	2.64331500	-0.37049300
C	3.29861300	1.78550700	-0.06924600
C	-2.41576200	-1.53095000	0.33823000
C	-2.65001900	0.96892400	0.21252400
C	-3.09700500	-0.32608900	0.53991800
H	-4.15199000	-0.40751200	0.79292300
C	6.17150500	0.04350700	1.21744100
H	6.19040000	-0.77605100	0.48760700
H	7.10535400	0.02872100	1.78980200
H	6.10272200	0.97834300	0.64505500
C	-0.29112700	-3.85511600	1.86333000
H	-0.75529200	-2.89955900	2.15666100
C	-0.54228000	-2.96956400	-1.90637900
C	0.26472400	-5.07446300	-0.25605300
H	0.58154200	-5.90178800	0.38319800
C	-1.12034400	3.61244200	0.65904900
C	2.14445800	0.54006000	5.16287900
C	-3.24284200	-2.79248500	0.41666300
H	-3.15720100	-3.37165100	-0.51382100
H	-4.29625100	-2.55501500	0.59817200
H	-2.87838200	-3.43415000	1.22862200
C	3.18394700	2.89438000	0.96425600
H	2.56573900	2.48329900	1.77769200
C	4.60052800	-0.47394000	5.89491200
H	4.46568200	0.45847000	6.45906200
H	5.63858600	-0.81073900	5.98989000
H	3.93002300	-1.21169600	6.35200800

C	1.30268400	-0.35286100	5.84627100
C	-0.72508400	3.01395500	-1.69312100
C	3.59121500	-0.24144200	-1.98706900
H	3.69737900	-1.02503000	-2.73906300
C	2.25439900	1.89867000	5.53520600
C	-1.42631300	3.27576800	2.11168600
H	-1.61006900	2.19491400	2.19243500
C	1.08128900	-1.79737700	5.42185100
H	1.60422800	-1.95034800	4.46730800
C	-1.12225600	-5.02212500	2.41939900
H	-0.57881000	-5.97330900	2.31133500
H	-2.08762500	-5.13935200	1.90810500
H	-1.31595000	-4.87641800	3.49272300
C	3.12923200	2.05270800	-1.43042900
H	2.87620100	3.06325700	-1.75155800
C	-3.76950200	1.98891100	0.13506200
H	-4.27897800	2.04081500	1.10739300
H	-4.50807000	1.63336800	-0.59777900
H	-3.44180900	2.99145600	-0.15381500
C	-0.87991400	4.95130800	0.32889700
H	-0.93459600	5.70834800	1.11437700
C	5.11913500	-2.65154900	-1.14221800
H	4.75176900	-2.81070100	-2.16635100
H	5.39367100	-3.63765400	-0.74074500
H	6.03100000	-2.03885700	-1.20879100
C	0.60908200	0.13259600	6.96193500
H	-0.04672500	-0.54448700	7.51256000
C	3.11739600	2.88752400	4.75567900
H	3.08164900	2.57537300	3.70122500
C	0.36316400	-5.20538100	-1.63559900
H	0.74904200	-6.12686800	-2.07436400
C	3.27639400	1.04941700	-2.38441400
H	3.13925300	1.27662100	-3.44297800
C	-0.72762600	1.99257500	-2.82188500
H	-0.25853900	1.07532500	-2.43116000
C	-1.02218100	-1.87492100	-2.84906300
H	-1.34669800	-1.01681900	-2.24330800
C	-0.55817100	5.33083900	-0.96687900
H	-0.36949800	6.37913000	-1.20346800
C	-0.21699500	3.58917900	2.99623700
H	0.68187200	3.07317900	2.63179500
H	-0.39777200	3.24046600	4.02564000
H	-0.02642200	4.67511700	3.02135500
C	0.72842200	1.45302600	7.37146600
H	0.17922300	1.80774800	8.24481200
C	2.45551500	4.12484000	0.43661000
H	2.22349400	4.80808900	1.26727300
H	1.50949000	3.84615300	-0.04511900
H	3.06738500	4.68089300	-0.29166400
C	2.75190600	-2.82670000	-0.31603900
H	2.00364100	-2.39049300	0.35646000
H	2.93014000	-3.86765900	-0.00711100

H	2.32524900	-2.83422200	-1.33225400
C	-0.04016700	-4.15398700	-2.45159200
H	0.02446900	-4.25716900	-3.53732700
C	-0.46541500	4.36183100	-1.96205400
H	-0.20571200	4.66649800	-2.97569500
C	-0.41095600	-2.05462800	5.17535100
H	-0.55757000	-3.06671200	4.76904900
H	-0.81401800	-1.32960900	4.45587900
H	-0.98344000	-1.99155100	6.11382000
C	4.54900600	3.29733400	1.53705500
H	5.23005400	3.60952100	0.72949600
H	5.03064200	2.48806300	2.10528700
H	4.43000000	4.14943900	2.22418200
C	1.10543000	-3.90045900	2.49908200
H	1.01920300	-4.05643700	3.58530500
H	1.64867100	-2.96005300	2.33649500
H	1.69672000	-4.73502400	2.08993600
C	1.53363300	2.33079400	6.65081300
H	1.59772300	3.37399600	6.96085500
C	4.58999000	2.89840800	5.19551900
H	5.11657200	3.72814100	4.70038700
H	5.12856800	1.97811400	4.93735000
H	4.66390700	3.05604100	6.28351100
C	-2.64748800	4.03624300	2.64520500
H	-2.44243800	5.11654000	2.70186800
H	-2.88745000	3.69363300	3.66256700
H	-3.53731100	3.90078500	2.01761800
C	-2.23392300	-2.34891700	-3.65920200
H	-1.97307300	-3.20249300	-4.30389500
H	-2.60773900	-1.54010200	-4.30494000
H	-3.05491300	-2.66396800	-2.99853600
C	1.60855200	-2.80485600	6.45089800
H	1.11196400	-2.66946400	7.42416300
H	2.69218200	-2.72669500	6.61375400
H	1.40019700	-3.83088000	6.11190700
C	0.10493800	-1.38835600	-3.76321400
H	0.93639000	-0.98563000	-3.16387700
H	-0.26214600	-0.59050100	-4.42715600
H	0.48719200	-2.20141000	-4.40025400
C	0.08985400	2.43390700	-4.03479300
H	-0.39636600	3.25839200	-4.57900800
H	0.19690500	1.59699000	-4.73965200
H	1.09719000	2.76320800	-3.74104100
C	-2.16033700	1.64767800	-3.24740200
H	-2.74039300	1.21968200	-2.41775800
H	-2.14900400	0.90985600	-4.06505000
H	-2.68311900	2.54775000	-3.60791800
C	2.58553800	4.32127000	4.83526200
H	2.81135300	4.77566200	5.81240800
H	1.50238100	4.36846300	4.67502900
H	3.07561300	4.94170500	4.07000900

Table S2**Al=As-Rea**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.01154500	-0.01030800	0.04827700
As	0.02054500	-0.05916600	2.53248700
Al	2.27294600	0.05691100	2.74688700
N	-1.35714000	-1.56146800	-0.13862700
N	3.18983800	0.03234800	4.42139600
N	3.84281300	0.15644700	1.67184700
N	-1.56944000	1.32734100	-0.19921400
C	4.50161600	-0.17524700	4.55872800
C	5.38548200	-0.27843800	3.47300500
H	6.43111000	-0.45298100	3.71408300
C	3.64042600	0.43035300	0.27129500
C	-0.78527900	-2.78359900	-0.61387100
C	5.08541300	-0.03099200	2.12434500
C	3.73429600	-0.61784700	-0.66306500
C	4.00805700	-2.05450100	-0.24770100
H	4.45607000	-2.05076000	0.75631800
C	-0.45053900	-3.84696100	0.25192300
C	-1.20922000	2.68392900	-0.48980900
C	3.29013000	1.74039300	-0.11485100
C	-2.66380700	-1.47381700	0.04713400
C	-2.85420200	1.03378900	-0.04318900
C	-3.35136500	-0.25766600	0.19859200
H	-4.42573000	-0.33400500	0.34449300
C	6.24349000	0.04810900	1.16230200
H	6.22603300	-0.79977200	0.46326100
H	7.19511000	0.04288600	1.70393000
H	6.17076000	0.95910200	0.55239300
C	-0.69654900	-3.82159800	1.75366200
H	-1.15315100	-2.85335600	2.01104700
C	-0.55514400	-2.89008300	-2.00497500
C	0.11137700	-5.00299000	-0.30461500
H	0.36911400	-5.83459100	0.35524100
C	-1.30920800	3.68255900	0.50801200
C	2.43992400	0.42152700	5.58932800
C	-3.50993900	-2.72508200	0.06170200
H	-3.18864500	-3.44517600	-0.70219700
H	-4.56657900	-2.47937200	-0.08975300
H	-3.40600800	-3.21445000	1.04118400
C	3.21158000	2.86783000	0.90490900
H	2.71107200	2.46798300	1.80432000
C	5.10856700	-0.22113100	5.93799100
H	5.23802400	0.80450300	6.31607100
H	6.09156400	-0.70430200	5.90565400
H	4.45603200	-0.74378600	6.64820700
C	1.54637900	-0.48634800	6.19399500

C	-0.77001800	3.01807600	-1.79552500
C	3.48716700	-0.32303300	-2.00650400
H	3.54716400	-1.12097900	-2.74859100
C	2.60627900	1.73387000	6.07893500
C	-1.63267300	3.38315600	1.96484400
H	-1.92334100	2.32545100	2.05144600
C	1.36061700	-1.90100200	5.66134700
H	1.34162200	-1.83462800	4.56215500
C	-1.63292400	-4.96049200	2.18391200
H	-1.12710700	-5.93489400	2.09979500
H	-2.54243800	-5.01153900	1.57001900
H	-1.92995500	-4.83190700	3.23557800
C	3.03219500	1.97983300	-1.46781500
H	2.73288500	2.97776300	-1.79021600
C	-3.89450200	2.11860000	-0.20768600
H	-3.84324600	2.83987600	0.61570000
H	-4.89965700	1.68513400	-0.23576900
H	-3.71528400	2.68117600	-1.13501300
C	-1.02209600	5.00833900	0.16247600
H	-1.10417500	5.78410300	0.92654000
C	4.98074300	-2.77410000	-1.18485900
H	4.53219400	-2.94274100	-2.17467200
H	5.23754300	-3.76097700	-0.77374000
H	5.91250200	-2.20634800	-1.33047900
C	0.84276800	-0.05176800	7.32205300
H	0.14141400	-0.72712400	7.80987800
C	3.47651000	2.76536700	5.37231100
H	4.16388300	2.24607200	4.68839500
C	0.34545900	-5.11880300	-1.66867900
H	0.78257400	-6.03154800	-2.07655600
C	3.13706600	0.95982200	-2.40821400
H	2.92922100	1.16316500	-3.46017100
C	-0.68093400	1.96778100	-2.89504700
H	-0.20774200	1.07516500	-2.45225300
C	-0.97353300	-1.79579700	-2.97423400
H	-1.28835300	-0.92185400	-2.38737300
C	-0.61155100	5.35033000	-1.11765600
H	-0.38776700	6.38886300	-1.36649800
C	-0.36301400	3.56799400	2.80015800
H	0.45315000	2.97087300	2.37582800
H	-0.51978100	3.21841400	3.83225300
H	-0.06222100	4.62927400	2.82491900
C	1.00881700	1.23125900	7.83215300
H	0.44582400	1.54494100	8.71232200
C	2.36236900	4.04307600	0.43110000
H	2.17796600	4.73317900	1.26792400
H	1.38900500	3.70388300	0.04904600
H	2.86755800	4.61316500	-0.36433700
C	2.68553400	-2.81520900	-0.14376600
H	1.99681400	-2.30651700	0.54611500
H	2.84534400	-3.84178500	0.21980200
H	2.18245500	-2.86844300	-1.12267000

C	0.01007600	-4.06352900	-2.51042700
H	0.17763700	-4.15628500	-3.58580800
C	-0.47216900	4.35486200	-2.07997200
H	-0.13847500	4.63089000	-3.07969000
C	0.02425600	-2.51312800	6.07707600
H	-0.11907700	-3.47861000	5.57267600
H	-0.81197200	-1.85564900	5.79915400
H	-0.01871800	-2.70829900	7.15955500
C	4.60697900	3.34548200	1.32628300
H	5.18809400	3.65080800	0.44204300
H	5.17154700	2.56743300	1.85992800
H	4.52702000	4.21596400	1.99425800
C	0.61344500	-3.92956300	2.54091100
H	0.39937000	-3.98522000	3.61791400
H	1.24624300	-3.04981900	2.37346300
H	1.17265100	-4.83641300	2.26008400
C	1.87959000	2.11647800	7.20972100
H	1.98882900	3.12928700	7.60110300
C	4.33018900	3.59444300	6.33504900
H	5.01974200	4.23699500	5.76861100
H	4.92583900	2.95980400	7.00798000
H	3.70980800	4.25382800	6.95941000
C	-2.74773300	4.26270200	2.54352700
H	-2.43068200	5.31468300	2.60678000
H	-2.98608300	3.93266600	3.56504500
H	-3.67463600	4.23538000	1.95406400
C	-2.17935400	-2.25230100	-3.80319000
H	-1.92778000	-3.13337500	-4.41395200
H	-2.51210000	-1.45195600	-4.48107900
H	-3.02563600	-2.52204200	-3.15409300
C	2.52187600	-2.81879000	6.05969700
H	2.62739200	-2.86366100	7.15536500
H	3.47676200	-2.48080200	5.63326800
H	2.34026800	-3.83997600	5.69202800
C	0.18763400	-1.35137700	-3.86420500
H	1.00991800	-0.95614700	-3.24807400
H	-0.14298700	-0.55890800	-4.55236000
H	0.57313000	-2.18012100	-4.47801300
C	0.18927300	2.40810200	-4.07237600
H	-0.29871100	3.19705100	-4.66548200
H	0.36842000	1.55809000	-4.74573000
H	1.16464100	2.78856900	-3.73639400
C	-2.07352600	1.57241300	-3.40420100
H	-2.68358500	1.09842900	-2.62256400
H	-1.98495000	0.85618700	-4.23579200
H	-2.61059400	2.45878200	-3.77800900
C	2.58682900	3.67122100	4.51494500
H	1.88715700	4.23741700	5.14940900
H	1.98044200	3.07716000	3.81710000
H	3.18937400	4.38949200	3.93825900

Table S3**Ga=As-Rea**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	-0.00772300	-0.00030800	0.05443100
As	-0.05148500	-0.05561600	2.54873600
Ga	2.21735300	0.05870400	2.76311000
N	-1.37482100	-1.54735700	-0.15595600
N	3.20760300	0.03208500	4.47469900
N	3.84622300	0.17743800	1.66091700
N	-1.57604000	1.33949100	-0.21760800
C	4.52353100	-0.14915400	4.57471000
C	5.39057000	-0.23419300	3.47280000
H	6.44090400	-0.39406600	3.70312800
C	3.64099500	0.43853000	0.26224600
C	-0.79362500	-2.77008900	-0.61987100
C	5.08357700	0.00493000	2.12278600
C	3.73299300	-0.61963000	-0.66155800
C	4.01085300	-2.05005400	-0.22776800
H	4.47612800	-2.03078200	0.76801000
C	-0.47253700	-3.82994600	0.25478600
C	-1.21039600	2.69350000	-0.51772200
C	3.28498000	1.74353600	-0.13681900
C	-2.68239100	-1.45710800	0.01841800
C	-2.86371200	1.05095400	-0.07016800
C	-3.36657400	-0.23815400	0.16958000
H	-4.44230400	-0.31152400	0.30752100
C	6.24388200	0.08875900	1.16107000
H	6.23143000	-0.76098600	0.46397600
H	7.19519500	0.09014400	1.70324300
H	6.16737700	0.99792600	0.54903100
C	-0.75999200	-3.80339000	1.74839300
H	-1.21941200	-2.83334100	1.99236800
C	-0.53973800	-2.87954500	-2.00621400
C	0.10683400	-4.98428500	-0.28702000
H	0.35510200	-5.81311600	0.37987800
C	-1.31089700	3.69967800	0.47220400
C	2.47507300	0.39387600	5.65716300
C	-3.53680600	-2.70304500	0.02789200
H	-3.16441200	-3.46586300	-0.66748100
H	-4.57595100	-2.45907900	-0.21923600
H	-3.51840400	-3.13602200	1.03940600
C	3.20203300	2.88080500	0.87211900
H	2.69761100	2.48910700	1.77239100
C	5.16167500	-0.19460800	5.94198800
H	5.26712700	0.82822000	6.33520800
H	6.15778000	-0.64733800	5.88316400
H	4.54015400	-0.74895700	6.65625300
C	1.60861900	-0.53609300	6.26739800
C	-0.76819000	3.01716000	-1.82494500

C	3.47696700	-0.34136800	-2.00660600
H	3.53530200	-1.14732000	-2.74015900
C	2.62610600	1.70443800	6.15843400
C	-1.63571300	3.41063300	1.93048800
H	-1.93107700	2.35479300	2.02295600
C	1.43401900	-1.94445100	5.71340200
H	1.35256000	-1.85417800	4.61792900
C	-1.71647200	-4.93601300	2.14916200
H	-1.21819500	-5.91459200	2.06884900
H	-2.61178800	-4.97221500	1.51387100
H	-2.03638000	-4.81233200	3.19464100
C	3.01970600	1.96667800	-1.49125900
H	2.71647900	2.96013100	-1.82372300
C	-3.89807200	2.13946000	-0.24533000
H	-3.83984300	2.87211400	0.56741500
H	-4.90588000	1.71186600	-0.26548100
H	-3.71741400	2.68799300	-1.18086600
C	-1.02259300	5.02266100	0.11737900
H	-1.10488700	5.80413800	0.87551800
C	4.96609700	-2.78730000	-1.16885400
H	4.50149900	-2.97120900	-2.14855900
H	5.22778600	-3.76784200	-0.74580600
H	5.89631900	-2.22353200	-1.33768800
C	0.92187200	-0.12806900	7.41619500
H	0.24184000	-0.82044900	7.91017400
C	3.45014800	2.75581100	5.42688500
H	4.17938100	2.24988100	4.77775800
C	0.36760800	-5.10193100	-1.64609600
H	0.81778600	-6.01307700	-2.04315600
C	3.12095900	0.93619900	-2.42058700
H	2.90711000	1.12743400	-3.47367500
C	-0.67445200	1.95859500	-2.91606000
H	-0.20043900	1.07021700	-2.46537300
C	-0.95889500	-1.79427600	-2.98467200
H	-1.26573300	-0.91282900	-2.40500600
C	-0.61089100	5.35470400	-1.16493300
H	-0.38650700	6.39119500	-1.42152300
C	-0.36571900	3.59546100	2.76552700
H	0.45230600	3.00009800	2.34207500
H	-0.52413500	3.24725500	3.79752800
H	-0.06448500	4.65656300	2.78948000
C	1.07986600	1.14986800	7.94092800
H	0.53272400	1.44160200	8.83849200
C	2.35765500	4.05261400	0.38119100
H	2.17150800	4.75305100	1.20894600
H	1.38498400	3.71204200	-0.00104700
H	2.86745100	4.61232200	-0.41873900
C	2.68821800	-2.80578400	-0.08994600
H	2.01028400	-2.28608400	0.60288600
H	2.85098600	-3.82752100	0.28602900
H	2.16985100	-2.87159400	-1.05995400
C	0.04068700	-4.05161000	-2.49750100

H	0.22635000	-4.14792300	-3.56945900
C	-0.47008600	4.35179800	-2.11919000
H	-0.13423900	4.62003800	-3.12025600
C	0.14397600	-2.60843000	6.19118700
H	0.00998000	-3.57411000	5.68486300
H	-0.73092800	-1.98093700	5.96879800
H	0.16776600	-2.81528900	7.27205500
C	4.59418900	3.36407800	1.29860400
H	5.18364700	3.65643800	0.41544700
H	5.15311100	2.59468900	1.85001000
H	4.50805700	4.24493500	1.95234500
C	0.52508400	-3.91655100	2.57376700
H	0.27900200	-3.93824500	3.64503300
H	1.18101600	-3.05484600	2.40159800
H	1.07315600	-4.84129400	2.33194500
C	1.92073900	2.05924000	7.31096100
H	2.02129900	3.06785500	7.71453600
C	4.23740100	3.67355500	6.36381800
H	4.90100300	4.32700200	5.77924000
H	4.85467200	3.10189500	7.07293400
H	3.57157600	4.32605800	6.94732700
C	-2.74866100	4.29620400	2.50373300
H	-2.43080000	5.34840200	2.55765200
H	-2.98562100	3.97490300	3.52834100
H	-3.67658600	4.26413600	1.91608700
C	-2.17448400	-2.25687500	-3.79605100
H	-1.93143100	-3.14754800	-4.39628500
H	-2.51090900	-1.46481600	-4.48179500
H	-3.01526500	-2.51470700	-3.13492000
C	2.63931700	-2.83914900	6.02529900
H	2.80200900	-2.90872700	7.11264600
H	3.56147300	-2.46570800	5.55940600
H	2.46425400	-3.85535800	5.64104600
C	0.19469500	-1.36332300	-3.89020300
H	1.02445700	-0.96505100	-3.28638900
H	-0.14019600	-0.57666800	-4.58282600
H	0.57156300	-2.19848400	-4.50042400
C	0.19813900	2.39151100	-4.09448200
H	-0.29012200	3.17463400	-4.69498600
H	0.38082300	1.53658800	-4.76051800
H	1.17182500	2.77664400	-3.75911200
C	-2.06513600	1.55787400	-3.42643100
H	-2.67668100	1.08681200	-2.64416100
H	-1.97335200	0.83778600	-4.25423800
H	-2.60251300	2.44151800	-3.80612700
C	2.52295500	3.56545100	4.51456600
H	1.79255300	4.13241000	5.11267400
H	1.94809700	2.90161200	3.85284100
H	3.09150100	4.27591700	3.89502600

Table S4

In=As-Rea

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	-0.11293200	-0.00237400	0.06656200
As	-0.40351300	-0.10346100	2.55568000
In	2.02789800	0.06811100	2.83864200
N	-1.46300000	-1.53403700	-0.28413300
N	3.29745500	0.09052900	4.63743600
N	3.88995300	0.23074400	1.69082500
N	-1.62895000	1.35033000	-0.31906300
C	4.62224200	-0.00188000	4.66240400
C	5.45063400	-0.06485300	3.52589400
H	6.51250400	-0.16929900	3.73450900
C	3.67301500	0.44758700	0.29312200
C	-0.84101700	-2.75584600	-0.69462900
C	5.12257700	0.10710600	2.16661200
C	3.74283400	-0.63956400	-0.59990900
C	4.01816200	-2.05457700	-0.11626300
H	4.52487500	-1.99737800	0.85770300
C	-0.58661000	-3.80784600	0.21071900
C	-1.23036000	2.69733300	-0.61249700
C	3.29452000	1.73689800	-0.13976000
C	-2.77569500	-1.43478900	-0.18386500
C	-2.92721400	1.07695500	-0.23434600
C	-3.45408400	-0.20900300	-0.04043300
H	-4.53631800	-0.27434200	0.04286900
C	6.28148000	0.17377500	1.19696800
H	6.26764200	-0.69389900	0.52159400
H	7.23748000	0.19478600	1.73034600
H	6.19626600	1.06600000	0.56116300
C	-1.03376000	-3.78580100	1.66374900
H	-1.51075800	-2.81393000	1.85967300
C	-0.46545600	-2.86537900	-2.05287500
C	0.06541600	-4.95098400	-0.26908600
H	0.26570200	-5.77333200	0.42153200
C	-1.33813300	3.70987700	0.36964700
C	2.58765200	0.36697600	5.84657600
C	-3.64964000	-2.66595400	-0.24473400
H	-3.17013000	-3.49628400	-0.77633900
H	-4.60778600	-2.42974600	-0.72274700
H	-3.85938600	-2.99555400	0.78474200
C	3.19355500	2.89701400	0.84280100
H	2.69480200	2.51906800	1.75443400
C	5.32868800	0.01481300	6.00045200
H	5.36034500	1.04374500	6.39109300
H	6.35724900	-0.34848400	5.89869200
H	4.79246100	-0.59027100	6.74270600
C	1.81881500	-0.64878200	6.45425500
C	-0.74692700	3.00622300	-1.90872800
C	3.46119700	-0.40460600	-1.94762500
H	3.50635300	-1.23337000	-2.65646800

C	2.61921400	1.67924000	6.36733600
C	-1.69588400	3.43161100	1.82184400
H	-1.99915600	2.37809000	1.91301700
C	1.76570900	-2.05394700	5.86646400
H	1.64989900	-1.94967300	4.77344000
C	-2.03920300	-4.90986600	1.95021300
H	-1.55243900	-5.89520400	1.88308800
H	-2.87866600	-4.90894800	1.24216500
H	-2.44378400	-4.80806900	2.96827400
C	3.00728900	1.91787000	-1.49607500
H	2.69057300	2.89850300	-1.85343800
C	-3.93516800	2.18312700	-0.44273600
H	-3.86724300	2.93409200	0.35223300
H	-4.95239300	1.77877600	-0.46665100
H	-3.72981600	2.70485900	-1.38889500
C	-1.02665300	5.02742200	0.01359400
H	-1.11621200	5.81428900	0.76535500
C	4.92385600	-2.84683900	-1.06115000
H	4.41660800	-3.06864300	-2.01162500
H	5.19214700	-3.81068900	-0.60515100
H	5.85212200	-2.30231200	-1.29154200
C	1.11845000	-0.32908000	7.62233700
H	0.51410600	-1.09064300	8.11370900
C	3.32353700	2.80788800	5.62582500
H	4.11081000	2.37572500	4.99173200
C	0.45475900	-5.06480000	-1.59746200
H	0.96116100	-5.96604200	-1.94653400
C	3.09907900	0.86032100	-2.39553900
H	2.86875600	1.01947300	-3.45054900
C	-0.61840100	1.93487300	-2.98376200
H	-0.15233800	1.05575500	-2.50616200
C	-0.85491600	-1.80081900	-3.06484700
H	-1.14059400	-0.89709600	-2.50962500
C	-0.58395600	5.34681700	-1.26143300
H	-0.34345000	6.37925300	-1.51974500
C	-0.44479700	3.61491300	2.68745200
H	0.38679800	3.02010400	2.28800400
H	-0.63289000	3.26873100	3.71490300
H	-0.14257900	4.67543700	2.71743000
C	1.16966100	0.94874500	8.16907300
H	0.61655800	1.17281500	9.08221800
C	2.33150000	4.04332600	0.32320700
H	2.13622900	4.76365100	1.13142400
H	1.36378400	3.67977300	-0.05008600
H	2.83311600	4.58823900	-0.49189100
C	2.69110000	-2.78675500	0.10203400
H	2.04173900	-2.24223500	0.80519400
H	2.85518900	-3.80019800	0.49979500
H	2.13310500	-2.87113000	-0.84392500
C	0.18222400	-4.02608200	-2.48273900
H	0.46377500	-4.12545700	-3.53289900
C	-0.42873200	4.33568100	-2.20486700

H	-0.06286100	4.59320900	-3.19815900
C	0.56326300	-2.86117900	6.35094300
H	0.52374700	-3.82091800	5.81747300
H	-0.37908500	-2.32549200	6.16703300
H	0.63568900	-3.09098900	7.42490300
C	4.57251900	3.41515100	1.26986600
H	5.15624800	3.71588800	0.38582200
H	5.14703400	2.66257000	1.82713000
H	4.46221000	4.29743900	1.91828500
C	0.14992900	-3.90719000	2.62675600
H	-0.20604900	-3.82537300	3.66435000
H	0.87307500	-3.09950700	2.46112600
H	0.66032000	-4.87711500	2.51141000
C	1.90836300	1.94477900	7.54005500
H	1.92132900	2.95078100	7.96203800
C	3.99419900	3.82128800	6.55414300
H	4.58401000	4.53823100	5.96501700
H	4.66674000	3.33002000	7.27306800
H	3.25455600	4.40153900	7.12515400
C	-2.81782600	4.32442300	2.36499100
H	-2.50354700	5.37822700	2.40815600
H	-3.07086000	4.01709300	3.39004500
H	-3.73629600	4.27988700	1.76350400
C	-2.08633000	-2.26505300	-3.85202300
H	-1.86481400	-3.18533400	-4.41490300
H	-2.40830500	-1.49384200	-4.56778800
H	-2.92935100	-2.47727500	-3.17751200
C	3.06129500	-2.83274200	6.12413900
H	3.25712900	-2.90516100	7.20556400
H	3.92911900	-2.36082800	5.64486300
H	2.97551400	-3.85396600	5.72402600
C	0.29533600	-1.41749300	-3.99352100
H	1.14449900	-1.02960100	-3.41125600
H	-0.03158300	-0.63431200	-4.69383600
H	0.64135700	-2.26931400	-4.59851100
C	0.28588600	2.35692900	-4.14226600
H	-0.18839100	3.13145000	-4.76472600
H	0.48819100	1.49460500	-4.79286500
H	1.24935800	2.74895300	-3.78635500
C	-1.98986300	1.51940000	-3.53327300
H	-2.62132200	1.04435700	-2.76956600
H	-1.86577700	0.79822600	-4.35584600
H	-2.52274100	2.39698100	-3.93279200
C	2.32529300	3.50135900	4.69138700
H	1.53215800	3.99708800	5.27239700
H	1.82531400	2.77876500	4.02818500
H	2.82299000	4.25830300	4.06556300

Table S5

TI=As-Rea

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

Ge	-0.17164700	-0.00449600	0.06531900
As	-0.51744000	-0.12185100	2.55552400
Tl	1.95016700	0.07495000	2.85913300
N	-1.51039700	-1.53211900	-0.30205200
N	3.39145400	0.11706000	4.66562000
N	3.91835800	0.26301600	1.68101000
N	-1.67303800	1.34823800	-0.32545200
C	4.71398600	0.05594400	4.65062200
C	5.51483900	0.00161300	3.49258300
H	6.58294500	-0.08404100	3.67722800
C	3.66701200	0.45712500	0.29193200
C	-0.87834600	-2.75193200	-0.70740600
C	5.15560100	0.15168300	2.13771200
C	3.71203400	-0.64201300	-0.58992900
C	3.99668500	-2.04974600	-0.09143000
H	4.52732000	-1.97758900	0.86852700
C	-0.62914800	-3.80328900	0.19982800
C	-1.26808300	2.69489200	-0.61886600
C	3.27140300	1.73858900	-0.15283000
C	-2.82316400	-1.43440700	-0.20277000
C	-2.97215900	1.07822800	-0.23836600
C	-3.49983200	-0.20824300	-0.04629600
H	-4.58207000	-0.27306300	0.03807200
C	6.29764400	0.20734800	1.14405800
H	6.27235000	-0.67047200	0.48189700
H	7.26437900	0.23756800	1.65756200
H	6.19918600	1.08994800	0.49669200
C	-1.10169600	-3.79258200	1.64500800
H	-1.59338700	-2.82743000	1.83665900
C	-0.48220800	-2.85457300	-2.06052200
C	0.04285900	-4.93822500	-0.27230700
H	0.24054900	-5.76023900	0.41931800
C	-1.36589200	3.70625400	0.36521400
C	2.69791800	0.36049400	5.88326700
C	-3.69638800	-2.66493500	-0.27572500
H	-3.20792500	-3.49562400	-0.79839700
H	-4.64653800	-2.42885300	-0.76969400
H	-3.92337700	-2.99348300	0.75049100
C	3.18809700	2.91012700	0.81728100
H	2.72124700	2.53657100	1.74705700
C	5.45852400	0.09557600	5.96998700
H	5.47492700	1.12641700	6.35673400
H	6.49306000	-0.24190300	5.84206700
H	4.95917500	-0.52012500	6.72931100
C	1.96500000	-0.68466100	6.48818700
C	-0.78741500	3.00197200	-1.91629800
C	3.39419500	-0.42788600	-1.93295500
H	3.42223200	-1.26761100	-2.63002000
C	2.68702300	1.66802200	6.41907200
C	-1.71306300	3.42770600	1.81969600

H	-2.02597700	2.37723900	1.91054700
C	1.95432400	-2.08261900	5.88263800
H	1.86013700	-1.96719700	4.78881900
C	-2.10100500	-4.92781200	1.90777500
H	-1.60421300	-5.90808000	1.84168500
H	-2.92917900	-4.92944400	1.18644300
H	-2.52239700	-4.83702100	2.91999900
C	2.94974500	1.90003500	-1.50381200
H	2.62303300	2.87549600	-1.86680800
C	-3.97651700	2.18831100	-0.43909900
H	-3.89805400	2.93950600	0.35500100
H	-4.99579400	1.78887300	-0.45512900
H	-3.77537500	2.70836500	-1.38710800
C	-1.05149200	5.02290200	0.00862700
H	-1.13309800	5.80934100	0.76163200
C	4.87508000	-2.86065600	-1.04609700
H	4.34322500	-3.09606200	-1.97989700
H	5.15266200	-3.81789300	-0.58164300
H	5.79848600	-2.32242700	-1.30813300
C	1.26538800	-0.40285900	7.66602700
H	0.69155500	-1.19047600	8.15364700
C	3.34321100	2.82553000	5.67854300
H	4.14141500	2.42402400	5.03835100
C	0.45694000	-5.04323000	-1.59360200
H	0.98085600	-5.93701800	-1.93578900
C	3.02052400	0.83028600	-2.39103000
H	2.76545200	0.97460000	-3.44256300
C	-0.66111100	1.92999300	-2.99090700
H	-0.19009900	1.05272400	-2.51446300
C	-0.88138900	-1.79599100	-3.07475300
H	-1.14344400	-0.88320200	-2.52280500
C	-0.61430000	5.34149300	-1.26837000
H	-0.37110700	6.37316100	-1.52704000
C	-0.45291300	3.59675900	2.67587900
H	0.37339000	2.99925200	2.26822400
H	-0.63601600	3.24998300	3.70395500
H	-0.14118100	4.65429700	2.70617400
C	1.28053600	0.86973100	8.22762700
H	0.73028500	1.06549300	9.14896600
C	2.30490700	4.04375500	0.30511200
H	2.12287700	4.77310700	1.10836900
H	1.33181700	3.66910100	-0.04253100
H	2.78289400	4.58254800	-0.52811600
C	2.67224800	-2.77338700	0.16908300
H	2.04352800	-2.21834600	0.88276400
H	2.84020100	-3.78365100	0.57354800
H	2.09053000	-2.86390400	-0.76184100
C	0.18697700	-4.00592800	-2.48168900
H	0.48751000	-4.10023300	-3.52675800
C	-0.46588500	4.33043500	-2.21283800
H	-0.10183300	4.58708100	-3.20694400
C	0.76511200	-2.92686300	6.33580200

H	0.75151000	-3.87447900	5.77939600
H	-0.18736300	-2.40756400	6.15616600
H	0.83192200	-3.17916100	7.40507600
C	4.57364000	3.44433500	1.20100300
H	5.12944800	3.74269700	0.29830700
H	5.16875800	2.70072700	1.74791200
H	4.47332800	4.33077800	1.84551000
C	0.06548400	-3.90455600	2.62904900
H	-0.30902300	-3.83350400	3.66093000
H	0.78297800	-3.08834100	2.48036800
H	0.58980200	-4.86731400	2.51718400
C	1.97953400	1.89641500	7.60157000
H	1.96343900	2.89772500	8.03476800
C	3.97979300	3.86054800	6.60686900
H	4.53930100	4.60140500	6.01770800
H	4.67391100	3.39179500	7.32018800
H	3.22184200	4.41045400	7.18409100
C	-2.82391500	4.32735900	2.37375200
H	-2.50276400	5.37899900	2.41634900
H	-3.07129400	4.01988100	3.40012300
H	-3.74691500	4.28921300	1.77855300
C	-2.13885600	-2.25515200	-3.82333500
H	-1.94278400	-3.18749000	-4.37560500
H	-2.46827400	-1.49134800	-4.54354800
H	-2.96768500	-2.44500100	-3.12503300
C	3.26675900	-2.82899400	6.15054400
H	3.44817900	-2.90701600	7.23399800
H	4.12621900	-2.32486200	5.68953000
H	3.21672800	-3.84771100	5.73809900
C	0.24530000	-1.43493900	-4.03978600
H	1.12063600	-1.06253400	-3.48738100
H	-0.09036600	-0.64630800	-4.72965200
H	0.55499700	-2.29227400	-4.65628000
C	0.23843900	2.35189900	-4.15315300
H	-0.23888900	3.12582700	-4.77393200
H	0.43798000	1.48911000	-4.80395800
H	1.20343500	2.74394800	-3.80164900
C	-2.03352200	1.51129300	-3.53560200
H	-2.66170200	1.03378100	-2.77069400
H	-1.91054500	0.79175100	-4.35964600
H	-2.56967500	2.38808800	-3.93229200
C	2.31533500	3.48545800	4.75160200
H	1.50480400	3.94540400	5.33802200
H	1.84478800	2.74857200	4.08261600
H	2.78121800	4.26539400	4.12956200

Table S6

CH₃I

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

C	-4.13541200	0.55847200	-0.00001900
I	-1.99233200	0.55852300	0.00002600
H	-4.46813400	-0.18866800	-0.72505500
H	-4.46803700	1.55996300	-0.28453600
H	-4.46802600	0.30415000	1.00957300

Table S7

B=As-TS

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.15111900	0.21758800	0.33722300
B	-0.78456000	-0.19838100	3.86500000
I	3.66054900	-0.26639200	4.01317000
C	2.18732100	0.08483300	1.90587200
H	2.97475800	0.57295500	1.33929800
H	1.49694500	0.66738400	2.50074600
H	2.00823200	-0.98361900	1.79281300
As	-1.28901900	-0.76531100	2.02810400
N	-0.68775900	1.15730200	4.50891600
N	-0.99658400	1.10960500	-1.14422900
N	0.39779400	-1.38214700	-0.96515700
N	-0.79764000	-1.28089800	4.91416500
C	-1.56527400	3.49261800	-0.85119700
C	-0.86107000	0.88263900	-2.44993700
C	-2.29586900	2.74837300	3.54025500
C	-0.48244500	1.32870700	5.83356700
C	-0.95020700	2.38492300	3.77930000
C	-1.92934700	2.13256500	-0.77259800
C	0.86617500	-2.64613300	-0.46808800
C	0.32970200	-1.30475600	-2.28962300
C	-0.13610000	-0.18243100	-2.99226900
H	-0.10196700	-0.24279300	-4.07622300
C	-2.55065600	-2.95779900	4.58842200
C	-1.17994700	-2.64507500	4.58730700
C	-2.53855300	4.45609000	-0.56401600
H	-2.27243000	5.51415600	-0.61162900
C	2.25937500	-2.86372200	-0.39143200
C	-3.25216000	1.74190700	-0.47115600
C	-0.51160900	-1.06011600	6.20539100
C	-3.46969100	1.82245900	3.86073100
H	-3.21923800	0.84671700	3.40890700
C	-0.18060800	3.94362000	-1.29536400
H	0.33987100	3.07157800	-1.71724100
C	-0.06043000	-3.68000600	-0.22758700
C	0.69032800	-2.50017300	-3.14980100
H	-0.08587900	-3.27104200	-3.05262900
H	1.62867900	-2.97445700	-2.84614300
H	0.75475600	-2.19894900	-4.20123900
C	-3.62599100	-1.90324200	4.79118100
H	-3.14983300	-0.91708800	4.71990300

C	-1.56608600	-3.45248100	-0.25307200
H	-1.73275700	-2.36831200	-0.20875500
C	0.12721300	3.25804100	3.52986100
C	-2.52681300	4.01979900	3.00808100
H	-3.54482500	4.33297500	2.78238100
C	-1.53033900	1.79476000	-3.45584100
H	-2.55710700	2.04934800	-3.16663000
H	-1.53732700	1.32425400	-4.44478700
H	-0.97165600	2.73851600	-3.52553700
C	-0.18888700	-3.62730800	4.42560500
C	-0.28731900	0.23530300	6.66458600
H	-0.08499700	0.39698500	7.71946000
C	2.70709500	-4.16421600	-0.13957700
H	3.77924200	-4.36164800	-0.09058200
C	-3.67752800	0.28220600	-0.54215700
H	-2.78444900	-0.32663200	-0.34979500
C	-0.63527900	2.67244700	6.49235700
H	-0.24125800	3.50897900	5.91395600
H	-0.17183700	2.65190600	7.48536600
H	-1.71414600	2.85326000	6.61720300
C	-0.45878800	-2.19133600	7.18801600
H	-1.36815300	-2.80461500	7.14263800
H	-0.32048700	-1.80104700	8.20158000
H	0.38188000	-2.85303600	6.94128300
C	3.27317300	-1.74757700	-0.63116200
H	2.75401500	-0.79297900	-0.47020300
C	-0.17486700	4.53282600	3.03818300
H	0.64084400	5.23440800	2.85197700
C	0.44020800	-4.96231600	0.02146300
H	-0.25935600	-5.78239700	0.19504300
C	-4.19656000	2.74370200	-0.23343500
H	-5.23336900	2.46464800	-0.03819800
C	-2.91723600	-4.29767900	4.43226700
H	-3.97600800	-4.56437500	4.43462400
C	-4.68341500	-1.96094600	3.68862200
H	-5.28782000	-2.87912700	3.75103700
H	-4.19922700	-1.91852900	2.70304600
H	-5.37092100	-1.10431100	3.77504300
C	-2.23461600	-3.97772700	-1.53001700
H	-1.97418300	-3.37863100	-2.41349100
H	-3.32894200	-3.93602600	-1.42133000
H	-1.95569400	-5.02553500	-1.72439500
C	1.28975700	-3.29386300	4.38129600
H	1.42671000	-2.23835300	4.65753500
C	-4.25609500	-2.01660400	6.18355400
H	-5.05132500	-1.26698800	6.31176600
H	-3.51269500	-1.85785000	6.97963900
H	-4.70281400	-3.01189700	6.33143800
C	-2.22759800	-4.06382300	0.98409800
H	-2.23734800	-5.16501000	0.93935800
H	-3.27282900	-3.72482600	1.05946800
H	-1.70514900	-3.74925900	1.89757600

C	-4.19458100	-0.07704200	-1.94136900
H	-4.54679900	-1.11946300	-1.95723100
H	-3.41179100	0.01807100	-2.70672800
H	-5.03725700	0.57252800	-2.22720900
C	-3.84437200	4.09077600	-0.26078300
H	-4.59694300	4.85711500	-0.06581000
C	-4.70652600	-0.09005200	0.52163700
H	-5.67448900	0.41059800	0.35980900
H	-4.33284900	0.16146500	1.52362700
H	-4.88948900	-1.17492500	0.49415900
C	-0.60720800	-4.95254000	4.26299700
H	0.14609200	-5.73099000	4.12705100
C	-1.48274400	4.91034800	2.77342700
H	-1.69737500	5.90446300	2.37693100
C	1.80846300	-5.21114100	0.03957500
H	2.17817100	-6.22187700	0.22062400
C	-1.95572800	-5.29123600	4.27756200
H	-2.25999900	-6.33221100	4.15833000
C	1.58678000	2.90876100	3.81169300
H	1.65144400	1.84411700	4.07270600
C	-4.78422800	2.29098900	3.23722400
H	-5.54689800	1.50756500	3.35540300
H	-4.67352800	2.49938800	2.16745200
H	-5.16243200	3.19844300	3.73430100
C	2.47082500	3.14041500	2.58045000
H	2.58137700	4.21550300	2.36679100
H	2.06668700	2.65695000	1.68304100
H	3.47008300	2.72332200	2.77476500
C	3.81504200	-1.72086100	-2.06835700
H	4.66058300	-1.02001700	-2.13088000
H	3.06188000	-1.38906000	-2.79495900
H	4.17846300	-2.71621000	-2.37014000
C	0.64186000	4.42182400	-0.10306700
H	1.67908700	4.64098100	-0.39979900
H	0.65236700	3.65869700	0.68230000
H	0.20149200	5.33544700	0.32640200
C	-0.23300200	5.04001500	-2.36595400
H	-0.58978700	5.99028300	-1.94159100
H	-0.89911800	4.78272200	-3.20179100
H	0.77411700	5.22213400	-2.76866300
C	-3.71990700	1.61364100	5.36226900
H	-3.88554900	2.57928800	5.86651000
H	-2.91517000	1.07595900	5.88073300
H	-4.63318600	1.01376900	5.49328500
C	4.44533500	-1.82168400	0.35275200
H	5.11530200	-2.66232000	0.11515100
H	4.11313800	-1.93185400	1.39445600
H	5.04667600	-0.90222500	0.29277400
C	1.79530800	-3.45801500	2.94842500
H	1.78662100	-4.51958100	2.65996100
H	2.82674300	-3.08401000	2.86541300
H	1.14869800	-2.91412300	2.24367100

C	2.14715800	-4.14521700	5.32262400
H	1.80117600	-4.12442900	6.36649800
H	3.18069500	-3.77003200	5.30118800
H	2.16633200	-5.19771600	5.00110800
C	2.20365200	3.68473800	4.98593500
H	3.28209500	3.47417100	5.01991100
H	1.79274200	3.39540200	5.96027100
H	2.06936800	4.77089900	4.85893200

Table S8

Al=As-TS

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.36374300	0.02040000	-0.19597600
Al	-0.17163600	0.11913000	3.72033000
I	2.70304000	0.51318700	4.07764400
C	2.37934200	0.55361700	1.62728100
H	3.38067000	0.73826100	1.23399700
H	1.66528300	1.37043700	1.63066500
H	2.01476400	-0.46434500	1.64865000
As	-1.17334600	-0.18529200	1.64444600
N	-0.62688200	1.59797700	4.88677200
N	-0.84918100	0.92216900	-1.54122000
N	0.23640200	-1.68472400	-1.37788600
N	-0.36532700	-1.24244800	5.04005300
C	-1.40621300	3.21126000	-0.82689600
C	-0.66918500	0.74971900	-2.84992300
C	-2.38897700	2.88821400	3.77615500
C	-0.46436800	1.50268000	6.20215400
C	-1.07490600	2.83507700	4.29450300
C	-1.80814600	1.89594300	-1.11746300
C	0.52980100	-2.95567800	-0.78463100
C	0.19674200	-1.58958700	-2.69712700
C	-0.05834100	-0.38559700	-3.39185800
H	0.03024000	-0.42368400	-4.47481100
C	-2.13345000	-2.90856200	4.74759700
C	-0.76430800	-2.58176500	4.68752900
C	-2.38357800	4.14284800	-0.46376200
H	-2.08523900	5.16600000	-0.22451700
C	1.84704300	-3.46561900	-0.82159700
C	-3.15957500	1.50331900	-1.02257000
C	-0.13684000	-0.98510800	6.33317300
C	-3.36069700	1.73248100	3.95492300
H	-2.80003300	0.79533500	3.82269900
C	0.05696200	3.61331500	-0.85281400
H	0.62223900	2.79449700	-1.32307500
C	-0.52004100	-3.69033500	-0.19325000
C	0.43122700	-2.81249900	-3.55314900
H	-0.03755400	-3.70421200	-3.11849300
H	1.50959300	-3.01491800	-3.62200500

H	0.04421900	-2.64878100	-4.56471600
C	-3.20345000	-1.88676600	5.09892700
H	-2.71460900	-0.91034500	5.23427400
C	-1.94730600	-3.17438300	-0.22468100
H	-1.88960700	-2.07993500	-0.18090100
C	-0.21946900	3.95399000	4.21933200
C	-2.81278200	4.06754500	3.16062700
H	-3.81371800	4.11925300	2.73439500
C	-1.16771600	1.80677400	-3.80491700
H	-2.25155600	1.95380900	-3.70720600
H	-0.92873300	1.54069400	-4.84026300
H	-0.70021600	2.77116700	-3.55647100
C	0.19807700	-3.54651800	4.33310000
C	-0.07672100	0.31157100	6.85455900
H	0.10802300	0.39419300	7.92354900
C	2.07876100	-4.73996100	-0.29164500
H	3.08873100	-5.15406000	-0.32201000
C	-3.59496200	0.07204300	-1.30324500
H	-2.69022500	-0.55290500	-1.27912600
C	-0.70314600	2.68531300	7.10856800
H	-1.32134800	3.45802000	6.63831000
H	0.26605800	3.13287600	7.37586200
H	-1.17977500	2.34782800	8.03703300
C	0.02016000	-2.13529300	7.29392800
H	-0.90197600	-2.73184100	7.33597300
H	0.26468400	-1.77450200	8.29842300
H	0.81282200	-2.81151200	6.94216400
C	3.02598300	-2.68865700	-1.39325200
H	2.63822500	-1.80876400	-1.92821700
C	-0.70526300	5.12169600	3.61793400
H	-0.05380300	5.99629100	3.55836300
C	-0.23013800	-4.94541500	0.34960500
H	-1.02887600	-5.52063000	0.81904700
C	-4.10535800	2.47382500	-0.68253700
H	-5.15947200	2.19569500	-0.61988000
C	-2.51609300	-4.22486400	4.47058800
H	-3.57344200	-4.49448200	4.52070600
C	-4.21124600	-1.74573900	3.95465700
H	-4.71611300	-2.70247200	3.74924400
H	-3.70801000	-1.41694600	3.03147600
H	-4.98700200	-1.01101400	4.21773200
C	-2.63858800	-3.55884100	-1.53770500
H	-2.14409700	-3.09918400	-2.40706900
H	-3.68481300	-3.21592700	-1.53223900
H	-2.63939500	-4.65149200	-1.67854800
C	1.67070800	-3.19595300	4.24722500
H	1.81916500	-2.25051300	4.78671500
C	-3.90623100	-2.23493500	6.41516600
H	-4.65419200	-1.46783700	6.66604900
H	-3.19353300	-2.29839100	7.25041500
H	-4.42728400	-3.20184200	6.34119400
C	-2.75867600	-3.61101200	0.99059400

H	-2.97902600	-4.69088200	0.98326500
H	-3.72062700	-3.07734300	1.00675100
H	-2.21866600	-3.36316500	1.91629600
C	-4.21600300	-0.06525300	-2.69856300
H	-4.55120200	-1.09969300	-2.86792300
H	-3.49649900	0.18449200	-3.49128800
H	-5.08883200	0.59825500	-2.80520400
C	-3.72573000	3.78472500	-0.40544300
H	-4.47970900	4.52647900	-0.13509000
C	-4.54709400	-0.45975600	-0.23032000
H	-5.49697200	0.09708300	-0.21159400
H	-4.07940600	-0.39786300	0.76328500
H	-4.79162100	-1.51325600	-0.43480100
C	-0.23413300	-4.84156900	4.03291600
H	0.50103900	-5.59367300	3.74022700
C	-1.98302800	5.18165400	3.08308200
H	-2.33761300	6.09635100	2.60465200
C	1.05409000	-5.47804200	0.28781700
H	1.25761700	-6.46730300	0.70187800
C	-1.57918700	-5.18706700	4.11203300
H	-1.89840000	-6.20624500	3.88758300
C	1.20498800	3.97409800	4.75325800
H	1.40534100	3.01858500	5.25819300
C	-4.46314800	1.72180200	2.90012300
H	-5.03961700	0.78903600	2.96554200
H	-4.02603800	1.78630200	1.89305600
H	-5.17054700	2.55473900	3.03749100
C	2.21245000	4.10211800	3.60656900
H	2.07826400	5.05818000	3.07616300
H	2.08884300	3.29166100	2.87748400
H	3.24256800	4.05935800	3.99115600
C	3.86438500	-3.52066800	-2.37173400
H	4.60734300	-2.88231000	-2.87170800
H	3.25107500	-4.00672900	-3.14363300
H	4.41738300	-4.31257700	-1.84503300
C	0.57269400	3.77315700	0.58094100
H	1.67004200	3.86274100	0.59504000
H	0.26214200	2.92084100	1.20921100
H	0.14759300	4.67603900	1.04712600
C	0.31370400	4.88533500	-1.66473000
H	-0.18067300	5.75642200	-1.20912200
H	-0.05486900	4.79349700	-2.69701500
H	1.39158700	5.10129500	-1.70347900
C	-3.94240000	1.73720500	5.37382300
H	-4.48766200	2.67466200	5.56465900
H	-3.15675100	1.63786600	6.13829200
H	-4.64533800	0.90003100	5.50491500
C	3.92276600	-2.17328800	-0.26309400
H	4.33962200	-3.01334600	0.31453300
H	3.35429500	-1.53841500	0.42600100
H	4.75920100	-1.58381800	-0.66839400
C	2.06312700	-2.96537700	2.78489700

H	2.04437000	-3.91526900	2.23050400
H	3.07507300	-2.53655000	2.71470500
H	1.34121100	-2.29716300	2.28527800
C	2.58001000	-4.24235300	4.89424500
H	2.28670500	-4.45365500	5.93368500
H	3.61950800	-3.88314400	4.89697700
H	2.56294500	-5.19234800	4.33942300
C	1.42419100	5.11204100	5.75899700
H	2.41269300	5.01632300	6.23210300
H	0.66009000	5.12270900	6.54824200
H	1.39356600	6.09122500	5.25805100

Table S9

Ga=As-TS

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.33889100	0.01618300	-0.19850800
Ga	-0.22483600	0.10704300	3.66982200
I	2.78875900	0.51532300	4.05019000
C	2.31964000	0.53773100	1.60352200
H	3.29840100	0.72246200	1.15922100
H	1.60973200	1.35622300	1.65602200
H	1.96449800	-0.48169200	1.66794000
As	-1.26246700	-0.19355100	1.59099700
N	-0.62375800	1.62651900	4.90641300
N	-0.85325900	0.92258000	-1.55585200
N	0.23296700	-1.68446100	-1.38300200
N	-0.37715000	-1.26638900	5.06658800
C	-1.42058700	3.20876800	-0.83873600
C	-0.66036000	0.75141200	-2.86313300
C	-2.38121500	2.91663000	3.79837600
C	-0.43663700	1.51345000	6.21422500
C	-1.06739400	2.86219100	4.31900600
C	-1.81784200	1.89436500	-1.13792700
C	0.52927300	-2.95547700	-0.78896700
C	0.20355600	-1.58834200	-2.70274500
C	-0.04591400	-0.38422400	-3.39950500
H	0.05287300	-0.42219400	-4.48157900
C	-2.14669900	-2.92681700	4.76881300
C	-0.77615700	-2.60262400	4.71943700
C	-2.40148700	4.13425200	-0.46891100
H	-2.10670200	5.15638900	-0.22110700
C	1.85080500	-3.45545200	-0.81668200
C	-3.16829700	1.49640000	-1.04732400
C	-0.12911300	-0.98739500	6.34839200
C	-3.35582500	1.76302400	3.97937900
H	-2.79977800	0.82219800	3.85321600
C	0.04122600	3.61583500	-0.85712400
H	0.61159700	2.80017000	-1.32683000
C	-0.51978800	-3.70115400	-0.21007700

C	0.44747500	-2.80992800	-3.55766400
H	-0.01431600	-3.70540700	-3.12356400
H	1.52763100	-3.00302900	-3.62546100
H	0.06051900	-2.64915400	-4.56972400
C	-3.21448800	-1.90438400	5.12575800
H	-2.72243900	-0.93062600	5.27058200
C	-1.95265800	-3.20172300	-0.25247200
H	-1.90798400	-2.10656800	-0.22637500
C	-0.20643900	3.97653400	4.23405100
C	-2.80249300	4.09577700	3.18039600
H	-3.80390100	4.14936900	2.75521400
C	-1.14817200	1.81067700	-3.82082300
H	-2.23228800	1.96078700	-3.73113100
H	-0.90195800	1.54506200	-4.85458100
H	-0.67946000	2.77322400	-3.56751000
C	0.18575700	-3.56355400	4.35307600
C	-0.05436700	0.31424400	6.85674000
H	0.14873000	0.39872700	7.92232300
C	2.08765100	-4.73019100	-0.29034700
H	3.10103700	-5.13626300	-0.31382900
C	-3.59690100	0.06448200	-1.33525400
H	-2.69222900	-0.55965100	-1.29022800
C	-0.64404100	2.69317600	7.13407400
H	-1.23787100	3.48906400	6.67120500
H	0.33702300	3.10809000	7.41060500
H	-1.13459000	2.35904600	8.05664200
C	0.03417500	-2.12862000	7.32022900
H	-0.89100100	-2.71929300	7.37869200
H	0.29181300	-1.75944400	8.31835300
H	0.81951000	-2.81242000	6.96673800
C	3.02927000	-2.66832500	-1.37534900
H	2.64040900	-1.78557100	-1.90489100
C	-0.69012300	5.14439000	3.63178100
H	-0.03535200	6.01620700	3.56703900
C	-0.22467400	-4.95634300	0.33009900
H	-1.02336000	-5.53995100	0.78927600
C	-4.11733000	2.46035400	-0.69884400
H	-5.17007700	2.17771600	-0.63587500
C	-2.53034600	-4.23934900	4.47553400
H	-3.58833800	-4.50798300	4.51762100
C	-4.22152500	-1.74990200	3.98230300
H	-4.73733400	-2.70054000	3.77563000
H	-3.71731000	-1.42497900	3.05820000
H	-4.98884800	-1.00700600	4.24774000
C	-2.63532800	-3.61133100	-1.56237100
H	-2.14142200	-3.15873400	-2.43580500
H	-3.68512300	-3.27934700	-1.56544600
H	-2.62432400	-4.70567100	-1.68835200
C	1.65534600	-3.20410200	4.25582300
H	1.80487600	-2.25711300	4.79263000
C	-3.91953800	-2.26136300	6.43842300
H	-4.66471600	-1.49383700	6.69612700

H	-3.20699300	-2.33560600	7.27281800
H	-4.44389800	-3.22573000	6.35502000
C	-2.76301700	-3.63120900	0.96675400
H	-2.97681200	-4.71230600	0.96851800
H	-3.72838600	-3.10328000	0.97659700
H	-2.22645400	-3.37222700	1.89158900
C	-4.18406600	-0.07683700	-2.74492700
H	-4.51950600	-1.11059400	-2.91772300
H	-3.44469700	0.16615200	-3.52116000
H	-5.05116200	0.58990900	-2.87510400
C	-3.74199300	3.77055400	-0.41188300
H	-4.49830300	4.50707900	-0.13402800
C	-4.57537600	-0.46818400	-0.28644000
H	-5.53554200	0.07026600	-0.31101900
H	-4.14708600	-0.38328100	0.72323600
H	-4.79273600	-1.52918000	-0.48268600
C	-0.24673200	-4.85536800	4.04017100
H	0.48800400	-5.60510100	3.74006600
C	-1.96978500	5.20761400	3.10074400
H	-2.32270600	6.12285800	2.62210800
C	1.06385500	-5.47884200	0.27706900
H	1.27150600	-6.46826500	0.68857400
C	-1.59284300	-5.19937700	4.11186400
H	-1.91282100	-6.21572800	3.87588400
C	1.22281500	3.98488400	4.75492300
H	1.42278600	3.02446100	5.25084100
C	-4.45796300	1.74911500	2.92387300
H	-5.03375900	0.81590100	2.99251400
H	-4.02138900	1.81113500	1.91612100
H	-5.16582200	2.58192600	3.05922800
C	2.21937500	4.11174800	3.59867300
H	2.08408200	5.06905500	3.07062000
H	2.08680900	3.30108200	2.87121900
H	3.25269800	4.06325800	3.97343300
C	3.87683200	-3.48813800	-2.35635000
H	4.62054700	-2.84234200	-2.84549100
H	3.27084700	-3.96967300	-3.13673000
H	4.42946600	-4.28259400	-1.83318200
C	0.54942900	3.77454200	0.57943500
H	1.64623400	3.86717400	0.59987700
H	0.23873900	2.92012000	1.20442300
H	0.11904500	4.67457800	1.04605100
C	0.29667300	4.89077100	-1.66489600
H	-0.20439200	5.75833100	-1.20993600
H	-0.06585500	4.79969200	-2.69938900
H	1.37370100	5.11185900	-1.69706000
C	-3.93646100	1.77182200	5.39865700
H	-4.48585200	2.70767700	5.58504700
H	-3.14825700	1.68107000	6.16151600
H	-4.63503700	0.93170100	5.53482700
C	3.91844500	-2.16027800	-0.23576500
H	4.34256800	-3.00450400	0.33029600

H	3.34355000	-1.54228800	0.46311600
H	4.75017400	-1.55716800	-0.63041600
C	2.02955300	-2.97060400	2.78913400
H	2.01241900	-3.92035100	2.23457500
H	3.03604600	-2.53167600	2.70817100
H	1.29629400	-2.30922200	2.29643000
C	2.57711200	-4.24604100	4.89175600
H	2.29841900	-4.45604600	5.93541200
H	3.61507900	-3.88271300	4.88010500
H	2.55571900	-5.19723500	4.33894000
C	1.45819000	5.11587400	5.76452400
H	2.45288700	5.01498400	6.22330500
H	0.70534200	5.12247200	6.56453500
H	1.42261400	6.09827100	5.26998600

Table S10

In=As-TS

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.29499100	-0.03145100	-0.31962500
In	-0.14659900	0.12875300	3.57616600
I	2.92915200	0.57614400	3.87857200
C	2.37592600	0.49052100	1.46235200
H	3.34178700	0.62511000	0.97352500
H	1.69225400	1.33333600	1.47689000
H	1.98400000	-0.51587300	1.54682300
As	-1.35430400	-0.26245700	1.42085300
N	-0.62084100	1.72265900	5.03904800
N	-0.85155600	0.91880500	-1.67414200
N	0.15093300	-1.72450900	-1.49681300
N	-0.35488500	-1.28889800	5.22177900
C	-1.41104100	3.17985000	-0.87045000
C	-0.64500100	0.74728300	-2.98017600
C	-2.36495600	2.98254100	3.89124100
C	-0.44706000	1.57143700	6.34088800
C	-1.06527500	2.94984700	4.45332500
C	-1.81362600	1.88669300	-1.24444000
C	0.44157300	-2.97523300	-0.85845700
C	0.15670400	-1.61868200	-2.81272100
C	-0.04575400	-0.39922800	-3.50658000
H	0.07924000	-0.43732000	-4.58695400
C	-2.08554200	-2.97336700	4.85804700
C	-0.71756000	-2.62663800	4.87147100
C	-2.38968000	4.09107600	-0.45954600
H	-2.08982100	5.09567600	-0.15262700
C	1.77363600	-3.44227900	-0.81889200
C	-3.16780700	1.49278700	-1.17798000
C	-0.14637100	-0.95895800	6.49276300
C	-3.31910600	1.80623300	4.03915400
H	-2.73852100	0.87634600	3.93207700

C	0.05225700	3.58202900	-0.84351800
H	0.63327300	2.77088100	-1.30848100
C	-0.60595800	-3.71056900	-0.26354500
C	0.37124800	-2.82333400	-3.70006900
H	0.44422900	-3.76398100	-3.14480400
H	1.29502900	-2.67422900	-4.27892400
H	-0.45481000	-2.89013600	-4.42135400
C	-3.17882400	-1.97453700	5.20767100
H	-2.70263700	-1.00187600	5.40615900
C	-2.04847400	-3.25311700	-0.37414800
H	-2.03306200	-2.15671300	-0.39816200
C	-0.20919000	4.06769100	4.35710000
C	-2.78484800	4.15020500	3.25077200
H	-3.77561000	4.18658100	2.79900600
C	-1.09010000	1.82713200	-3.93502300
H	-2.16995500	2.00940500	-3.85399800
H	-0.84221900	1.56341800	-4.96898200
H	-0.59422900	2.77242000	-3.66802800
C	0.26671400	-3.55578400	4.47872700
C	-0.08669500	0.35784500	6.97739500
H	0.09618100	0.44654100	8.04666700
C	2.02641600	-4.67630100	-0.20897200
H	3.04972900	-5.05782800	-0.18428800
C	-3.59697200	0.07202400	-1.51548000
H	-2.69652400	-0.55757400	-1.45786100
C	-0.64860700	2.74056000	7.28033500
H	-1.21577400	3.55635100	6.81776200
H	0.33517600	3.13039400	7.58343800
H	-1.16571000	2.40465400	8.18771800
C	-0.00987400	-2.07349600	7.50299400
H	-0.94219700	-2.65382700	7.55584300
H	0.22852500	-1.68286100	8.49775700
H	0.77516400	-2.77419400	7.18368300
C	2.94490800	-2.67800300	-1.42042500
H	2.56262100	-1.75216300	-1.87525500
C	-0.69021400	5.22388200	3.73108900
H	-0.03966400	6.09872400	3.66189500
C	-0.29625800	-4.92184800	0.36062500
H	-1.09277900	-5.49562400	0.83519700
C	-4.11350200	2.44176000	-0.78433100
H	-5.16710500	2.16045500	-0.73432500
C	-2.43993100	-4.27546700	4.49204000
H	-3.49500000	-4.55885600	4.48397200
C	-4.14346600	-1.78832100	4.03190700
H	-4.65373100	-2.73201200	3.78328800
H	-3.61060800	-1.44345100	3.13118900
H	-4.91868600	-1.04994000	4.28787900
C	-2.66543500	-3.73936500	-1.69033600
H	-2.10839400	-3.35846100	-2.55964400
H	-3.70719900	-3.39367100	-1.77848800
H	-2.66462200	-4.83959400	-1.74092300
C	1.73079300	-3.16643500	4.39471100

H	1.84617400	-2.18412600	4.87434900
C	-3.93445700	-2.38501900	6.47578600
H	-4.69542700	-1.63236300	6.73132100
H	-3.25685300	-2.48811600	7.33556600
H	-4.44777100	-3.34855000	6.33351800
C	-2.89491100	-3.65886500	0.83026600
H	-3.09177900	-4.74280700	0.85167000
H	-3.86855000	-3.14798200	0.79156900
H	-2.39593900	-3.36900500	1.76756800
C	-4.14171400	-0.03764900	-2.94479300
H	-4.47987900	-1.06540800	-3.14639100
H	-3.37784900	0.21325400	-3.69400100
H	-4.99944600	0.63849500	-3.08774800
C	-3.73231600	3.73383800	-0.42948100
H	-4.48551100	4.45884200	-0.11538400
C	-4.61054500	-0.48053400	-0.51090900
H	-5.57968100	0.03704200	-0.58204100
H	-4.23386900	-0.38625300	0.51870100
H	-4.79549000	-1.54601100	-0.71611600
C	-0.13553500	-4.84013600	4.10160300
H	0.61930500	-5.56302900	3.78390200
C	-1.96241900	5.27085800	3.17893300
H	-2.31444700	6.17773800	2.68406100
C	1.00565500	-5.41293700	0.37752300
H	1.22441800	-6.36881600	0.85713300
C	-1.47713500	-5.20700100	4.11812100
H	-1.77451100	-6.21607900	3.82750000
C	1.22215900	4.07154400	4.87158900
H	1.42349900	3.10347400	5.35378800
C	-4.39160100	1.76602600	2.95333900
H	-4.94773200	0.81994500	3.01213300
H	-3.93376600	1.83272200	1.95474300
H	-5.12093900	2.58312400	3.06914200
C	2.20735800	4.21404100	3.70657300
H	2.07929200	5.18570100	3.20368000
H	2.05363100	3.42330700	2.96031800
H	3.24515700	4.14314000	4.06517400
C	3.65935700	-3.49130000	-2.50692300
H	4.44258900	-2.88545300	-2.98611100
H	2.96567400	-3.83790000	-3.28450800
H	4.14502800	-4.37954700	-2.07520300
C	0.52383900	3.72551700	0.60789600
H	1.61736300	3.84551800	0.65468400
H	0.22136900	2.84991800	1.20669700
H	0.06203700	4.60397500	1.08599500
C	0.32757200	4.86612000	-1.63054700
H	-0.19203000	5.72618500	-1.18207900
H	-0.00447200	4.78291800	-2.67575700
H	1.40405000	5.09233900	-1.62902900
C	-3.93781000	1.79160500	5.44231000
H	-4.52325000	2.70823100	5.61356800
H	-3.16642500	1.72718300	6.22442300

H	-4.61060600	0.92777600	5.55885400
C	3.94501000	-2.27380700	-0.33216700
H	4.40690800	-3.16150700	0.12733900
H	3.45076100	-1.70566800	0.46545900
H	4.74961200	-1.65377700	-0.75543100
C	2.14361800	-3.02809600	2.92434900
H	2.16823600	-4.01514700	2.43913300
H	3.14157200	-2.57068900	2.83787600
H	1.41273200	-2.42499100	2.35602500
C	2.65314200	-4.14584300	5.12403300
H	2.36546500	-4.26643500	6.17889200
H	3.69092700	-3.78287000	5.09094300
H	2.63473300	-5.14108000	4.65471400
C	1.46246200	5.18734000	5.89577300
H	2.47033700	5.09931300	6.32769600
H	0.73037500	5.16143600	6.71428900
H	1.39262200	6.17729300	5.42002600

Table S11

Tl=As-TS

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.25243300	-0.05504500	-0.35528900
Tl	-0.19765500	0.12519200	3.49505100
I	3.07657900	0.54730100	3.73863000
C	2.28399500	0.43138000	1.35719600
H	3.20639700	0.55111700	0.78958500
H	1.62903000	1.28955700	1.45926500
H	1.90766700	-0.57014300	1.52712200
As	-1.44313100	-0.37018500	1.34097400
N	-0.60856900	1.75159100	5.08751700
N	-0.87469800	0.90374100	-1.70711500
N	0.15524300	-1.72985700	-1.53543800
N	-0.39402000	-1.28393700	5.28385500
C	-1.44527000	3.15147600	-0.87249500
C	-0.65443800	0.74273300	-3.01276000
C	-2.33183200	3.02184100	3.93110400
C	-0.41702000	1.59394200	6.38427600
C	-1.03224600	2.97639000	4.49745100
C	-1.84261100	1.86491900	-1.27192000
C	0.45677900	-2.97981700	-0.89589300
C	0.16562200	-1.61830400	-2.85160100
C	-0.04327400	-0.39693000	-3.54040200
H	0.09046400	-0.42815100	-4.61988100
C	-2.12200700	-2.96176700	4.90350000
C	-0.75279000	-2.61334700	4.92503100
C	-2.42917200	4.05061900	-0.44647700
H	-2.13412900	5.04969700	-0.11798800
C	1.79995800	-3.40872200	-0.81865100
C	-3.19499700	1.46306300	-1.21355600

C	-0.16273600	-0.94553100	6.54362900
C	-3.29919600	1.85650900	4.08584000
H	-2.72935500	0.91830500	3.99331500
C	0.01627100	3.55810700	-0.82885800
H	0.60407100	2.75663000	-1.30221700
C	-0.58740600	-3.74639600	-0.33587600
C	0.38443100	-2.81902200	-3.74231900
H	0.52059200	-3.75285200	-3.18760400
H	1.26877000	-2.63682600	-4.37027900
H	-0.47488500	-2.92217900	-4.41967900
C	-3.21199500	-1.96547800	5.26979600
H	-2.73045800	-0.99767100	5.47826600
C	-2.03929500	-3.32415100	-0.46691900
H	-2.04928300	-2.22752000	-0.50412400
C	-0.16297500	4.08431600	4.38724600
C	-2.73986600	4.19039700	3.28440700
H	-3.73117600	4.23547800	2.83407400
C	-1.09435900	1.82914600	-3.96159600
H	-2.17354100	2.01518100	-3.88072300
H	-0.84550900	1.57137900	-4.99674400
H	-0.59471500	2.77043500	-3.68722800
C	0.22839800	-3.53470900	4.50337600
C	-0.08301800	0.37432000	7.02115800
H	0.11410100	0.46399100	8.08793700
C	2.06739800	-4.64278000	-0.21553800
H	3.09942900	-4.99672200	-0.16325500
C	-3.61308300	0.04290500	-1.56726400
H	-2.71276200	-0.58545600	-1.48760100
C	-0.57288500	2.77159200	7.32514900
H	-1.12628400	3.60087800	6.86939500
H	0.42476500	3.13733900	7.61229500
H	-1.08511200	2.45183400	8.24117000
C	-0.02381100	-2.05537000	7.56122300
H	-0.95916300	-2.62997400	7.62491400
H	0.22533600	-1.66151700	8.55219200
H	0.75490300	-2.76189700	7.23971500
C	2.96801200	-2.60586400	-1.37500000
H	2.58031400	-1.65827500	-1.77795700
C	-0.63283400	5.24271400	3.75716300
H	0.02813700	6.10924800	3.68122500
C	-0.26325600	-4.95638400	0.28367100
H	-1.05691500	-5.55560700	0.73075800
C	-4.14553000	2.39966700	-0.80372200
H	-5.19744100	2.11230200	-0.75664900
C	-2.47808300	-4.25555300	4.51190900
H	-3.53343400	-4.53830500	4.50089300
C	-4.18071200	-1.76198200	4.10020000
H	-4.70429500	-2.69789100	3.84988100
H	-3.64938100	-1.42150500	3.19699400
H	-4.94516300	-1.01420300	4.36166900
C	-2.63311500	-3.83260900	-1.78529600
H	-2.07737700	-3.44517400	-2.65206600

H	-3.68218400	-3.51328100	-1.88442900
H	-2.60532900	-4.93267600	-1.82760700
C	1.69125800	-3.14316500	4.40941300
H	1.80269200	-2.13991500	4.84471000
C	-3.96499200	-2.38912000	6.53492300
H	-4.72334300	-1.63786700	6.80237800
H	-3.28409200	-2.50400200	7.39041300
H	-4.48049000	-3.35008900	6.38279400
C	-2.89034200	-3.74361400	0.73095500
H	-3.07156900	-4.83007100	0.74462700
H	-3.87165700	-3.24807000	0.68458700
H	-2.40559500	-3.45287600	1.67538800
C	-4.11500100	-0.06751600	-3.01220200
H	-4.45156200	-1.09413800	-3.22171900
H	-3.32856300	0.17864800	-3.73903400
H	-4.96524100	0.61208000	-3.18044200
C	-3.76997000	3.68702600	-0.42551600
H	-4.52641900	4.40207800	-0.09717600
C	-4.65560500	-0.51552500	-0.59581500
H	-5.63008000	-0.01752700	-0.71467700
H	-4.32892400	-0.39846900	0.44856000
H	-4.81238000	-1.58703500	-0.79221300
C	-0.17528200	-4.81199500	4.10356800
H	0.57897500	-5.52769300	3.76761700
C	-1.90627100	5.30279900	3.20818200
H	-2.24956400	6.21224300	2.71175700
C	1.04985600	-5.41357000	0.33121100
H	1.28021100	-6.36860200	0.80678300
C	-1.51631100	-5.18081400	4.11847200
H	-1.81438400	-6.18440300	3.81005800
C	1.27364800	4.06786300	4.88615400
H	1.46625800	3.09666300	5.36576400
C	-4.37249500	1.81716300	3.00032400
H	-4.94000500	0.87845100	3.07072200
H	-3.91728400	1.86820700	1.99942800
H	-5.09226300	2.64373300	3.10790000
C	2.24559400	4.19397500	3.70819900
H	2.12284200	5.16502400	3.20241100
H	2.07485100	3.39886700	2.97034400
H	3.28677900	4.11065500	4.05353600
C	3.68373300	-3.35511200	-2.50599800
H	4.48081300	-2.73041500	-2.93547800
H	2.99590200	-3.64023100	-3.31270200
H	4.15060200	-4.27659100	-2.12608400
C	0.47651800	3.68341300	0.62811400
H	1.56901300	3.80508100	0.68571600
H	0.17385100	2.80042700	1.21564200
H	0.00887600	4.55334500	1.11533900
C	0.29171500	4.85457500	-1.59532700
H	-0.23644000	5.70522400	-1.13916600
H	-0.03068500	4.78431100	-2.64450000
H	1.36682000	5.08624200	-1.58071100

C	-3.91846400	1.85918300	5.48889500
H	-4.49855800	2.78103300	5.64999100
H	-3.14584800	1.79892000	6.26980500
H	-4.59561600	0.99998200	5.61468100
C	3.97189300	-2.26099600	-0.26909500
H	4.46856400	-3.16752900	0.10975000
H	3.47975400	-1.77617200	0.58320000
H	4.75275300	-1.58704600	-0.65231500
C	2.11477300	-3.06902300	2.93778100
H	2.14926000	-4.07571100	2.49498100
H	3.11071600	-2.61000200	2.84187600
H	1.38722400	-2.49272000	2.33806800
C	2.61147000	-4.08955200	5.18438000
H	2.32614600	-4.15690800	6.24438200
H	3.65090100	-3.73354500	5.13160200
H	2.58451800	-5.10670500	4.76436300
C	1.54293400	5.18192700	5.90489300
H	2.55494400	5.08002200	6.32384900
H	0.82144000	5.16816600	6.73299300
H	1.48154300	6.17188700	5.42763400

Table S12

B=As-Prod

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.12949600	0.06539800	0.23256100
B	-0.28442400	-0.07812300	3.87808300
I	2.17363500	0.05590300	3.63346100
C	1.85730900	0.95368000	-0.02417500
H	1.84560700	1.94553800	0.44343900
H	2.04301500	1.05460200	-1.10503900
H	2.65828500	0.36991100	0.44297600
As	-1.24447100	-0.40065300	2.04498300
N	-0.61591100	1.24493500	4.67067700
N	-0.94810900	1.00358000	-1.17212900
N	0.43676000	-1.48999500	-1.03769800
N	-0.49100200	-1.27936900	4.85361000
C	-1.60728100	3.33038300	-0.69620200
C	-0.69741100	0.87370700	-2.47635200
C	-2.34995000	2.70705300	3.68569000
C	-0.45314000	1.28069200	5.99543400
C	-0.99640300	2.50478500	4.04677700
C	-1.94832900	1.96902100	-0.80047600
C	0.77414100	-2.80106500	-0.54245700
C	0.45945700	-1.33614800	-2.35703800
C	0.07151600	-0.15860600	-3.02051000
H	0.19955700	-0.14922900	-4.09918800
C	-2.34987200	-2.84990500	4.54902800
C	-0.96356400	-2.60201400	4.47693100
C	-2.62399600	4.24813200	-0.41404600

H	-2.37613800	5.30704900	-0.31666000
C	2.12079100	-3.22585900	-0.53127300
C	-3.27842600	1.52945800	-0.65553600
C	-0.24375700	-1.12989500	6.16334100
C	-3.42844400	1.66939500	3.95728900
H	-3.01723700	0.69318600	3.67122800
C	-0.18084900	3.81875300	-0.88451100
H	0.40092800	2.99828800	-1.32944100
C	-0.27359600	-3.67430300	-0.19429700
C	0.88785800	-2.48015200	-3.24540500
H	1.96321600	-2.66801700	-3.13078800
H	0.67733800	-2.24634000	-4.29396200
H	0.37401300	-3.40921400	-2.96532900
C	-3.35163700	-1.77237100	4.92346000
H	-2.82486000	-0.80973500	4.92519300
C	-1.72217600	-3.22542400	-0.25177500
H	-1.72137200	-2.13871600	-0.11474400
C	-0.06869000	3.56987600	3.98124800
C	-2.72476300	3.95094300	3.17220600
H	-3.75497000	4.11337600	2.85996900
C	-1.28796300	1.86151500	-3.45396100
H	-2.37077700	1.96923300	-3.31048700
H	-1.08520700	1.54822700	-4.48329400
H	-0.84826600	2.85471200	-3.28922400
C	-0.05786800	-3.65671100	4.25547100
C	-0.10062200	0.13534100	6.71611500
H	0.07726800	0.22634400	7.78425800
C	2.38447200	-4.56372500	-0.22496400
H	3.41740400	-4.91681400	-0.22329100
C	-3.65361600	0.06900500	-0.85144300
H	-2.74935600	-0.52627700	-0.66748500
C	-0.67846700	2.52788700	6.80863100
H	0.28581200	3.03350700	6.95680800
H	-1.06225600	2.24757000	7.79692700
H	-1.36736300	3.23463800	6.33465800
C	-0.16676600	-2.31800100	7.08192400
H	-1.06346700	-2.94707400	7.01135500
H	-0.03448000	-1.98285200	8.11613300
H	0.68723900	-2.94760000	6.79850000
C	3.28524200	-2.28901100	-0.82144700
H	2.88032400	-1.36976600	-1.27103900
C	-0.51467600	4.80821400	3.50129700
H	0.19529700	5.63599700	3.45008400
C	0.04444600	-4.99706900	0.13092300
H	-0.75642600	-5.68694000	0.40078400
C	-4.26480800	2.48667100	-0.40444500
H	-5.30456800	2.17009900	-0.30467600
C	-2.81405500	-4.15138900	4.34046100
H	-3.88552500	-4.35139700	4.40243500
C	-4.48620100	-1.68382600	3.90298000
H	-5.07094200	-2.61555200	3.86783600
H	-4.08367300	-1.48724100	2.89834800

H	-5.17870500	-0.87297600	4.17300500
C	-2.35025200	-3.52872100	-1.61550400
H	-1.85792700	-2.96912700	-2.42615400
H	-3.41391300	-3.24422900	-1.61289400
H	-2.28661300	-4.60318200	-1.85000100
C	1.44588700	-3.47519600	4.30621300
H	1.65641500	-2.48867500	4.73948300
C	-3.89717300	-1.99832900	6.33869700
H	-4.63167500	-1.22122000	6.59785700
H	-3.09541300	-1.96580200	7.09099700
H	-4.39633300	-2.97667300	6.41571100
C	-2.54763400	-3.79104100	0.89793300
H	-2.70143600	-4.87873200	0.81316200
H	-3.54056000	-3.31588100	0.91762700
H	-2.05126700	-3.57163700	1.85258400
C	-4.09970600	-0.19395800	-2.29563400
H	-4.44326900	-1.23282200	-2.40833300
H	-3.28028500	-0.03736500	-3.01208200
H	-4.93206900	0.47221900	-2.57267900
C	-3.94361100	3.83509700	-0.27413800
H	-4.72769200	4.56619900	-0.06918600
C	-4.71033600	-0.40652000	0.14288000
H	-5.69032900	0.06269100	-0.03708300
H	-4.39203500	-0.18577500	1.17077600
H	-4.84672400	-1.49484300	0.05031100
C	-0.57206200	-4.93681700	4.01419700
H	0.12352200	-5.75422900	3.81537500
C	-1.81895100	5.00097400	3.08052000
H	-2.13869400	5.97042100	2.69352200
C	1.35872000	-5.44847400	0.08986400
H	1.58804700	-6.48927100	0.32498200
C	-1.93625100	-5.19157800	4.05897600
H	-2.31496200	-6.20022400	3.88595600
C	1.38286700	3.51074800	4.44122200
H	1.56324500	2.54189300	4.92636400
C	-4.68264000	1.88256400	3.11283500
H	-5.35152800	1.01626300	3.20657000
H	-4.42203700	2.00343700	2.05389700
H	-5.24940900	2.76853000	3.43941800
C	2.34542700	3.61185100	3.25287900
H	2.23901400	4.59065700	2.75786100
H	2.16240700	2.81814700	2.51964100
H	3.38459500	3.51092700	3.60066600
C	4.31144000	-2.88166500	-1.79431400
H	5.05654900	-2.11888800	-2.06290600
H	3.85507800	-3.25518700	-2.72217100
H	4.85637900	-3.71898000	-1.33425100
C	0.44634900	4.14746900	0.46926000
H	1.52894200	4.32130000	0.36955400
H	0.27882900	3.34024300	1.19826600
H	-0.01085500	5.05641600	0.88679000
C	-0.07914700	5.03091900	-1.81606500

H	-0.54572300	5.91876400	-1.36438100
H	-0.56685200	4.85898300	-2.78658800
H	0.97695300	5.27612900	-2.00072700
C	-3.80802200	1.63660100	5.44394900
H	-4.13108300	2.63388100	5.78216600
H	-2.98186100	1.30361800	6.08829900
H	-4.64575200	0.93975200	5.60111100
C	3.98930200	-1.89816900	0.48355700
H	4.47274000	-2.78102500	0.93101400
H	3.28885100	-1.49480600	1.22811200
H	4.76781300	-1.14379400	0.29158500
C	2.02009300	-3.48893000	2.89338500
H	1.91162900	-4.49161700	2.45604900
H	3.08729800	-3.22255900	2.90859200
H	1.49091300	-2.77279800	2.24746300
C	2.14697900	-4.53581800	5.16307800
H	1.70501700	-4.63443800	6.16585400
H	3.20810900	-4.27186200	5.28075100
H	2.10876400	-5.52743300	4.68775800
C	1.72264500	4.63583400	5.43332000
H	2.69026800	4.43024100	5.91422700
H	0.96401800	4.76344400	6.21717400
H	1.81770200	5.60250600	4.91638300

Table S13

Al=As-Prod

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

Ge	0.04473600	0.00453900	0.00680800
Al	0.00937200	0.01017100	3.74152500
I	2.60290500	0.09627800	3.69942200
C	1.77617500	0.90588800	-0.15302300
H	1.72184900	1.89504500	0.32022800
H	2.03970700	1.01966800	-1.21579000
H	2.55405500	0.33108000	0.36411100
As	-1.30449000	-0.40541900	1.81539900
N	-0.44129500	1.52935200	4.87174700
N	-1.01935800	0.92726500	-1.37983100
N	0.35390100	-1.55688300	-1.20934500
N	-0.43113300	-1.33117300	5.05578800
C	-1.84152100	3.15528200	-0.72051000
C	-0.71214300	0.82431100	-2.67429700
C	-2.12351200	3.03300100	3.90891800
C	-0.36533700	1.42196000	6.19896500
C	-0.79503100	2.82202300	4.33604300
C	-2.10033200	1.80514200	-1.01621800
C	0.68181000	-2.85111700	-0.66229100
C	0.41559200	-1.40268900	-2.52737400
C	0.06991600	-0.21115800	-3.19670700
H	0.24944000	-0.19051600	-4.26827400

C	-2.31569500	-2.83663400	4.64794800
C	-0.91931400	-2.63745800	4.69521700
C	-2.92441500	3.99213600	-0.43100900
H	-2.73872000	5.03945300	-0.18476400
C	2.03146900	-3.26075300	-0.59230800
C	-3.41352900	1.29472800	-1.02698200
C	-0.26080200	-1.08192500	6.35657200
C	-3.16024500	1.92431400	3.94944300
H	-2.62207600	0.97396500	3.85818100
C	-0.42912300	3.70951100	-0.69711700
H	0.23056900	2.97036100	-1.17555600
C	-0.36457800	-3.70788900	-0.26702000
C	0.85133900	-2.55685100	-3.39490400
H	1.92042700	-2.75836800	-3.24788600
H	0.67192100	-2.33142100	-4.45103600
H	0.31667400	-3.47495300	-3.11695200
C	-3.30025400	-1.71065300	4.92373900
H	-2.74366700	-0.76359900	4.88347000
C	-1.82053900	-3.28577700	-0.35813900
H	-1.84735000	-2.19410900	-0.26054000
C	0.14752900	3.87531400	4.31066200
C	-2.50436600	4.31896100	3.51135400
H	-3.53112500	4.49334100	3.18744500
C	-1.25919400	1.84360600	-3.64084300
H	-2.35736900	1.84899100	-3.62708100
H	-0.90861600	1.64055000	-4.65810300
H	-0.93946100	2.85054000	-3.33596200
C	-0.02883500	-3.69770100	4.44598400
C	-0.12911900	0.21147500	6.87843000
H	0.00214100	0.28477600	7.95486200
C	2.30332900	-4.56934000	-0.18337800
H	3.34036000	-4.90638300	-0.13026600
C	-3.71175200	-0.16214000	-1.34306800
H	-2.75827600	-0.70932400	-1.32611700
C	-0.56920500	2.63974500	7.06683100
H	0.27293600	3.33431800	6.95345100
H	-0.65080300	2.35017100	8.11942500
H	-1.47343100	3.18638100	6.76571300
C	-0.24089500	-2.22927100	7.33487500
H	-1.16488300	-2.82006300	7.27303300
H	-0.10750800	-1.86627900	8.35928300
H	0.58356600	-2.91097000	7.08045000
C	3.19900700	-2.33206300	-0.89328500
H	2.80314200	-1.42070100	-1.36638000
C	-0.28919400	5.14723800	3.92539600
H	0.42562200	5.97249500	3.91734200
C	-0.03737300	-5.00011900	0.15664900
H	-0.83429000	-5.67645600	0.46718500
C	-4.46664300	2.17551500	-0.76434900
H	-5.49231400	1.80177200	-0.78094700
C	-2.79807300	-4.11932600	4.37439300
H	-3.87587100	-4.29115500	4.34839100

C	-4.40056800	-1.64594300	3.86284900
H	-5.04155800	-2.54042000	3.88609200
H	-3.96282400	-1.55489200	2.85746600
H	-5.04999100	-0.77580200	4.04193600
C	-2.41657600	-3.64987700	-1.72193500
H	-1.90710600	-3.11976500	-2.54202700
H	-3.48183700	-3.37399800	-1.75936400
H	-2.33867600	-4.73213700	-1.91123300
C	1.47538600	-3.50668300	4.47285600
H	1.68583500	-2.51473100	4.89620000
C	-3.89714400	-1.82932100	6.33106000
H	-4.62564800	-1.02468300	6.51147400
H	-3.12056700	-1.75734000	7.10625800
H	-4.41519400	-2.79336600	6.45421200
C	-2.65300000	-3.83355300	0.79837500
H	-2.79191100	-4.92450800	0.73638100
H	-3.65223200	-3.37374500	0.79275900
H	-2.17418000	-3.58903500	1.75783400
C	-4.30970900	-0.31822300	-2.74608100
H	-4.53260300	-1.37548400	-2.95352200
H	-3.61874900	0.03650100	-3.52467100
H	-5.24765700	0.25151100	-2.83748200
C	-4.22923900	3.51368000	-0.46694200
H	-5.06416900	4.18278600	-0.25286700
C	-4.62070800	-0.78982000	-0.28477800
H	-5.61576100	-0.31922500	-0.27415800
H	-4.17089900	-0.68837500	0.71382600
H	-4.76663900	-1.85962700	-0.49726600
C	-0.55794600	-4.95825400	4.14586600
H	0.12513500	-5.78473200	3.93848300
C	-1.60508900	5.37831700	3.54386300
H	-1.92478100	6.38021300	3.25183100
C	1.28107700	-5.43946800	0.17547200
H	1.51486000	-6.45673900	0.49417200
C	-1.92983400	-5.17688000	4.12234600
H	-2.32500600	-6.16969700	3.90083400
C	1.61943400	3.68987900	4.64996200
H	1.75184900	2.69459300	5.09903600
C	-4.11813500	1.98159800	2.76234500
H	-4.74013200	1.07447300	2.73663800
H	-3.55001300	2.02566700	1.82177700
H	-4.79794000	2.84704300	2.81085800
C	2.45652200	3.72925600	3.36572500
H	2.39106300	4.72591700	2.89943900
H	2.11022700	2.98086700	2.64106300
H	3.51257300	3.51530700	3.58827600
C	4.23722600	-2.94687000	-1.83903600
H	4.99962200	-2.19750400	-2.09671700
H	3.79619600	-3.32021300	-2.77416300
H	4.75814700	-3.78936800	-1.36113000
C	0.03095700	3.89456500	0.74993600
H	1.08517800	4.20832800	0.79152000

H	-0.09222800	2.97034600	1.33856400
H	-0.57546900	4.66787400	1.24180400
C	-0.29304500	5.02215400	-1.47405000
H	-0.85311600	5.83455400	-0.98800100
H	-0.66283500	4.93189200	-2.50634400
H	0.76204700	5.32978100	-1.51242900
C	-3.89909400	1.91392900	5.29145200
H	-4.39032300	2.88214200	5.47718500
H	-3.21275300	1.70982700	6.12821100
H	-4.67422500	1.13218200	5.29685400
C	3.88119600	-1.92224700	0.41763500
H	4.37520200	-2.79312700	0.87663800
H	3.16207300	-1.53296200	1.15137400
H	4.64650500	-1.15172000	0.23731200
C	2.02276800	-3.53157000	3.04460900
H	1.91542400	-4.53979700	2.61793600
H	3.08777900	-3.25454300	3.03185300
H	1.47327700	-2.83346700	2.39158700
C	2.19256100	-4.54913400	5.33588400
H	1.79170900	-4.58759400	6.35971400
H	3.26451300	-4.31091800	5.39698800
H	2.10326500	-5.55809500	4.90557700
C	2.15307800	4.74114000	5.63096300
H	3.17705000	4.48041100	5.93514200
H	1.53998000	4.82934200	6.53905200
H	2.19528100	5.73703200	5.16512800

Table S14

Ga=As-Prod

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	0.02791700	-0.01303100	-0.01393200
Ga	0.01075900	0.01603200	3.68961300
I	2.64893900	0.11496800	3.70661600
C	1.76257200	0.88399000	-0.14210000
H	1.70663900	1.86805400	0.34121500
H	2.03700400	1.00788600	-1.20098100
H	2.53337600	0.30157700	0.37685000
As	-1.34776100	-0.42513800	1.78265400
N	-0.44500600	1.56819100	4.89003000
N	-1.02507700	0.91623700	-1.39933700
N	0.34056700	-1.57088700	-1.22672900
N	-0.42671400	-1.34667100	5.08222700
C	-1.83977400	3.14465900	-0.72991100
C	-0.71242500	0.81486700	-2.69291400
C	-2.12783500	3.05772200	3.91667400
C	-0.36094400	1.44017500	6.21165400
C	-0.80179200	2.85598300	4.35777400
C	-2.10341700	1.79757900	-1.03462700
C	0.66427800	-2.86358700	-0.67291400

C	0.40985500	-1.41543700	-2.54424000
C	0.06840100	-0.22248900	-3.21359100
H	0.25349500	-0.20032900	-4.28419100
C	-2.29994300	-2.85038900	4.64019900
C	-0.90447400	-2.65075900	4.71970000
C	-2.92009200	3.98350400	-0.43636100
H	-2.73084300	5.02848800	-0.18309500
C	2.01314500	-3.27183700	-0.58612100
C	-3.41814900	1.29103300	-1.04677300
C	-0.25295300	-1.07539300	6.37370100
C	-3.15481600	1.93990400	3.95649800
H	-2.60789200	0.99545300	3.85591400
C	-0.42552900	3.69352200	-0.69628800
H	0.23465300	2.95337500	-1.17266400
C	-0.38631600	-3.71661800	-0.27918900
C	0.85172200	-2.56882900	-3.40893600
H	1.92125300	-2.76508800	-3.25796400
H	0.67499600	-2.34552100	-4.46598000
H	0.32009900	-3.48869800	-3.13121200
C	-3.28460000	-1.72177000	4.90472100
H	-2.73211400	-0.77475600	4.82226100
C	-1.84143100	-3.29596700	-0.39250100
H	-1.87165400	-2.20578500	-0.27863100
C	0.13715200	3.91240100	4.32687600
C	-2.51142900	4.33810800	3.50468300
H	-3.53601100	4.50518400	3.17003900
C	-1.25045500	1.83981200	-3.65810900
H	-2.34856900	1.85286000	-3.64643000
H	-0.89900000	1.63724400	-4.67513900
H	-0.92426500	2.84356900	-3.34934900
C	-0.00769900	-3.70575100	4.47047400
C	-0.12041100	0.22473500	6.88365500
H	0.01661100	0.30012200	7.95927800
C	2.28113500	-4.57494400	-0.15698300
H	3.31774900	-4.91071700	-0.08918800
C	-3.72068300	-0.16339900	-1.37026700
H	-2.76955600	-0.71487300	-1.35155300
C	-0.56135100	2.65140300	7.09199100
H	0.27955700	3.34783600	6.97991300
H	-0.63774900	2.35417600	8.14282700
H	-1.46810400	3.19891300	6.79981200
C	-0.22656900	-2.21276300	7.36551500
H	-1.14212100	-2.81641300	7.30149600
H	-0.10676700	-1.83902300	8.38777300
H	0.60959400	-2.88533500	7.12477000
C	3.18512400	-2.34911600	-0.88843400
H	2.79403500	-1.43692000	-1.36405900
C	-0.30203300	5.17922700	3.92765100
H	0.40970100	6.00722900	3.91644400
C	-0.06263100	-5.00207100	0.16634400
H	-0.86138900	-5.67459600	0.47979600
C	-4.46823500	2.17340600	-0.77795500

H	-5.49504400	1.80295100	-0.79490800
C	-2.77517700	-4.13084100	4.34576900
H	-3.85164500	-4.30406400	4.29424900
C	-4.41374300	-1.68914800	3.87346200
H	-5.06575200	-2.57229800	3.95340800
H	-4.00591800	-1.64565500	2.85230800
H	-5.04693500	-0.80356600	4.03422300
C	-2.41140500	-3.63731000	-1.77337200
H	-1.89178900	-3.08919200	-2.57490800
H	-3.47746300	-3.36639600	-1.82343600
H	-2.32446900	-4.71548000	-1.98095900
C	1.49513000	-3.50522500	4.50721100
H	1.69672300	-2.50960400	4.92698000
C	-3.84338200	-1.79897600	6.33065000
H	-4.58058700	-1.00023000	6.50166700
H	-3.04850400	-1.68606500	7.08191000
H	-4.34106700	-2.76680200	6.50007900
C	-2.69825300	-3.86415100	0.73605400
H	-2.83882000	-4.95300200	0.64755900
H	-3.69612000	-3.40203500	0.71837700
H	-2.23931000	-3.64234900	1.71060900
C	-4.31122300	-0.31045300	-2.77747900
H	-4.53890500	-1.36546200	-2.99096700
H	-3.61377900	0.04387400	-3.55040200
H	-5.24529300	0.26513500	-2.87154000
C	-4.22635000	3.50943700	-0.47432200
H	-5.05899500	4.17989800	-0.25576600
C	-4.63866600	-0.79359500	-0.32111200
H	-5.63280100	-0.32117500	-0.31618200
H	-4.19856800	-0.69832200	0.68261600
H	-4.78532500	-1.86193900	-0.54025500
C	-0.52901100	-4.96494400	4.15168500
H	0.15885600	-5.78820800	3.94673200
C	-1.61632900	5.40151500	3.53479700
H	-1.93775900	6.39949300	3.23142000
C	1.25609800	-5.43963800	0.20574700
H	1.48711700	-6.45161700	0.54274100
C	-1.89997300	-5.18527800	4.10237100
H	-2.28948500	-6.17671600	3.86498200
C	1.60825500	3.73073500	4.67120100
H	1.74079300	2.73670400	5.12343400
C	-4.12408100	1.99403200	2.77857700
H	-4.73245500	1.07759800	2.75063600
H	-3.56693100	2.05521900	1.83244200
H	-4.81640500	2.84860100	2.84221000
C	2.44946700	3.76651400	3.38967900
H	2.38016700	4.75939600	2.91583800
H	2.11034300	3.01058700	2.66931800
H	3.50588900	3.55969900	3.61708200
C	4.22029800	-2.97261000	-1.83215900
H	4.98845900	-2.22916400	-2.08984100
H	3.77852900	-3.34496300	-2.76725200

H	4.73415500	-3.81798800	-1.35171000
C	0.02585800	3.87340900	0.75448700
H	1.08090700	4.18299600	0.80354200
H	-0.10447300	2.94824700	1.34002000
H	-0.58046900	4.64733100	1.24567200
C	-0.27999400	5.00768200	-1.46896700
H	-0.84188500	5.82019200	-0.98526700
H	-0.64192200	4.92077700	-2.50433300
H	0.77610500	5.31274600	-1.49830300
C	-3.88329800	1.91093800	5.30381000
H	-4.38262600	2.87275800	5.50070100
H	-3.18854800	1.70636100	6.13330500
H	-4.65054400	1.12132500	5.30784600
C	3.87083100	-1.94016400	0.42105600
H	4.36370000	-2.81180500	0.87973800
H	3.15564700	-1.54823200	1.15713100
H	4.63793900	-1.17197100	0.23864100
C	2.05231500	-3.53261400	3.08241500
H	1.95708200	-4.54377900	2.65931000
H	3.11457900	-3.24514900	3.07509000
H	1.50122100	-2.84302300	2.42154300
C	2.21218000	-4.54035200	5.37898500
H	1.80721000	-4.57316600	6.40128600
H	3.28343900	-4.29967100	5.44278900
H	2.12592400	-5.55210400	4.95443200
C	2.13518600	4.78660000	5.65072400
H	3.15901500	4.53087100	5.95963500
H	1.51767700	4.87482200	6.55582100
H	2.17495600	5.78120200	5.18175900

Table S15

In=As-Prod

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	-0.04805300	-0.05928800	-0.13260000
In	0.15521600	0.04907800	3.57549900
I	2.94131000	0.20150100	3.71129700
C	1.70254200	0.81240200	-0.21560600
H	1.65041200	1.79554300	0.26989000
H	2.00644300	0.93785700	-1.26623800
H	2.45536400	0.21961700	0.31774600
As	-1.43166700	-0.46070000	1.66178900
N	-0.41753200	1.66652400	4.99117300
N	-1.06365100	0.90103900	-1.51197400
N	0.24638400	-1.61670700	-1.33162000
N	-0.35321600	-1.37083300	5.19084400
C	-1.84662800	3.11932800	-0.76681800
C	-0.74459700	0.79422700	-2.80290100
C	-2.11643300	3.11076800	3.98948400
C	-0.34214700	1.49224300	6.30493500

C	-0.79663700	2.94444700	4.46926200
C	-2.12938000	1.79082600	-1.13109000
C	0.54425100	-2.90127400	-0.74473500
C	0.33798400	-1.46021400	-2.64728000
C	0.01888700	-0.26060000	-3.31808400
H	0.21730200	-0.23897000	-4.38644500
C	-2.17156700	-2.89771000	4.64658300
C	-0.78493800	-2.68034900	4.81883500
C	-2.91455400	3.95701600	-0.42813900
H	-2.71010500	4.98684400	-0.12855100
C	1.88602300	-3.31050200	-0.59109100
C	-3.45003400	1.29893100	-1.14754800
C	-0.20189500	-1.05259900	6.46932700
C	-3.11001600	1.96189100	4.01279700
H	-2.53316300	1.03695000	3.88854200
C	-0.42688000	3.65187000	-0.70643100
H	0.23044200	2.91312900	-1.18905600
C	-0.52544200	-3.72617700	-0.33604800
C	0.78758600	-2.61786000	-3.50003700
H	1.85626900	-2.80864200	-3.33487300
H	0.62282800	-2.40316900	-4.56084100
H	0.25513900	-3.53654500	-3.22029400
C	-3.17718000	-1.78229600	4.88832500
H	-2.64839300	-0.82937500	4.73506500
C	-1.97484300	-3.30578700	-0.51807400
H	-2.01363000	-2.21743400	-0.38199200
C	0.12552200	4.01422300	4.41908100
C	-2.51295200	4.37233400	3.53553900
H	-3.53138200	4.51196400	3.17069300
C	-1.25310700	1.83677100	-3.76383300
H	-2.35095000	1.86718500	-3.76370100
H	-0.89362300	1.64055400	-4.77929800
H	-0.91449600	2.83114900	-3.43765100
C	0.14207500	-3.70917900	4.56697800
C	-0.09809300	0.26362800	6.95958700
H	0.02904000	0.34048700	8.03662300
C	2.13193900	-4.58210600	-0.06285800
H	3.16427800	-4.91481100	0.06295400
C	-3.77377700	-0.13975800	-1.51975200
H	-2.82874900	-0.70246300	-1.54133700
C	-0.55726900	2.68466500	7.21125200
H	0.26402100	3.40434100	7.09574100
H	-0.61378700	2.37407700	8.25942500
H	-1.48155500	3.21301900	6.93754200
C	-0.15898200	-2.16744000	7.48968300
H	-1.03719300	-2.82102100	7.39663800
H	-0.10423800	-1.77306700	8.50981100
H	0.72287000	-2.79685400	7.29805600
C	3.07954700	-2.42305600	-0.91396100
H	2.71232100	-1.51429900	-1.41478400
C	-0.32458200	5.26196800	3.97370100
H	0.37555700	6.09976300	3.94742000

C	-0.22295100	-4.97691400	0.20939600
H	-1.03263000	-5.62311900	0.54725000
C	-4.48656000	2.17989900	-0.82690800
H	-5.51751500	1.82136700	-0.84491300
C	-2.60664500	-4.17063500	4.27142800
H	-3.67406900	-4.35663900	4.14201100
C	-4.35091600	-1.82220200	3.90918800
H	-5.00745600	-2.68684400	4.09146900
H	-3.99454200	-1.86487400	2.86869200
H	-4.96787700	-0.91863800	4.02778300
C	-2.47459400	-3.61550800	-1.93372500
H	-1.92306200	-3.04496400	-2.69675400
H	-3.53891900	-3.34942200	-2.02828100
H	-2.37089600	-4.68789400	-2.16225900
C	1.63931300	-3.47479800	4.64424800
H	1.80772000	-2.46845000	5.05532300
C	-3.67694500	-1.79334400	6.33859600
H	-4.44771800	-1.02266700	6.48880000
H	-2.86252400	-1.59134300	7.04854200
H	-4.11746000	-2.77198800	6.58636800
C	-2.89333900	-3.90538100	0.54480400
H	-3.03717300	-4.98813300	0.40380900
H	-3.88533500	-3.43496500	0.49145600
H	-2.48434900	-3.72970000	1.55109400
C	-4.39447200	-0.22907600	-2.91889400
H	-4.62931200	-1.27450000	-3.16892900
H	-3.71391700	0.15508900	-3.69233300
H	-5.32888700	0.35124200	-2.96932000
C	-4.22624300	3.49937300	-0.47076100
H	-5.04855400	4.16832100	-0.21228500
C	-4.68016900	-0.80132000	-0.47928500
H	-5.66430000	-0.31128900	-0.43037400
H	-4.22028200	-0.76317700	0.51973800
H	-4.85290200	-1.85457000	-0.74640400
C	-0.33887000	-4.96423400	4.17661500
H	0.37367600	-5.76686500	3.97239000
C	-1.63505700	5.45146800	3.55152000
H	-1.96622600	6.43454200	3.21212400
C	1.09196500	-5.41222800	0.33162700
H	1.30522800	-6.39569600	0.75394900
C	-1.70051700	-5.20267200	4.04027100
H	-2.05901700	-6.18921900	3.74110600
C	1.59624800	3.85108500	4.77253100
H	1.73631400	2.86047000	5.23085300
C	-4.09768800	2.00806900	2.84926400
H	-4.66597600	1.06666400	2.80493400
H	-3.56344500	2.12032500	1.89429100
H	-4.82526100	2.82918900	2.95109100
C	2.44036200	3.88858400	3.49291100
H	2.35673100	4.87499100	3.00814800
H	2.11321400	3.12191000	2.77731400
H	3.49949300	3.69826500	3.72152000

C	4.09800700	-3.10127200	-1.83875100
H	4.89245100	-2.39065000	-2.10914700
H	3.64831900	-3.48126900	-2.76674400
H	4.57885800	-3.95276300	-1.33541200
C	0.01286200	3.80558200	0.75277600
H	1.06938000	4.10800100	0.81465100
H	-0.12670900	2.87004900	1.31907200
H	-0.59149500	4.57339100	1.25739300
C	-0.26168400	4.97584200	-1.45850100
H	-0.82967000	5.78374500	-0.97424200
H	-0.60596200	4.90267100	-2.50089600
H	0.79590300	5.27701400	-1.46567200
C	-3.82562600	1.87394300	5.36448900
H	-4.34962600	2.81587800	5.59111400
H	-3.11964800	1.66391600	6.18266200
H	-4.57117400	1.06380700	5.34950500
C	3.77867200	-1.99951800	0.38413100
H	4.25736400	-2.86933500	0.86057400
H	3.07664200	-1.57892900	1.11679300
H	4.55900800	-1.24948600	0.18383000
C	2.23825300	-3.50947700	3.23493600
H	2.19510500	-4.53084500	2.82542400
H	3.28708100	-3.17665200	3.24790600
H	1.67770600	-2.85906600	2.54317600
C	2.35153200	-4.48205800	5.55156600
H	1.92740300	-4.49382000	6.56619000
H	3.41984600	-4.23223600	5.62901200
H	2.27761400	-5.50367900	5.14851000
C	2.10239700	4.91651900	5.75159600
H	3.13364900	4.68675900	6.05626700
H	1.48496800	4.98388400	6.65856000
H	2.11296700	5.91307600	5.28494000

Table S16

Tl=As-Prod

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ge	-0.07054600	-0.07140100	-0.16396300
Tl	0.19354100	0.04497200	3.47430700
I	3.01981500	0.18503600	3.83482100
C	1.67562500	0.80694600	-0.15994600
H	1.59770900	1.78509000	0.33172100
H	2.02473600	0.94434700	-1.19476500
H	2.40805300	0.21191000	0.39917200
As	-1.48135700	-0.49402300	1.62435400
N	-0.41652200	1.68632800	5.01825700
N	-1.06642000	0.89369400	-1.54075200
N	0.25303200	-1.61682600	-1.35370100
N	-0.39515600	-1.37943100	5.21720600
C	-1.85831000	3.10356000	-0.77804500

C	-0.73206400	0.79230400	-2.82929500
C	-2.10350500	3.12907900	4.00964400
C	-0.32183500	1.49829400	6.32573600
C	-0.78650000	2.96011000	4.49973000
C	-2.13742500	1.77999500	-1.16242400
C	0.54947200	-2.89859700	-0.75816300
C	0.36156400	-1.45689400	-2.66789300
C	0.04179100	-0.25734500	-3.33895600
H	0.25348400	-0.23073200	-4.40463300
C	-2.20209000	-2.89579300	4.63118200
C	-0.81790800	-2.68136000	4.83674700
C	-2.92974600	3.93449400	-0.43413100
H	-2.72879100	4.95990300	-0.11766600
C	1.89081300	-3.29536700	-0.57381200
C	-3.45689600	1.28579400	-1.19321900
C	-0.21442600	-1.05511900	6.48580700
C	-3.09157100	1.97577000	4.02749500
H	-2.50674600	1.05536500	3.90254800
C	-0.44036100	3.63797200	-0.69662100
H	0.22535000	2.90239800	-1.17284700
C	-0.52304000	-3.72756400	-0.36480200
C	0.83364000	-2.60928100	-3.51410900
H	1.90188000	-2.78817400	-3.33292600
H	0.68196000	-2.39655400	-4.57721000
H	0.30729800	-3.53340000	-3.24080900
C	-3.20370600	-1.77836400	4.87661000
H	-2.67432400	-0.82907200	4.70068300
C	-1.97220300	-3.31732000	-0.57330900
H	-2.02208300	-2.22844800	-0.43861300
C	0.13869600	4.02795200	4.43943400
C	-2.49744500	4.38941900	3.55078700
H	-3.51513400	4.52962700	3.18341600
C	-1.23483700	1.83708100	-3.78970100
H	-2.33277400	1.86112000	-3.80121600
H	-0.86307900	1.64865000	-4.80213300
H	-0.90568600	2.83130100	-3.45357900
C	0.11003100	-3.71093400	4.58254000
C	-0.08634200	0.26282100	6.97149000
H	0.05894900	0.33664400	8.04664800
C	2.13463000	-4.56162600	-0.03174000
H	3.16648600	-4.88523700	0.11895700
C	-3.77779600	-0.14859100	-1.58489300
H	-2.83179500	-0.70962300	-1.62107000
C	-0.51137000	2.68830300	7.24459700
H	0.30740700	3.40847800	7.11446400
H	-0.54539700	2.37362600	8.29265400
H	-1.44182700	3.21840000	6.99470100
C	-0.16526400	-2.16504900	7.51431400
H	-1.03594400	-2.82864400	7.41876300
H	-0.12144700	-1.76599000	8.53333000
H	0.72568700	-2.78498600	7.33354000
C	3.08521500	-2.40177200	-0.87578000

H	2.72160800	-1.49180900	-1.37733200
C	-0.30682900	5.27460700	3.98680000
H	0.39645200	6.10975600	3.95558900
C	-0.22261100	-4.97196000	0.19551600
H	-1.03333700	-5.62127700	0.52430200
C	-4.49648800	2.15988700	-0.86387200
H	-5.52668000	1.79977900	-0.89080000
C	-2.63299700	-4.16006900	4.22407000
H	-3.69796900	-4.34088300	4.06955300
C	-4.39971300	-1.83063200	3.92599400
H	-5.05635100	-2.68790100	4.14045400
H	-4.07038400	-1.89774100	2.87760500
H	-5.00948200	-0.92169000	4.04036000
C	-2.44485100	-3.62596000	-1.99854400
H	-1.88318800	-3.05136300	-2.75092500
H	-3.50887800	-3.36601600	-2.11141100
H	-2.33095500	-4.69729200	-2.22650400
C	1.60636100	-3.47985500	4.68358600
H	1.77042400	-2.47745100	5.10586100
C	-3.67162100	-1.77015100	6.33761200
H	-4.44235500	-1.00080700	6.49476200
H	-2.84192100	-1.55440700	7.02523300
H	-4.10192800	-2.74728700	6.60840900
C	-2.90614600	-3.92731800	0.47041400
H	-3.03924100	-5.00995600	0.31995500
H	-3.90070000	-3.46476900	0.40089300
H	-2.51753200	-3.75620300	1.48560300
C	-4.40625800	-0.22034500	-2.98157200
H	-4.63677300	-1.26310300	-3.24611400
H	-3.73308300	0.17999800	-3.75311500
H	-5.34418400	0.35515600	-3.01716300
C	-4.24015800	3.47469500	-0.48846500
H	-5.06472300	4.13798000	-0.22303600
C	-4.67887000	-0.82732300	-0.55044200
H	-5.66466400	-0.34180200	-0.49425400
H	-4.22308400	-0.79891900	0.45099700
H	-4.84733300	-1.87803200	-0.82936800
C	-0.36610600	-4.95819200	4.16265400
H	0.34885600	-5.75921700	3.95950500
C	-1.61720400	5.46717200	3.56431900
H	-1.94547900	6.45010900	3.22159900
C	1.09288700	-5.39632100	0.34728600
H	1.30451200	-6.37450800	0.78228900
C	-1.72517100	-5.19134700	3.99409200
H	-2.07988100	-6.17198400	3.67156700
C	1.60967500	3.85377500	4.78472000
H	1.74090400	2.86833100	5.25647000
C	-4.08345800	2.02197600	2.86732800
H	-4.64580200	1.07694900	2.81975500
H	-3.55611700	2.14545700	1.90965800
H	-4.81651500	2.83719000	2.97780800
C	2.44285800	3.85937800	3.49750400

H	2.36373600	4.83704500	2.99432000
H	2.10176300	3.08148300	2.79987600
H	3.50207600	3.66191600	3.71927200
C	4.11741400	-3.07269500	-1.79086800
H	4.91659500	-2.36056800	-2.04251200
H	3.68243500	-3.44459000	-2.72905700
H	4.58919100	-3.92890000	-1.28702900
C	-0.02210900	3.78978500	0.76938400
H	1.03393700	4.08963300	0.84767500
H	-0.17206800	2.85531900	1.33479200
H	-0.63131300	4.55828000	1.26681000
C	-0.26811600	4.96427500	-1.44314400
H	-0.84911700	5.76793600	-0.96751600
H	-0.59282500	4.89162100	-2.49182900
H	0.78782500	5.27074800	-1.43024600
C	-3.80453900	1.87732200	5.37976200
H	-4.33411100	2.81523800	5.61019900
H	-3.09426000	1.66917900	6.19447600
H	-4.54475600	1.06231000	5.36326400
C	3.76824200	-1.98373000	0.43313400
H	4.24929100	-2.85345500	0.90712500
H	3.05842400	-1.57521500	1.16518500
H	4.54478100	-1.22631100	0.24710400
C	2.22523700	-3.50189700	3.28268200
H	2.18316400	-4.51846700	2.86098800
H	3.27475100	-3.17239200	3.31267000
H	1.67573300	-2.84188000	2.59101700
C	2.30470400	-4.49747700	5.59006100
H	1.86441600	-4.51994800	6.59745900
H	3.37190800	-4.24934900	5.68680500
H	2.23600000	-5.51461500	5.17458900
C	2.13579900	4.92684800	5.74402900
H	3.16635700	4.68929500	6.04519000
H	1.52450200	5.01242000	6.65369800
H	2.15454300	5.91694400	5.26380300
