

Supporting Information

Reactivity for the [2 + 5] Cycloaddition Reactions of Norbornene-Linked Group 14 Element/P-Based and Si/Group 15 Element-Based Frustrated Lewis Pairs with Benzaldehyde: Insights from Computational Study

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Table S1. Results of EDA-NOCV at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level of **Si/G15-TS** using two different models. Energy values are in kcal/mol.

Fragments	<u>Si/N-TS</u>		<u>Si/P-TS</u>		<u>Si/As-TS</u>		<u>Si/Sb-TS</u>		<u>Si/Bi-TS</u>	
	Si/N-Rea (S)	Si/N-Rea (T)	Si/P-Rea (S)	Si/P-Rea (T)	Si/As-Rea (S)	Si/As-Rea (T)	Si/Sb-Rea (S)	Si/Sb-Rea (T)	Si/Bi-Rea (S)	Si/Bi-Rea (T)
	+	+	+	+	+	+	+	+	+	+
	Ph(H)C=O (S)	Ph(H)C=O (T)	Ph(H)C=O (S)	Ph(H)C=O (T)	Ph(H)C=O (S)	Ph(H)C=O (T)	Ph(H)C=O (S)	Ph(H)C=O (T)	Ph(H)C=O (S)	Ph(H)C=O (T)
$\Delta E_{\text{INT}}^{(a)}$	-24.0	-139.0	-28.0	-130.4	-30.3	-133.2	-24.4	-130.0	-19.8	-128.2
ΔE_{Pauli}	80.8	132.3	143.5	204.7	130.3	179.5	104.8	131.1	56.8	67.1
$\Delta E_{\text{Elstat}}^{(b)}$	-51.9 (49.5 %)	-63.0 (23.2 %)	-81.5 (47.5 %)	-101.5 (30.3 %)	-77.6 (48.3 %)	-88.9 (28.4 %)	-63.5 (49.1 %)	-64.4 (24.7 %)	-38.3 (50.0 %)	-32.0 (16.4 %)
$\Delta E_{\text{Orb}}^{(b)}$	-40.2 (38.4 %)	-195.6 (72.1 %)	-78.8 (46.0 %)	-222.5 (66.4 %)	-73.7 (45.9 %)	-214.5 (68.6 %)	-56.5 (43.7 %)	-187.4 (71.8 %)	-29.3 (38.3 %)	-154.3 (79.0 %)
$\Delta E_{\text{Orb}(1)}^{(c)}$	-21.6 (53.7 %)	-175.5 (89.7 %)	-46.4 (58.9 %)	-185.5 (83.4 %)	-43.0 (58.4 %)	-180.8 (84.3 %)	-32.7 (57.9 %)	-160.4 (85.6 %)	-16.2 (55.2 %)	-141.0 (91.3 %)
$\Delta E_{\text{Orb}(2)}^{(c)}$	-6.5 (16.3 %)	-8.4 (4.3 %)	-10.5 (13.4 %)	-18.7 (8.4 %)	-10.4 (14.1 %)	-18.2 (8.5 %)	-7.8 (13.8 %)	-15.8 (8.4 %)	-4.1 (14.1 %)	-5.9 (3.8 %)
$\Delta E_{\text{Rest}}^{(c)}$	-12.1 (30.0 %)	-11.8 (6.0 %)	-21.9 (27.7 %)	-18.3 (8.2 %)	-20.3 (27.5 %)	-15.5 (7.2 %)	-16.0 (28.3 %)	-11.3 (6.0 %)	-9.0 (30.8 %)	-7.5 (4.9 %)
$\Delta E_{\text{Disper}}^{(b)}$	-12.7 (12.1 %)	-12.7 (4.7 %)	-11.2 (6.5 %)	-11.2 (3.3 %)	-9.3 (5.8 %)	-9.3 (3.0 %)	-9.3 (7.2 %)	-9.3 (3.5 %)	-19.8 (11.7 %)	-9.0 (4.6 %)

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

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

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

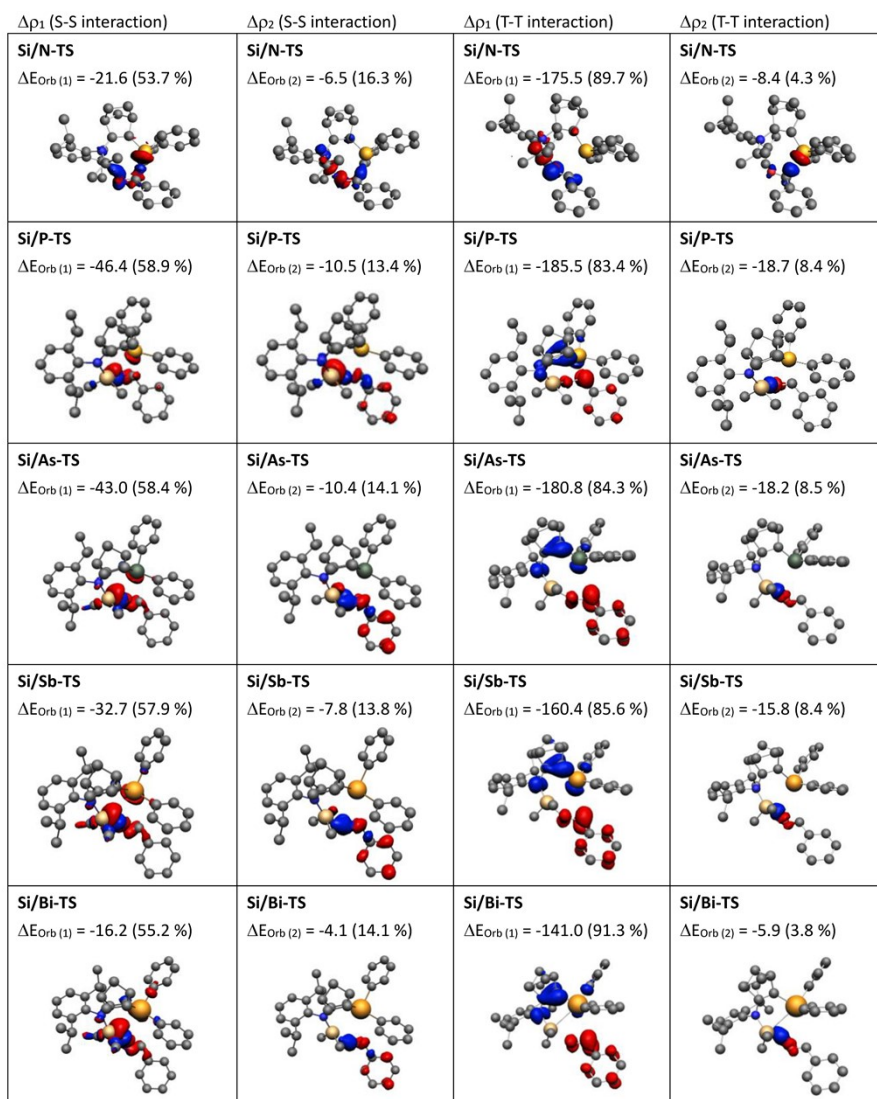
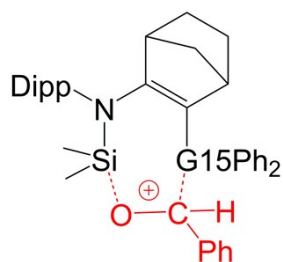


Figure S1: Plots of deformation densities, $\Delta\rho(r)$, of the pair-wise orbital interactions in **Si/G15-TS** at the ZORA-B3LYP-D3(BJ)/TZ2P//B3LYP-D3(BJ)/def2-TZVP level. Also see Table 2. The contour value is $|\Delta\rho| = 0.002$ a.u. The associated orbital interaction energies are given in kcal/mol. The color code of the charge flow is red/blue.

C/P-Rea

C	-0.50488200	-0.15965400	0.50196600
H	-0.99962800	0.81436800	0.42819200
C	0.83890400	-0.25718000	-0.22419000
C	1.08904000	-1.58662200	-0.31707600
C	-0.25348300	-0.62534500	1.97351500
H	-1.15172200	-0.43945500	2.57937400
H	0.57229700	-0.06938900	2.43678800
C	0.02489000	-2.14825200	1.81882300
H	1.00412600	-2.45769300	2.21342000
H	-0.73566700	-2.75532900	2.33060500
C	-0.08117000	-2.35753800	0.27361300
H	-0.17891100	-3.39649400	-0.05336900
C	-1.23314900	-1.39366600	-0.07521300
H	-1.41408100	-1.32371500	-1.15759300
H	-2.17324400	-1.63106800	0.44452200
N	2.26420700	-2.24380800	-0.80601700
P	1.90052600	1.15182400	-0.76710600
C	1.40557700	2.38848100	0.51116800
C	0.75331200	4.19067300	2.56821000
C	2.04700000	2.31278200	1.76060700
C	0.45070300	3.39365700	0.29775200
C	0.12937400	4.28934000	1.32204500
C	1.71569500	3.19956700	2.78608500
H	2.81921300	1.55866200	1.93492500
H	-0.04337300	3.48466700	-0.67064300
H	-0.61344800	5.07010400	1.14240700
H	2.21880800	3.12617100	3.75310400
H	0.49884300	4.89166800	3.36610300
C	1.02009100	1.72152500	-2.28037700
C	-0.14134600	2.72832200	-4.63406000
C	1.81469000	2.33564700	-3.26326400
C	-0.36351100	1.60722200	-2.49760900
C	-0.93897800	2.10896100	-3.66647500

C	1.23705900	2.83985300	-4.43159700
H	2.89364200	2.42163300	-3.10968300
H	-1.00190300	1.13059300	-1.75430600
H	-2.01602400	2.01533600	-3.82334600
H	1.86561500	3.32003300	-5.18506700
H	-0.59429000	3.12103800	-5.54701000
C	2.00826300	-3.30927700	-1.78143100
C	1.49858000	-5.31539600	-3.60977600
C	1.77687100	-2.94731200	-3.12120700
C	1.98534300	-4.64295700	-1.31969800
C	1.72190000	-5.63629800	-2.27212500
C	1.52768900	-3.98663500	-4.02743900
H	1.69414900	-6.68137400	-1.95923500
H	1.35730900	-3.74862500	-5.07840400
H	1.30102200	-6.10926100	-4.33313600
C	1.84384400	-1.50918100	-3.60961200
H	1.87864300	-0.84890200	-2.73446000
C	3.13033200	-1.25581100	-4.41239100
H	4.03172900	-1.49138400	-3.82515700
H	3.18621300	-0.19771500	-4.71059800
H	3.15841100	-1.86886400	-5.32715100
C	0.59879000	-1.11920700	-4.41513300
H	-0.31990900	-1.27108600	-3.82844600
H	0.51235600	-1.70797700	-5.34177300
H	0.64967000	-0.05937200	-4.69793100
C	2.24456900	-5.04896800	0.12751300
H	2.34048100	-4.13662800	0.73573000
C	3.56032500	-5.83698400	0.25605300
H	4.41692100	-5.28885700	-0.16109300
H	3.49581500	-6.79704500	-0.27863900
H	3.77520800	-6.05860100	1.31273900
C	1.08298800	-5.86443100	0.71890600
H	0.12247800	-5.33570100	0.63912700
H	1.26915500	-6.07219900	1.78361800
H	0.97350100	-6.83331200	0.20882500
C	3.48035000	-2.00504100	-0.37412700
C		3.75223300	-1.12428800 0.79080300

C	4.66476300	-2.59752000	-1.05468800
H	5.23284600	-3.21346300	-0.34049600
H	4.41472300	-3.19321300	-1.93695900
H	5.33127800	-1.76652200	-1.34320200
H	4.61776200	-1.51222700	1.34653700
H	4.01126800	-0.11815500	0.41715500
H	2.88279800	-1.01918300	1.44949400

Si/P-Rea

C	-1.28122900	-0.29331200	0.31216900
H	-1.79328700	0.67671400	0.30793400
C	0.12800300	-0.30660700	-0.26750700
C	0.43045900	-1.61716100	-0.56513100
C	-1.20607300	-0.98753800	1.70662300
H	-2.18241200	-0.94187700	2.21116400
H	-0.47186400	-0.50312800	2.36423200
C	-0.82670100	-2.45409800	1.34173100
H	0.13408800	-2.77378900	1.76793500
H	-1.58915700	-3.16882700	1.68270700
C	-0.78977400	-2.44453100	-0.22754100
H	-0.83655700	-3.43365400	-0.69698900
C	-1.91502800	-1.42753300	-0.53094500
H	-1.99739700	-1.17844500	-1.59794000
H	-2.89554900	-1.75392300	-0.15388200
N	1.66972100	-2.06317400	-0.94482900
P	1.44084400	0.83321100	-0.52743300
C	1.68115300	2.01026400	0.82716700
C	2.01698200	3.76707900	2.97581200
C	1.84136800	1.50660100	2.13036300
C	1.67928500	3.39549900	0.60525700
C	1.84871400	4.26858600	1.68312400
C	2.01039700	2.38536900	3.19892500
H	1.82128400	0.43056000	2.31095500
H	1.53745000	3.79558400	-0.39954200

H	1.84368000	5.34659500	1.50934400	
H	2.13294800	1.99229000	4.21026700	
H	2.14826100	4.45368100	3.81479400	
C	1.27464500	1.71079200	-2.10719000	
C	1.10377100	2.87968300	-4.63834200	
C	2.35372500	2.45897100	-2.60857700	
C	0.11769800	1.53815900	-2.87987800	
C	0.03423500	2.12821800	-4.14310200	
C	2.26292400	3.04479000	-3.87140800	
H	3.26584200	2.58119100	-2.01851300	
H	-0.70532100	0.93192600	-2.49750000	
H	-0.86865900	1.99781200	-4.74330300	
H	3.10009600	3.62719100	-4.26177200	
H	1.03727000	3.33621600	-5.62819200	
C	1.83272700	-3.28462500	-1.69594800	
C	2.19034700	-5.61496900	-3.17711100	
C	1.58298300	-3.26069700	-3.08890200	
C	2.25801300	-4.45733300	-1.03776300	
C	2.43182200	-5.61764800	-1.80544000	
C	1.76751100	-4.44640700	-3.81014400	
H	2.75722700	-6.53940900	-1.31894500	
H	1.57718500	-4.45744800	-4.88496000	
H	2.33016000	-6.52947200	-3.75765400	
C	1.08687900	-2.00881900	-3.80008800	
H	1.21264300	-1.15891900	-3.11607100	
C	1.88001200	-1.68610900	-5.07380600	
H	2.96362100	-1.66446200	-4.88544700	
H	1.57910500	-0.70225900	-5.46698300	
H	1.69676500	-2.42633500	-5.86764800	
C	-0.41503400	-2.11748700	-4.10816100	
H	-0.99880300	-2.33179300	-3.20181600	
H	-0.61030700	-2.92961700	-4.82588500	
H	-0.79073200	-1.17992900	-4.54815200	
C	2.50700200	-4.49993000	0.46152700	
H	2.31644700	-3.49086900	0.85331200	
C	3.96456300	-4.86112400	0.78459700	
H		4.67181400	-4.19360800	0.26754800

H	4.20159700	-5.89015600	0.47268500
H	4.15316200	-4.79120800	1.86739300
C	1.52896600	-5.45424600	1.16442300
H	0.48334200	-5.19050200	0.94555800
H	1.66969700	-5.41946000	2.25627900
H	1.68372400	-6.49558500	0.84182700
Si	2.98745000	-0.87224600	-0.72941700
C	3.90682400	-1.09726600	0.87702800
H	4.47260000	-0.18681200	1.13050600
H	4.62180400	-1.92895800	0.77865200
H	3.22710100	-1.33175600	1.70831000
C	4.08524800	-0.71116500	-2.21885600
H	4.94470200	-0.06088600	-1.99362900
H	3.54649700	-0.30179900	-3.08362700
H	4.47205000	-1.70651400	-2.49253700

Ge/P-Rea

C	-1.27584400	-0.26990400	0.25308000
H	-1.78041100	0.70408600	0.23694700
C	0.13908800	-0.29533000	-0.31529300
C	0.43874500	-1.61446100	-0.60335300
C	-1.21723300	-0.95308500	1.65262400
H	-2.19651800	-0.89744300	2.15071300
H	-0.48300200	-0.46937700	2.31094600
C	-0.84557100	-2.42466800	1.29953400
H	0.10958400	-2.74830200	1.73507000
H	-1.61565700	-3.13190000	1.63915800
C	-0.79668900	-2.42582000	-0.26901600
H	-0.84777200	-3.41839800	-0.73081600
C	-1.91140400	-1.40316800	-0.58818900
H	-1.98377900	-1.15911900	-1.65702800
H	-2.89721400	-1.72090500	-0.21735000
N	1.66106700	-2.08837300	-0.96238300
P	1.42642400	0.87019500	- 0.53625900

C	1.64455200	2.00440200	0.85802300
C	1.91918600	3.68073600	3.07809400
C	1.89408300	1.45542300	2.12855300
C	1.52259500	3.39355300	0.70483300
C	1.66175400	4.22642500	1.81840200
C	2.03266700	2.29416400	3.23291600
H	1.96693500	0.37366600	2.25581300
H	1.31092800	3.82653600	-0.27372500
H	1.56314100	5.30730500	1.69874200
H	2.22580900	1.86625700	4.21878400
H	2.02711600	4.33608200	3.94494100
C	1.27044400	1.79554300	-2.08949300
C	1.12769700	3.02774200	-4.59254200
C	2.30604900	2.64709900	-2.51215900
C	0.17308900	1.55114400	-2.92744800
C	0.10299300	2.17328200	-4.17627100
C	2.22880300	3.26392200	-3.76093300
H	3.17309000	2.82718200	-1.87109500
H	-0.61342400	0.86711200	-2.60362700
H	-0.75451300	1.98776800	-4.82646700
H	3.03132500	3.92751300	-4.08972200
H	1.07210300	3.50990500	-5.57084900
C	1.82915700	-3.32217800	-1.68179100
C	2.20719400	-5.68747900	-3.10549800
C	1.58601300	-3.33507200	-3.07712900
C	2.26304600	-4.47655700	-0.99579100
C	2.44555900	-5.65440500	-1.73360900
C	1.77993100	-4.53713200	-3.76827100
H	2.77556100	-6.56173100	-1.22356200
H	1.59315700	-4.57608000	-4.84301900
H	2.35350700	-6.61526800	-3.66289700
C	1.08436800	-2.10382700	-3.82051100
H	1.22150200	-1.23323700	-3.16406000
C	1.85832100	-1.82376600	-5.11594800
H	2.94461000	-1.79683200	-4.94654400
H	1.55215200	-0.85300300	-5.53680900
H	1.66086200	-2.58833900	- 5.88279500

C	-0.42189900	-2.21835500	-4.10580100
H	-0.99466500	-2.40685800	-3.18728600
H	-0.62609800	-3.05010900	-4.79813700
H	-0.80293500	-1.29331300	-4.56759200
C	2.51075400	-4.47824600	0.50409800
H	2.32506000	-3.45651900	0.86516100
C	3.96552500	-4.83878700	0.83982800
H	4.67731600	-4.19295400	0.30224500
H	4.19585100	-5.87903300	0.56196100
H	4.15406600	-4.73544500	1.92002100
C	1.52638800	-5.40718000	1.23179800
H	0.48264200	-5.14446800	1.00335300
H	1.66506000	-5.34322500	2.32265500
H	1.67668000	-6.45768800	0.93786900
Ge	3.06888000	-0.81383700	-0.80290100
C	4.09064900	-1.10176500	0.83154000
H	4.61420200	-0.17573600	1.11064000
H	4.83251700	-1.89446700	0.66013600
H	3.42942300	-1.40791900	1.65272900
C	4.09920100	-0.66000400	-2.44118100
H	5.03115100	-0.11116800	-2.24477400
H	3.52182100	-0.14048700	-3.21617500
H	4.34578400	-1.67275600	-2.79346400

Sn/P-Rea

C	-1.19823900	-0.18251100	0.18523500
H	-1.66873300	0.80850500	0.16049600
C	0.21584200	-0.25626400	-0.38634200
C	0.47599900	-1.59086800	-0.66543900
C	-1.16004100	-0.85260900	1.59059300
H	-2.13467800	-0.75874800	2.09243700
H	-0.40568000	-0.38899500	2.24089400
C	-0.84080200	-2.33880200	1.24808000
H	0.10214400	-2.69211000	1.68649200

H	-1.63514000	-3.01598900	1.59339500
C	-0.79306100	-2.35305100	-0.31963700
H	-0.87814200	-3.34755200	-0.77224800
C	-1.87322200	-1.29826600	-0.64584700
H	-1.94045000	-1.05887200	-1.71611200
H	-2.86837400	-1.58055600	-0.27081400
N	1.66122700	-2.13614600	-1.02147500
P	1.48209900	0.93668700	-0.55921600
C	1.62515800	2.03246400	0.87786700
C	1.75365100	3.62731800	3.17071500
C	2.01618500	1.47058700	2.10619400
C	1.29198200	3.39301300	0.80315700
C	1.35873000	4.18534100	1.95271800
C	2.08048100	2.26825200	3.24734200
H	2.25897200	0.40750300	2.17348900
H	0.97495700	3.83381900	-0.14319200
H	1.09610900	5.24366700	1.89411300
H	2.38448400	1.83017500	4.20028400
H	1.80505200	4.25102600	4.06564900
C	1.30820500	1.91962600	-2.07727400
C	1.14610100	3.25970900	-4.52410900
C	2.25874600	2.90277800	-2.40313700
C	0.28786600	1.59885900	-2.98450500
C	0.20761600	2.27468900	-4.20480400
C	2.17134300	3.57284300	-3.62347300
H	3.06422100	3.14808400	-1.70583000
H	-0.43216000	0.81782500	-2.73255600
H	-0.59129100	2.02978400	-4.90791300
H	2.90620700	4.34035600	-3.87552600
H	1.08227900	3.78509400	-5.47941200
C	1.76270300	-3.40816500	-1.67546200
C	2.02196400	-5.85923000	-2.98190400
C	1.53456600	-3.47673600	-3.07246300
C	2.13192700	-4.55121400	-0.93322000
C	2.25477300	-5.77170500	-1.61132400
C	1.66565600	-4.71991100	-3.70321000
H	2.53397800	-6.66928300	- 1.05553700

H	1.48630900	-4.80052000	-4.77686200
H	2.11934900	-6.81981700	-3.49245000
C	1.11737600	-2.25264900	-3.87779000
H	1.33475100	-1.36192900	-3.26995600
C	1.88706800	-2.10697100	-5.19735800
H	2.97526200	-2.15528300	-5.04497600
H	1.64979300	-1.14107200	-5.67054800
H	1.61731800	-2.89518200	-5.91672900
C	-0.39816200	-2.26087600	-4.13560100
H	-0.96723700	-2.34336200	-3.19970200
H	-0.68036100	-3.11567700	-4.77019000
H	-0.71234000	-1.33896400	-4.65114600
C	2.39128200	-4.48758100	0.56351100
H	2.20876100	-3.44984400	0.87946200
C	3.85216100	-4.82927300	0.89435200
H	4.55352900	-4.19575000	0.32904100
H	4.08444600	-5.87608200	0.64397700
H	4.05416400	-4.69174000	1.96850500
C	1.41930400	-5.38276400	1.34658200
H	0.37231000	-5.13677800	1.11455600
H	1.56750300	-5.26204400	2.43137900
H	1.57223900	-6.44661300	1.10721500
Sn	3.32062900	-0.81657300	-0.89203200
C	4.43285100	-1.19274300	0.91441500
H	4.79898800	-0.23696400	1.31428000
H	5.28249100	-1.85224800	0.69397300
H	3.76927400	-1.67592600	1.64340600
C	4.30998700	-0.67465000	-2.79092800
H	5.29297800	-0.20154300	-2.66457900
H	3.68661800	-0.08423400	-3.47469300
H	4.43269800	-1.69321400	-3.18464000

Pb/P-Rea

C	-1.16827200	-0.18136200	0.25316200
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H	-1.62971900	0.81424900	0.25330300
C	0.23836100	-0.25460100	-0.34006700
C	0.48552600	-1.59074200	-0.64972600
C	-1.12239600	-0.87886500	1.64403400
H	-2.09107800	-0.78690700	2.15789200
H	-0.35768600	-0.43504000	2.29592600
C	-0.81982100	-2.36069200	1.26858100
H	0.12548300	-2.72996600	1.68830700
H	-1.61529000	-3.03799800	1.61124500
C	-0.79151700	-2.34435900	-0.29866800
H	-0.89184500	-3.32930700	-0.76901300
C	-1.86459300	-1.27354800	-0.59115600
H	-1.94410400	-1.01208800	-1.65537200
H	-2.85770000	-1.55371500	-0.20871000
N	1.64697900	-2.14479400	-1.03062400
P	1.47647800	0.95666900	-0.52757800
C	1.58455900	2.08616100	0.88438300
C	1.67939100	3.73001100	3.14442000
C	1.94051900	1.54741500	2.13401300
C	1.27182900	3.44911800	0.77184000
C	1.32062200	4.26559500	1.90531000
C	1.98775200	2.36905100	3.25861100
H	2.16832700	0.48264100	2.22818100
H	0.98213800	3.87226500	-0.19118600
H	1.07190900	5.32529000	1.81760400
H	2.26320100	1.94879800	4.22815200
H	1.71675400	4.37268300	4.02654100
C	1.31974500	1.89631400	-2.07514400
C	1.19712000	3.15036300	-4.57061000
C	2.26946500	2.87540100	-2.41675700
C	0.32041900	1.53690500	-2.99137200
C	0.26003900	2.16907700	-4.23594100
C	2.20129600	3.50310500	-3.66055100
H	3.06032300	3.14910100	-1.71313500
H	-0.39775500	0.75879900	-2.72612000
H	-0.52253000	1.89306000	-4.94594800
H	2.93490800	4.26801000	- 3.92412300

H	1.14887600	3.64182100	-5.54469500
C	1.74512400	-3.40620400	-1.69048500
C	2.01022200	-5.84499800	-3.02409300
C	1.52731200	-3.46073400	-3.09114700
C	2.11362300	-4.55884000	-0.96144600
C	2.23763000	-5.77205000	-1.65163700
C	1.65990400	-4.69685800	-3.73471200
H	2.51456800	-6.67571200	-1.10447200
H	1.48689700	-4.76561800	-4.81018200
H	2.10853200	-6.80016100	-3.54452300
C	1.11937600	-2.22377300	-3.88102100
H	1.37684700	-1.34317100	-3.27370500
C	1.85189400	-2.08908600	-5.22244100
H	2.94266100	-2.17284800	-5.10655000
H	1.63039000	-1.11121000	-5.67838200
H	1.53515800	-2.86033800	-5.94109200
C	-0.40240400	-2.19209800	-4.09616700
H	-0.94709000	-2.25596900	-3.14479500
H	-0.72415900	-3.04157200	-4.71901500
H	-0.70658500	-1.26410400	-4.60685200
C	2.37895500	-4.50701700	0.53436200
H	2.18478500	-3.47417500	0.85974500
C	3.84678500	-4.83219500	0.85140100
H	4.53527500	-4.18421900	0.28600900
H	4.09096900	-5.87313300	0.58811600
H	4.05631300	-4.70294000	1.92527800
C	1.42418300	-5.42076200	1.31646200
H	0.37281900	-5.18429900	1.09453700
H	1.57911500	-5.30841200	2.40126200
H	1.58732700	-6.48059300	1.06622700
Pb	3.43714400	-0.78718600	-0.85582600
C	4.46299300	-1.25494900	1.09475600
H	4.72840300	-0.29812600	1.56140100
H	5.35439900	-1.85809600	0.88722700
H	3.74053800	-1.81148600	1.70305600
C	4.37240500	-0.69972000	-2.89192800
H	5.40197700	-0.33654700	- 2.79091500

H	3.75817800	-0.02341000	-3.49791700
H	4.34237700	-1.72374400	-3.28390700

Si/N-Rea

C	-1.17813200	0.33279400	-0.50920000
H	-1.52042500	1.36277100	-0.66941800
C	0.23988100	0.00909300	-0.95174600
C	0.35394600	-1.33640400	-1.07401500
C	-1.39939800	-0.21107100	0.93900000
H	-2.42479400	0.02064400	1.26260600
H	-0.71644000	0.23543900	1.66986200
C	-1.19840300	-1.74404300	0.76831500
H	-0.33338700	-2.12648000	1.32738600
H	-2.07911300	-2.31276300	1.09905200
C	-1.00561200	-1.92403100	-0.78016800
H	-1.18464800	-2.93941500	-1.14812000
C	-1.90378300	-0.78007000	-1.31460400
H	-1.83176000	-0.65088800	-2.40363800
H	-2.95717700	-0.89750900	-1.02224000
N	1.59695400	-1.92777700	-1.19600400
N	1.51417700	0.74257800	-0.77334900
C	1.62905400	1.09954900	0.67671100
C	1.62570000	1.68090400	3.40801300
C	1.92303500	0.09556200	1.60178300
C	1.30075200	2.38529100	1.10881200
C	1.30316700	2.67046700	2.47741600
C	1.92996700	0.39069300	2.96512800
H	2.10250900	-0.92604100	1.27613100
H	1.03544000	3.16242400	0.39368900
H	1.04547400	3.67701000	2.81281800
H	2.16298300	-0.39846800	3.68266200
H	1.62972600	1.91068800	4.47514700
C	1.70544700	1.91821200	-1.66189700
C	2.18398500	4.04070900	-3.40058100

C	2.87950200	2.66714800	-1.53069500
C	0.77286300	2.21553300	-2.65064900
C	1.01729500	3.28439400	-3.52045700
C	3.11505900	3.72931400	-2.40320100
H	3.59870300	2.43364600	-0.74366300
H	-0.12592500	1.60864700	-2.75171500
H	0.28652300	3.52167000	-4.29615300
H	4.02932500	4.31735700	-2.30140800
H	2.37000200	4.87335700	-4.08161400
C	1.76211800	-3.31703600	-1.55436100
C	2.08337300	-6.01349700	-2.20836600
C	1.33106900	-3.77866400	-2.82205700
C	2.35077200	-4.19512000	-0.61529300
C	2.50781400	-5.54121700	-0.96909400
C	1.49732200	-5.13804900	-3.11926600
H	2.95815700	-6.23392100	-0.25558300
H	1.16699700	-5.51698300	-4.08832600
H	2.20750600	-7.06776800	-2.46484100
C	0.70582600	-2.87242700	-3.87610300
H	0.68907800	-1.84703100	-3.48276200
C	1.53551600	-2.86130300	-5.17087500
H	2.59344300	-2.63123900	-4.97923400
H	1.14274800	-2.11185300	-5.87598200
H	1.49923000	-3.83885200	-5.67552900
C	-0.74930500	-3.26417000	-4.18201500
H	-1.37492800	-3.25998600	-3.27870000
H	-0.80620500	-4.27250600	-4.62020900
H	-1.19228800	-2.56273900	-4.90640900
C	2.76460100	-3.74063100	0.77532300
H	2.65486400	-2.64955700	0.80172400
C	4.23019400	-4.06707000	1.09206500
H	4.91049400	-3.67151900	0.32263500
H	4.39889000	-5.15308600	1.15356600
H	4.52170300	-3.63597200	2.06286300
C	1.82090500	-4.31582200	1.84333700
H	0.77143900	-4.06539200	1.62722500
H	2.07241700	-3.92239600	2.84136500

H	1.89608400	-5.41346100	1.88796700
Si	2.78090300	-0.63642200	-1.44625000
C	4.36314600	-0.68938800	-0.48320100
H	4.94454500	0.22487300	-0.67799600
H	4.94885400	-1.53774600	-0.87502900
H	4.25142500	-0.81850000	0.59836400
C	3.09100000	-0.27606100	-3.23713800
H	3.74065400	0.60103400	-3.36530800
H	2.16348400	-0.11585300	-3.80096800
H	3.60628000	-1.15200300	-3.66373100

Si/As-Rea

C	-1.28612600	-0.36305400	0.34613700
H	-1.82085300	0.59465100	0.34295400
C	0.10243600	-0.35750000	-0.27524600
C	0.43455400	-1.65861500	-0.55174400
C	-1.15028700	-1.03311400	1.74936600
H	-2.10806100	-0.99399300	2.28893800
H	-0.40030000	-0.52447100	2.37075500
C	-0.75890700	-2.49944400	1.39582000
H	0.21666800	-2.79980300	1.80249900
H	-1.50290000	-3.21879600	1.76677000
C	-0.76079900	-2.50984800	-0.17328000
H	-0.79748600	-3.50547000	-0.63005500
C	-1.91735500	-1.52500700	-0.46027800
H	-2.03531400	-1.29376200	-1.52788900
H	-2.87909900	-1.86616700	-0.04936900
N	1.68515500	-2.10306400	-0.92722300
As	1.50749900	0.86798600	-0.53344800
C	1.68571000	2.15273200	0.88558700
C	1.91583000	3.98331700	2.97441300
C	1.88476900	1.69131800	2.19550500
C	1.59739100	3.52408000	0.61623700

C	1.71422200	4.43698600	1.66847400
C	1.99907800	2.61160700	3.23791300
H	1.94154400	0.62188900	2.40719700
H	1.43136500	3.88280400	-0.40116000
H	1.64295100	5.50735100	1.46434100
H	2.15113600	2.25730500	4.25956200
H	2.00546600	4.70080800	3.79275600
C	1.28311900	1.77479500	-2.21962300
C	1.03078000	2.91073400	-4.75147700
C	2.32155000	2.56654300	-2.73165000
C	0.12583700	1.53981000	-2.97142800
C	0.00212100	2.11460700	-4.23881300
C	2.18873400	3.13695000	-3.99940500
H	3.23184700	2.73909300	-2.15127800
H	-0.66490600	0.90072100	-2.57334900
H	-0.90027800	1.93832800	-4.82804200
H	2.99265900	3.75575600	-4.40345900
H	0.93194400	3.35593000	-5.74378700
C	1.83811600	-3.30911200	-1.70690900
C	2.17369600	-5.61134300	-3.23787100
C	1.59732600	-3.25166800	-3.10038000
C	2.24632100	-4.50170900	-1.07343600
C	2.40900300	-5.64713500	-1.86562400
C	1.76986200	-4.42341900	-3.84688300
H	2.72115400	-6.58328700	-1.39824100
H	1.58593800	-4.40794400	-4.92274900
H	2.30443100	-6.51458800	-3.83783900
C	1.12514000	-1.97702700	-3.78649200
H	1.26809100	-1.14397600	-3.08531200
C	1.92368400	-1.64256100	-5.05360100
H	3.00780300	-1.64593100	-4.86552800
H	1.64146800	-0.64480700	-5.42489800
H	1.72651700	-2.36178100	-5.86326700
C	-0.37871200	-2.05183000	-4.09402500
H	-0.96528400	-2.25847100	-3.18762700
H	-0.59109800	-2.85575400	-4.81610900
H	-0.73485300	-1.10435600	- 4.52852600

C	2.49519100	-4.57932200	0.42456000
H	2.30375000	-3.57998000	0.83956600
C	3.95427200	-4.94518000	0.73606900
H	4.65921000	-4.26371200	0.23370300
H	4.19323600	-5.96539900	0.39776300
H	4.14526100	-4.90175600	1.81988000
C	1.51981900	-5.54972000	1.10827800
H	0.47360100	-5.27950500	0.90050700
H	1.66513600	-5.54043400	2.20002400
H	1.67213400	-6.58346300	0.76107700
Si	3.04011400	-0.97466900	-0.67341000
C	3.86213200	-1.18519000	0.98768900
H	4.46342400	-0.29829400	1.24268600
H	4.53152200	-2.05918200	0.96317900
H	3.11977300	-1.35010800	1.78212300
C	4.19710400	-0.87425700	-2.12214400
H	5.07221600	-0.25407900	-1.87430300
H	3.70178600	-0.45486500	-3.00853600
H	4.55256600	-1.88661900	-2.37497300

Si/Sb-Rea

C	-1.25616700	-0.45359300	0.30636900
H	-1.81060200	0.49257300	0.27921000
C	0.13148800	-0.43439400	-0.31739700
C	0.48841200	-1.73416300	-0.55111700
C	-1.09628300	-1.07598900	1.72967000
H	-2.04767300	-1.03070700	2.28010100
H	-0.34457800	-0.53690300	2.32388600
C	-0.68997200	-2.54799600	1.41928000
H	0.28852300	-2.82754700	1.83459500
H	-1.42733800	-3.26298800	1.81160100
C	-0.69188600	-2.60043400	-0.14761800
H	-0.70808200	-3.60826300	-0.57835900

C	-1.86870700	-1.65065000	-0.46037400
H	-1.99473900	-1.45424600	-1.53403200
H	-2.82259000	-1.99692000	-0.03535000
N	1.74662200	-2.19847000	-0.90710700
Sb	1.66188400	0.95715900	-0.62053600
C	1.75026300	2.39495700	0.94221700
C	1.81961700	4.27300000	2.99975800
C	2.06761600	1.98482900	2.24498700
C	1.46801300	3.73786800	0.66209400
C	1.50441700	4.67518500	1.69917600
C	2.09919000	2.92982500	3.27269900
H	2.28402100	0.93833800	2.46955800
H	1.21396700	4.05916800	-0.35043000
H	1.28243800	5.72338900	1.48723700
H	2.34229200	2.61551700	4.29006200
H	1.84641300	5.00896200	3.80611700
C	1.21630300	1.98403600	-2.43114300
C	0.63858300	3.20370200	-4.86857700
C	2.05417500	2.99939100	-2.91277800
C	0.09616800	1.57081900	-3.16324700
C	-0.19022900	2.18683000	-4.38471500
C	1.75744600	3.61029200	-4.13417700
H	2.93407100	3.32050800	-2.34908900
H	-0.54627500	0.77148000	-2.78640400
H	-1.06474200	1.87200500	-4.95855200
H	2.40415100	4.40403100	-4.51455700
H	0.41217800	3.68252100	-5.82365800
C	1.87597200	-3.39258300	-1.71080100
C	2.16762300	-5.67777100	-3.27595300
C	1.66540000	-3.30310400	-3.10662100
C	2.23478000	-4.60874900	-1.09150800
C	2.37639000	-5.74494500	-1.90040300
C	1.81404100	-4.46694700	-3.87072900
H	2.65122500	-6.69830500	-1.44446400
H	1.65253800	-4.42691200	-4.94955600
H	2.28100400	-6.57404200	-3.88973600
C	1.25425300	-2.00127700	- 3.78123500

H	1.40526700	-1.18591100	-3.05935800
C	2.09871800	-1.67149300	-5.01950300
H	3.17700200	-1.70447600	-4.80046000
H	1.85237500	-0.66333200	-5.38779400
H	1.90930800	-2.37692600	-5.84291500
C	-0.24165200	-2.02427200	-4.13222300
H	-0.86020800	-2.20173400	-3.24099100
H	-0.46055000	-2.82669300	-4.85392800
H	-0.55087000	-1.06965700	-4.58574800
C	2.46583300	-4.71544900	0.40782900
H	2.25395100	-3.72867900	0.84189500
C	3.92939800	-5.06113600	0.72298000
H	4.62494700	-4.34903300	0.25004400
H	4.19285800	-6.06411400	0.35274800
H	4.10995700	-5.04927800	1.80950600
C	1.50145700	-5.71366200	1.06521000
H	0.45284400	-5.45321600	0.85647800
H	1.63998300	-5.72240300	2.15776700
H	1.67008700	-6.73895100	0.70105200
Si	3.15692800	-1.17735300	-0.58562900
C	3.76014200	-1.30539500	1.17841500
H	4.40956000	-0.45546400	1.44031700
H	4.34019800	-2.23332500	1.30221700
H	2.91322400	-1.33774500	1.88004200
C	4.46041700	-1.31930500	-1.89824400
H	5.32922900	-0.68969600	-1.65317600
H	4.07385100	-1.03067400	-2.88517700
H	4.79668500	-2.36755800	-1.95810400

Si/Bi-Rea

C	-1.01257000	-0.33513400	0.29696300
H	-1.50661100	0.64245900	0.23597400
C	0.36163100	-0.43183300	-0.34580200
C	0.62226900	-1.75291700	-0.52443100

C	-0.85789600	-0.89597200	1.74776800
H	-1.78992000	-0.75629800	2.31510300
H	-0.05785500	-0.37798700	2.29608700
C	-0.56070000	-2.40651200	1.50723600
H	0.40409300	-2.73295300	1.92221300
H	-1.33813200	-3.04655400	1.94883400
C	-0.59382400	-2.53337000	-0.05357400
H	-0.68020400	-3.55760100	-0.43565500
C	-1.71556000	-1.52908600	-0.39631300
H	-1.84686900	-1.38248200	-1.47774700
H	-2.68249400	-1.78895600	0.06006900
N	1.85880200	-2.30839500	-0.87776700
Bi	2.02877700	0.97652700	-0.75404300
C	1.82870800	2.49850800	0.87603500
C	1.49733700	4.39072400	2.88635200
C	2.29105700	2.21691800	2.16558500
C	1.20948000	3.71440900	0.57509000
C	1.04505700	4.66171900	1.59219600
C	2.11855700	3.17123200	3.17309300
H	2.77872000	1.26866000	2.40121400
H	0.85180600	3.93157100	-0.43427900
H	0.56016500	5.61460000	1.36802100
H	2.47281800	2.95967600	4.18456900
H	1.36673500	5.13377500	3.67589100
C	1.22667800	2.03323000	-2.56209400
C	0.18560800	3.28704300	-4.81338200
C	1.93612700	3.08618800	-3.14793700
C	0.00741000	1.59638400	-3.08536600
C	-0.51251400	2.23193700	-4.21825300
C	1.40541400	3.71467900	-4.27962900
H	2.89013900	3.42785600	-2.73803200
H	-0.53365000	0.76871600	-2.62067300
H	-1.46688900	1.90084100	-4.63431300
H	1.94906200	4.53993400	-4.74514300
H	-0.22334200	3.78007500	-5.69789900
C	1.91219300	-3.46343900	-1.74436200
C	2.08346600	-5.68671700	- 3.40711800

C	1.72971900	-3.29471300	-3.13513600
C	2.17268100	-4.72835900	-1.17348600
C	2.25792700	-5.83233900	-2.03208800
C	1.81766800	-4.43025600	-3.95023100
H	2.45898400	-6.82224800	-1.61780200
H	1.67866600	-4.33063600	-5.02845500
H	2.15241800	-6.55905800	-4.06068300
C	1.41906500	-1.93913400	-3.75431200
H	1.55780500	-1.17414600	-2.97751300
C	2.35878900	-1.58134200	-4.91368800
H	3.41752500	-1.65060200	-4.61841400
H	2.16486800	-0.55262600	-5.25512500
H	2.21499300	-2.24815300	-5.77747900
C	-0.05096400	-1.87177200	-4.19615000
H	-0.72957600	-2.05623100	-3.35035600
H	-0.26363100	-2.62942400	-4.96641900
H	-0.28366200	-0.88327400	-4.62016300
C	2.36082400	-4.91196200	0.32560500
H	2.11240000	-3.95535200	0.80587700
C	3.82366200	-5.23816000	0.66604800
H	4.51342200	-4.46890300	0.28175800
H	4.13223800	-6.19747700	0.22215000
H	3.96717100	-5.31145500	1.75573800
C	1.40443800	-5.96398000	0.90451700
H	0.35672300	-5.72164000	0.67011900
H	1.50648600	-6.01464900	1.99977900
H	1.61332700	-6.96909000	0.50682800
Si	3.31104900	-1.45500200	-0.45062900
C	3.65216400	-1.39526700	1.38083400
H	4.37720900	-0.60747700	1.63552300
H	4.07737800	-2.36680900	1.68323100
H	2.72309800	-1.23501800	1.94664100
C	4.73379300	-1.76821600	-1.59290700
H	5.59049900	-1.12535200	-1.34170800
H	4.44365800	-1.59870800	-2.63912200
H	5.04665800	-2.82106900	-1.49562200

benzaldehyde

C	0.21630400	0.30475400	1.07492800
O	-0.12034400	0.01038400	-0.04829200
C	1.40738800	-0.24005700	1.77020000
C	3.64574900	-1.26973700	3.08517400
C	2.23827700	-1.16778100	1.12017800
C	1.70422500	0.16854100	3.07814000
C	2.82268500	-0.34579700	3.73631600
C	3.35391000	-1.68007100	1.77707400
H	1.98298400	-1.46751800	0.10160600
H	1.05263500	0.89209300	3.57685600
H	3.05446800	-0.02864200	4.75559000
H	4.00243200	-2.40189200	1.27500800
H	4.52126200	-1.67424000	3.59907500
H	-0.37875900	1.03665900	1.68289600

C/P-PC

C	-0.78625400	-1.79417800	-0.12512700
C	-1.12641800	-2.55400200	-1.35374500
C	0.46162800	-2.16918700	0.59126700
H	-0.86558100	-3.61476400	-1.24769200
H	-2.16665000	-2.43727700	-1.67147600
H	-0.46996000	-2.13471300	-2.14633500
P	1.22542000	0.98133900	-0.10494400
N	-1.55851900	-0.81301100	0.28877200
H	0.49742600	-3.26576400	0.67132300
H	0.52990500	-1.71001000	1.58219100
H	1.33797500	-1.87085400	-0.00254600
C	0.90000200	2.61520300	-0.88776100

C	2.76266200	1.26411700	0.87133200
C	-0.03708700	0.92799900	1.23400100
C	-2.94666400	-0.70707200	-0.16884000
C	-1.15925600	0.16711500	1.25033900
C	0.93994400	2.65632600	-2.29156800
C	0.63480800	3.79954100	-0.17906600
C	3.21275600	0.23070200	1.71441200
C	3.56709600	2.40272300	0.71311500
C	-0.06366200	1.69921200	2.55534500
C	-3.89702300	-1.54287700	0.45620000
C	-3.27002600	0.21810700	-1.17412800
C	-1.94951700	0.46698800	2.51296500
C	0.73815200	3.86034900	-2.97274500
H	1.10010700	1.73747300	-2.85853800
C	0.42319600	4.99852400	-0.86088400
H	0.60271200	3.79374400	0.91029300
C	4.41749400	0.34766800	2.40737600
H	2.62412400	-0.68183000	1.82477000
C	4.78182500	2.51212600	1.39852100
H	3.24949800	3.21032700	0.05248400
C	0.16696200	0.65639500	3.69828200
C	-1.58083100	1.95478800	2.70279300
H	0.61152500	2.55982200	2.60521200
C	-3.54129300	-2.54833900	1.54592800
C	-5.22209000	-1.43432700	0.01688900
C	-2.24084900	1.12703900	-1.82303400
C	-4.61269800	0.28127000	-1.57305900
C	-1.13840300	-0.18896300	3.67680900
H	-3.01290900	0.21022900	2.48053200
C	0.48010900	5.03258300	-2.25869200
H	0.77367700	3.87817700	-4.06423700
H	0.21670600	5.91250900	-0.29954100
C	5.20787700	1.49129300	2.25042300
H	4.74511300	-0.45967500	3.06648500
H	5.39611800	3.40547900	1.26530600
H	1.07648000	0.06527600	3.53326600
H	0.28975300	1.18178000	4.65621000

H	-1.98737300	2.59935900	1.91068400
H	-1.86558400	2.35134400	3.68872800
C	-4.43579800	-2.40302000	2.78627400
C	-3.59056700	-3.98845500	1.00692000
H	-2.50963300	-2.35408000	1.87405700
C	-5.57727400	-0.53549800	-0.98852100
H	-5.98922900	-2.06476800	0.46931600
C	-2.14086100	0.88880200	-3.33634400
C	-2.54355700	2.59607300	-1.49409000
H	-1.25592100	0.88920000	-1.40034700
H	-4.90274000	0.98202700	-2.35768000
H	-0.96237700	-1.26141800	3.50679600
H	-1.69788100	-0.09882100	4.61893500
H	0.31847700	5.97337800	-2.78947100
H	6.15434400	1.58257100	2.78755500
H	-4.08686700	-3.07377400	3.58621700
H	-5.48038300	-2.67072900	2.56699400
H	-4.42928500	-1.37446100	3.17666400
H	-4.60890500	-4.24900600	0.67917700
H	-3.29596700	-4.70494700	1.78932700
H	-2.92215600	-4.12919600	0.14499800
H	-6.61680900	-0.47116700	-1.31686500
H	-3.09030400	1.11410100	-3.84623700
H	-1.36655400	1.53932400	-3.76802000
H	-1.86436300	-0.15108100	-3.56402800
H	-2.55345700	2.76511800	-0.40697000
H	-3.52514700	2.89807500	-1.89117600
H	-1.78352500	3.25480800	-1.93388700
C	2.09826900	-0.84651000	-2.79091000
O	0.99856900	-0.96299300	-3.29646400
C	2.80463800	-1.91208100	-2.05056100
C	4.06341400	-3.87631400	-0.51597700
C	2.39320500	-3.25293500	-2.15200700
C	3.86353600	-1.56545500	-1.19683200
C	4.48119700	-2.54499800	-0.41798600
C	3.02735300	-4.23234400	-1.39153000
H	1.58656800	-3.50757300	- 2.84221700

H	4.18211100	-0.52306000	-1.12318000
H	5.29055500	-2.27012900	0.26123500
H	2.72503200	-5.27826200	-1.48046800
H	4.55607000	-4.64597100	0.08277900
H	2.65022000	0.12194000	-2.84691600

Si/P-PC

Si	-0.63666800	-0.93087400	-0.57912500
C	-1.02903500	-0.98009900	-2.39021400
C	-0.06352700	-2.54632400	0.15241600
H	-0.22538200	-1.50272000	-2.92641300
H	-1.97737700	-1.52276700	-2.53455700
H	-1.14395500	0.02762700	-2.80997800
P	0.71926500	0.80224800	0.12738500
N	-1.99637500	-0.24208900	0.37600200
H	-0.78596900	-3.33617000	-0.10446000
H	0.01334600	-2.49954200	1.24802200
H	0.91160200	-2.80734300	-0.27952500
C	0.74338300	2.14293100	-1.09955600
C	2.40735800	0.45984300	0.68657000
C	-0.36426800	1.19069800	1.46034600
C	-3.37757500	-0.37802000	-0.01346200
C	-1.61916300	0.63578400	1.35775200
C	1.13629300	1.87329400	-2.42153400
C	0.28169000	3.41882800	-0.74469900
C	2.63543300	-0.59902400	1.57894400
C	3.47804100	1.25557200	0.25329900
C	-0.29809300	1.90043700	2.80589100
C	-4.12957200	-1.47867700	0.44685000
C	-3.93603600	0.59417400	-0.87754500
C	-2.38559100	1.02884400	2.60214100
C	1.07614000	2.88799400	-3.37833500
H	1.46259000	0.86789300	-2.69540000

C	0.22910800	4.42825000	-1.70782800
H	-0.05255300	3.61367900	0.27596100
C	3.93007700	-0.86505100	2.02463300
H	1.80517900	-1.21725200	1.92298900
C	4.76989200	0.98655500	0.71192500
H	3.30407400	2.08246200	-0.43737000
C	-0.31578300	0.79167600	3.90343300
C	-1.75772800	2.41067400	2.89875300
H	0.49920900	2.64545400	2.91944000
C	-3.54406600	-2.51841600	1.38886600
C	-5.46188400	-1.59172700	0.02470200
C	-3.14089900	1.80448000	-1.34832200
C	-5.27152700	0.43908300	-1.26780500
C	-1.73466600	0.16751900	3.74083100
H	-3.47670600	0.95379900	2.53135400
C	0.62483500	4.16365700	-3.02280700
H	1.37349600	2.68018400	-4.40847000
H	-0.12821900	5.42276100	-1.43236400
C	4.99809000	-0.07288600	1.59292400
H	4.10700900	-1.69632300	2.70957300
H	5.60215100	1.60867200	0.37600300
H	0.49388300	0.06379700	3.75707200
H	-0.18688800	1.23498300	4.90202100
H	-1.99825400	3.16717900	2.13908100
H	-2.02281200	2.79301700	3.89577800
C	-4.27286200	-2.52591700	2.74139200
C	-3.53533500	-3.91653500	0.75308700
H	-2.50117900	-2.23132800	1.58199500
C	-6.02946700	-0.64441200	-0.82397900
H	-6.06502500	-2.43391100	0.37024400
C	-3.24894400	2.04856200	-2.85949500
C	-3.54918400	3.06114700	-0.56352600
H	-2.08193900	1.61972600	-1.12635300
H	-5.72763500	1.17743100	-1.92999400
H	-1.71317500	-0.89948200	3.47951700
H	-2.33021900	0.26724900	4.65958200
H	0.57491900	4.95326600	- 3.77574600

H	6.01058300	-0.28694500	1.94004800
H	-3.79342700	-3.23281700	3.43697900
H	-5.32499100	-2.83101900	2.62918600
H	-4.26360400	-1.52895400	3.20717500
H	-4.55834500	-4.28917000	0.58804900
H	-3.02013100	-4.63919300	1.40545800
H	-3.02890900	-3.91261100	-0.22511800
H	-7.06941600	-0.74891500	-1.14116900
H	-4.25860100	2.37761800	-3.14991400
H	-2.54479600	2.83842000	-3.16473100
H	-3.01802300	1.14055700	-3.43628300
H	-3.45835000	2.90525600	0.52077000
H	-4.59662000	3.33052700	-0.77202100
H	-2.91497800	3.91703400	-0.84393100
C	3.35066000	-1.07392400	-2.01744600
O	2.14521000	-1.23989400	-1.92297900
C	4.38048500	-1.89914700	-1.37743600
C	6.37735400	-3.38346000	-0.10995400
C	4.03807000	-3.01943100	-0.59963700
C	5.72936700	-1.53424800	-1.52029400
C	6.72652000	-2.27265200	-0.88553000
C	5.03422300	-3.75896000	0.02994800
H	2.98824300	-3.29632300	-0.49945000
H	5.98965200	-0.66165400	-2.12533200
H	7.77514300	-1.98905100	-0.99548700
H	4.77242500	-4.63257700	0.63062500
H	7.15769200	-3.96636000	0.38494000
H	3.74944200	-0.22019900	-2.61751900

Ge/P-PC

Ge	-0.57089900	-0.95787500	-0.65827200
C	-1.03341800	-0.93943700	-2.53935400
C	-0.05253000	-2.66013100	0.13086800

H	-0.30587000	-1.54870300	-3.08986700
H	-2.04467900	-1.35693200	-2.65356300
H	-1.02383100	0.08618300	-2.92743600
P	0.74739000	0.83162100	0.14595000
N	-2.01430100	-0.24479300	0.38911100
H	-0.81554300	-3.41160400	-0.11502400
H	0.01926900	-2.57398800	1.22321200
H	0.91120800	-2.96401700	-0.29335700
C	0.77729400	2.17671500	-1.07723600
C	2.43308400	0.48107500	0.70461200
C	-0.35741900	1.17973400	1.46032200
C	-3.38906800	-0.39512500	0.00276700
C	-1.62205000	0.63130500	1.34882300
C	1.19224200	1.91965600	-2.39510100
C	0.29125900	3.44406500	-0.72431200
C	2.64859700	-0.58145400	1.59621300
C	3.51356200	1.26151200	0.26791600
C	-0.30308900	1.91347500	2.79494400
C	-4.13447900	-1.49737800	0.47209800
C	-3.95374700	0.55848500	-0.87953300
C	-2.39321800	1.05556200	2.58362000
C	1.13232000	2.93774200	-3.34824900
H	1.53163500	0.91943600	-2.67147600
C	0.23936400	4.45757900	-1.68332400
H	-0.06194500	3.62847100	0.29182600
C	3.94024300	-0.86604700	2.03814000
H	1.80897400	-1.18687000	1.94204500
C	4.80269700	0.97452400	0.72361800
H	3.34901100	2.09122700	-0.42168700
C	-0.34027500	0.82748500	3.91286200
C	-1.75859600	2.43742800	2.86250200
H	0.49872900	2.65471000	2.90304600
C	-3.54106900	-2.52110300	1.42629000
C	-5.46469500	-1.62646200	0.04859200
C	-3.16467300	1.76709900	-1.36553600
C	-5.28657100	0.38722800	-1.27189200
C		-1.76098700	0.20911600
			3.74289100

H	-3.48421500	0.98704900	2.50401700
C	0.65873400	4.20551000	-2.99331400
H	1.44683500	2.73886800	-4.37503800
H	-0.13614800	5.44550000	-1.40851800
C	5.01812600	-0.08836200	1.60355000
H	4.10775700	-1.69961300	2.72267200
H	5.64283600	1.58512600	0.38624700
H	0.46622100	0.09174700	3.78986500
H	-0.22160700	1.28800300	4.90504700
H	-1.98431600	3.18224100	2.08692500
H	-2.03290200	2.83945200	3.84936500
C	-4.25738800	-2.50306200	2.78545800
C	-3.54122000	-3.93105500	0.81716300
H	-2.49569700	-2.23104800	1.60272100
C	-6.03782200	-0.69524300	-0.81414000
H	-6.06200100	-2.46887400	0.40371800
C	-3.29381100	2.00844600	-2.87543900
C	-3.56200100	3.02642000	-0.57916500
H	-2.10235400	1.58255600	-1.15657500
H	-5.74648600	1.11198300	-1.94630000
H	-1.74217100	-0.86185000	3.49857900
H	-2.36677200	0.32641000	4.65287800
H	0.60923800	4.99810900	-3.74310200
H	6.02841000	-0.31646900	1.94814500
H	-3.77270700	-3.19728900	3.49019700
H	-5.31064000	-2.80927900	2.68710400
H	-4.24401500	-1.49771800	3.23244500
H	-4.56617900	-4.30772900	0.67509100
H	-3.01580100	-4.64108200	1.47528700
H	-3.05022900	-3.94582700	-0.16877700
H	-7.07620400	-0.81198400	-1.13218000
H	-4.30633700	2.34067800	-3.15182500
H	-2.59254400	2.79637200	-3.19235000
H	-3.07353600	1.09924600	-3.45404900
H	-3.45842500	2.87366400	0.50415100
H	-4.61189400	3.29504100	-0.77602900
H	-2.93084500	3.88134100	-0.86949500

C	3.32853400	-1.07504200	-2.00692800
O	2.12351500	-1.24823100	-1.91283600
C	4.36544900	-1.89541700	-1.37341800
C	6.38001800	-3.37360000	-0.12661900
C	4.03465600	-3.01531100	-0.59012600
C	5.71191300	-1.52701900	-1.53081200
C	6.71783900	-2.26270800	-0.90695200
C	5.03938300	-3.75170500	0.02917800
H	2.98691900	-3.29387500	-0.47685000
H	5.96341800	-0.65442100	-2.13945700
H	7.76444600	-1.97675000	-1.02894400
H	4.78627500	-4.62479100	0.63423800
H	7.16718700	-3.95424300	0.36001600
H	3.72102600	-0.21722300	-2.60501600

Sn/P-PC

Sn	-0.40790500	-1.09441400	-0.86513300
C	-1.07864900	-0.96005300	-2.89121700
C	0.07427900	-2.97121400	0.06828800
H	-0.51524000	-1.67691400	-3.50128100
H	-2.15294000	-1.18785700	-2.91330400
H	-0.90929700	0.06112300	-3.25390900
P	0.82482500	0.90455200	0.14031100
N	-1.98945200	-0.26922700	0.36227000
H	0.51609800	-3.63996500	-0.68104100
H	-0.84603900	-3.41190300	0.46923900
H	0.78712800	-2.80034900	0.88478000
C	0.79927600	2.28529300	-1.04843400
C	2.52911500	0.62845300	0.68667000
C	-0.30347500	1.13437100	1.44938700
C	-3.36675500	-0.42475000	0.00614300
C	-1.57565100	0.58290900	1.31892000
C	1.17774500	2.07225600	-2.38503900

C	0.30569800	3.53546900	-0.64843600
C	2.77681100	-0.37730300	1.63523000
C	3.59563800	1.37585500	0.16442300
C	-0.26750800	1.87058600	2.78575400
C	-4.11792600	-1.50663700	0.51471700
C	-3.93444600	0.49446400	-0.91326400
C	-2.35202500	1.01396700	2.55469400
C	1.07513800	3.11377000	-3.30909400
H	1.52851500	1.08783700	-2.70260500
C	0.20985000	4.57336200	-1.57767900
H	-0.01951300	3.68738400	0.38230400
C	4.08235800	-0.63970100	2.04763000
H	1.94563600	-0.95033200	2.05273000
C	4.89959600	1.11504800	0.59276800
H	3.40693500	2.16519300	-0.56527500
C	-0.31656500	0.79281800	3.90926900
C	-1.72210400	2.39601100	2.83768000
H	0.53369000	2.61210600	2.89960700
C	-3.52276100	-2.50470900	1.49451300
C	-5.45030300	-1.64649100	0.10114700
C	-3.14089700	1.68337500	-1.43995600
C	-5.26840900	0.31268300	-1.29634300
C	-1.73368900	0.17134900	3.72255200
H	-3.44231900	0.94567600	2.46506300
C	0.59300800	4.36376900	-2.90613600
H	1.36289800	2.94740000	-4.34946800
H	-0.17262700	5.54735600	-1.26507400
C	5.14508700	0.10621700	1.52698100
H	4.27310000	-1.42824100	2.77798600
H	5.72751700	1.70427900	0.19265800
H	0.49178600	0.05655100	3.80271800
H	-0.21247700	1.25892900	4.90069200
H	-1.93922100	3.14068600	2.05967100
H	-2.00765500	2.79927700	3.82112400
C	-4.24114300	-2.46358000	2.85171400
C	-3.51510700	-3.92771900	0.91531100
H	-2.47859300	-2.20426600	1.66515100

C	-6.02363800	-0.74760700	-0.79465200
H	-6.04897500	-2.47328900	0.48952200
C	-3.34611700	1.94586600	-2.93733900
C	-3.45773800	2.94706800	-0.62450200
H	-2.07376900	1.46615300	-1.28947500
H	-5.72744200	1.01212400	-1.99732400
H	-1.70800200	-0.89980000	3.48099300
H	-2.35072200	0.28826200	4.62510500
H	0.50862200	5.17519700	-3.63226700
H	6.16639300	-0.10111800	1.85184700
H	-3.75087700	-3.13667900	3.57297300
H	-5.29092300	-2.78306700	2.75839200
H	-4.23924700	-1.44863900	3.27600700
H	-4.53824300	-4.30894600	0.77287600
H	-2.99443900	-4.62391400	1.59224400
H	-3.01676000	-3.96284200	-0.06653700
H	-7.06345600	-0.87231500	-1.10482700
H	-4.35915400	2.31910900	-3.15288900
H	-2.63630100	2.71304800	-3.28482000
H	-3.19118500	1.03772500	-3.53801800
H	-3.29126200	2.78497300	0.44887200
H	-4.51175600	3.23893600	-0.75556400
H	-2.82530900	3.78867300	-0.94839700
C	3.25296500	-1.08078900	-1.99724900
O	2.03430000	-1.21376800	-1.98026700
C	4.21970900	-1.91621000	-1.28770200
C	6.11586800	-3.45466800	0.06620100
C	3.80763500	-2.99963100	-0.49007300
C	5.58729200	-1.61217700	-1.40086200
C	6.53392700	-2.37997500	-0.72525600
C	4.75342500	-3.76480600	0.18328200
H	2.74554700	-3.22650600	-0.41264400
H	5.90198700	-0.76735900	-2.01876500
H	7.59654200	-2.14616000	-0.81507000
H	4.43793800	-4.60943800	0.79929200
H	6.85668900	-4.06001900	0.59374000
H	3.70184200	-0.25571600	- 2.59740100

Pb/P-PC

Pb	-0.38097800	-1.15296900	-0.97336100
C	-1.11043900	-0.85617700	-3.06324400
C	0.08515600	-3.09272000	0.05919100
H	-0.56548200	-1.55357400	-3.70929300
H	-2.18858800	-1.05682800	-3.05204100
H	-0.90230200	0.18680800	-3.32605000
P	0.84302300	0.90788500	0.12196900
N	-2.02325800	-0.23653500	0.34935700
H	0.48140100	-3.78879500	-0.68964900
H	-0.84965100	-3.46311400	0.49330400
H	0.82642800	-2.87998100	0.83808700
C	0.79869300	2.27180800	-1.08620800
C	2.54841700	0.65240100	0.67102200
C	-0.28817300	1.12075100	1.42351200
C	-3.39903100	-0.40334700	0.02027100
C	-1.57672700	0.59013600	1.29998100
C	1.24901800	2.06746300	-2.40228100
C	0.21403600	3.49445400	-0.72631200
C	2.80241200	-0.35984500	1.61187900
C	3.60954600	1.42010900	0.16655500
C	-0.22489900	1.84054500	2.76904500
C	-4.13397000	-1.49757800	0.52867200
C	-3.98912500	0.51317300	-0.88947800
C	-2.32634200	1.02414100	2.55509000
C	1.12865500	3.09144000	-3.34323400
H	1.66801700	1.10102100	-2.69156700
C	0.09989300	4.51518100	-1.67273400
H	-0.16623800	3.63557700	0.28684800
C	4.10633300	-0.60383200	2.03926900
H	1.97505400	-0.95072100	2.01218000
C	4.91210500	1.17732300	0.60952100
H	3.41670800	2.21311500	- 0.55803300

C	-0.27996100	0.75541500	3.88390000
C	-1.66897000	2.39155500	2.84265900
H	0.58996200	2.56757400	2.87949200
C	-3.51417200	-2.49674800	1.49155300
C	-5.46941100	-1.64931600	0.13041800
C	-3.21053800	1.71125300	-1.41684500
C	-5.32540100	0.31959300	-1.25746800
C	-1.70928700	0.15967200	3.70665600
H	-3.41889500	0.97558600	2.47911500
C	0.55572400	4.31525000	-2.97923300
H	1.47366500	2.93177300	-4.36718400
H	-0.35323000	5.46791100	-1.39036800
C	5.16254200	0.16539400	1.53933400
H	4.30142800	-1.39650300	2.76396100
H	5.73495300	1.78416300	0.22540700
H	0.51441600	0.00632000	3.76257200
H	-0.15774300	1.21074900	4.87840500
H	-1.88252300	3.14786100	2.07477100
H	-1.93564700	2.79050200	3.83328600
C	-4.20968200	-2.47096100	2.86093500
C	-3.50419900	-3.91605900	0.90322300
H	-2.46979400	-2.18733100	1.64634400
C	-6.06374100	-0.75136800	-0.75280300
H	-6.05451400	-2.48492600	0.52086700
C	-3.45303800	1.99884100	-2.90385400
C	-3.50908900	2.96086000	-0.57312200
H	-2.14018300	1.49084400	-1.29416200
H	-5.80028200	1.01806600	-1.94884900
H	-1.70364400	-0.90909400	3.45387300
H	-2.31399500	0.27662900	4.61759500
H	0.45772500	5.11264500	-3.71908900
H	6.18281900	-0.02669700	1.87658200
H	-3.70139100	-3.14349000	3.57025400
H	-5.25783000	-2.79973800	2.78252500
H	-4.21036900	-1.45843100	3.29070900
H	-4.52625200	-4.30523600	0.77572700
H	-2.96671900	-4.61293100	1.56642600

H	-3.02337200	-3.94081200	-0.08783900
H	-7.10593600	-0.88530600	-1.05087500
H	-4.47139800	2.37422800	-3.08865300
H	-2.75291700	2.77272500	-3.25619700
H	-3.31231900	1.10148500	-3.52435500
H	-3.30895400	2.78404500	0.49216700
H	-4.56824500	3.24826800	-0.66782800
H	-2.89218200	3.81143300	-0.90348800
C	3.37923600	-1.07690500	-2.01586400
O	2.16302400	-1.20685700	-2.08403900
C	4.29229900	-1.92899300	-1.25437300
C	6.07928200	-3.49965300	0.20705700
C	3.81942300	-3.02270100	-0.50642400
C	5.66543100	-1.63198700	-1.26567400
C	6.55787600	-2.41654300	-0.53675200
C	4.71016600	-3.80340000	0.22174900
H	2.75354700	-3.24568200	-0.51215800
H	6.02731000	-0.77958800	-1.84618500
H	7.62546700	-2.18822000	-0.54766600
H	4.34745900	-4.65582100	0.80005700
H	6.77750000	-4.11726800	0.77679300
H	3.87127300	-0.24294200	-2.56847800

Si/N-PC

Si	-0.34566500	-1.58647600	-0.39133000
C	-1.06385200	-2.54051400	-1.81288000
C	0.39426300	-2.53235700	1.04346000
H	-0.34932700	-3.28031600	-2.20539200
H	-1.98667700	-3.06243800	-1.52901000
H	-1.31714900	-1.83951300	-2.62290400
N	0.98225600	1.59273800	0.49615400
N	-1.48127100	-0.39703000	0.16856500

H	-0.04384500	-3.54302000	1.05577500
H	0.11258200	-2.03972000	1.98416600
H	1.48624500	-2.63264800	1.02402600
C	0.76232600	2.68852700	-0.41480900
C	2.28488900	1.20029100	0.77917900
C	-0.09862300	1.31173500	1.38299800
C	-2.86007400	-0.52731700	-0.28088100
C	-1.20154600	0.54715500	1.16961100
C	0.82403900	2.47964300	-1.79813900
C	0.50334500	3.97540600	0.07502100
C	2.52982500	0.09023500	1.62129800
C	3.40480000	1.87087600	0.22566900
C	-0.27740300	1.98673300	2.74849100
C	-3.70836000	-1.49837800	0.30271100
C	-3.31263900	0.31134100	-1.32253800
C	-2.13078400	0.78404700	2.36388900
C	0.64972300	3.54842200	-2.68014800
H	0.98058100	1.47448400	-2.18433800
C	0.31431900	5.03919200	-0.80948700
H	0.46250700	4.14592200	1.15038300
C	3.82829100	-0.32271200	1.90584400
H	1.68348600	-0.42556000	2.06706500
C	4.69795400	1.44850500	0.52359100
H	3.25156400	2.74139400	-0.41106200
C	-0.21998900	0.89855500	3.86684900
C	-1.79817500	2.25117800	2.70455300
H	0.38722000	2.84121000	2.92564300
C	-3.27879900	-2.39028100	1.46212000
C	-5.01109700	-1.62418300	-0.19911700
C	-2.42354300	1.38967400	-1.91548200
C	-4.62684900	0.15393700	-1.78167100
C	-1.49227400	0.04936800	3.58527500
H	-3.18072700	0.54007900	2.17408400
C	0.39404900	4.83138400	-2.18932800
H	0.70278000	3.37427300	-3.75704000
H	0.11377000	6.03806600	-0.41625600
C		4.92677400	0.34598500 1.35703200

H	3.98248400	-1.17882000	2.56667100
H	5.54342000	1.99792600	0.10222600
H	0.70972300	0.31585300	3.83727900
H	-0.27107100	1.37670900	4.85612300
H	-2.08942000	2.95299400	1.91057800
H	-2.21952300	2.58090700	3.66657100
C	-4.19465300	-2.21703400	2.68495300
C	-3.20508800	-3.87424300	1.06737500
H	-2.27267300	-2.07587000	1.76588100
C	-5.46919600	-0.81007400	-1.23254400
H	-5.68211800	-2.36902600	0.23349700
C	-2.41112000	1.37759700	-3.44874000
C	-2.81603300	2.77078800	-1.36835300
H	-1.40003400	1.18896700	-1.57906200
H	-4.99528600	0.79605400	-2.58376700
H	-1.27066900	-1.00400200	3.36378000
H	-2.18537300	0.05701800	4.43899400
H	0.25364200	5.66570100	-2.87947700
H	5.94423400	0.02732100	1.58957800
H	-3.79667500	-2.77835700	3.54471600
H	-5.20848900	-2.59557500	2.48344800
H	-4.28619800	-1.16237600	2.98006100
H	-4.18935900	-4.25080500	0.74855700
H	-2.87673900	-4.48530200	1.92293000
H	-2.50354800	-4.05179400	0.23908100
H	-6.48904700	-0.92368500	-1.60673500
H	-3.39103800	1.64539000	-3.87351600
H	-1.68216300	2.11085800	-3.82621300
H	-2.13707300	0.38597500	-3.84372300
H	-2.77063300	2.78681500	-0.26957200
H	-3.84284800	3.03650600	-1.66681200
H	-2.13492900	3.54654600	-1.74728500
C	2.25743000	-0.73530200	-1.38033400
O	0.99729400	-0.75735800	-1.21842500
C	3.17818400	-1.82087100	-1.27143400
C	5.11812400	-3.82725400	-1.08585500
C	2.78868900	-3.17991900	- 1.15965900

C	4.55624700	-1.49337600	-1.32206700
C	5.51717200	-2.49398600	-1.21648800
C	3.75425500	-4.16945800	-1.07031600
H	1.73570500	-3.45481900	-1.18319300
H	4.85335800	-0.45127800	-1.43686000
H	6.57783800	-2.23825400	-1.24394900
H	3.45723800	-5.21749000	-1.00031800
H	5.87174500	-4.61466800	-1.01305800
H	2.66169400	0.22962900	-1.70933000

Si/As-PC

Si	-0.68562800	-1.03053600	-0.52062600
C	-1.08322700	-1.16292300	-2.32542700
C	-0.06590300	-2.58907900	0.29411900
H	-0.27049600	-1.68997900	-2.84342900
H	-2.02293400	-1.72521500	-2.44851900
H	-1.21526800	-0.17249700	-2.78092900
As	0.75820600	0.77296100	0.10067700
N	-2.01436100	-0.27634900	0.40943500
H	-0.77049200	-3.41291300	0.10281800
H	0.02700200	-2.46550700	1.38304000
H	0.91120400	-2.85566100	-0.13142300
C	0.75788500	2.20266800	-1.19456500
C	2.55411800	0.48076900	0.72049400
C	-0.42092700	1.21504000	1.50390700
C	-3.39125700	-0.38620800	-0.00605100
C	-1.65029300	0.62132600	1.39231300
C	1.08376200	1.92378800	-2.53002000
C	0.33344300	3.48108400	-0.81127500
C	2.82598400	-0.59291200	1.57758700
C	3.58059200	1.33446400	0.29817900
C	-0.36389700	1.88869300	2.86573600
C	-4.17312100	-1.46793600	0.44965700

C	-3.91454400	0.58859100	-0.88888900
C	-2.42656600	0.96696200	2.64809100
C	0.99442100	2.94240000	-3.48209100
H	1.38276900	0.91381000	-2.81940800
C	0.25171900	4.49297700	-1.77070500
H	0.04948000	3.67950300	0.22440900
C	4.13501500	-0.81463800	2.00838100
H	2.02679100	-1.26083900	1.90302000
C	4.88616700	1.10849400	0.74213500
H	3.36508000	2.16987200	-0.37125200
C	-0.34608600	0.74738300	3.93168700
C	-1.83605500	2.35656000	2.97829200
H	0.41371700	2.65130500	2.99767700
C	-3.61983300	-2.51776000	1.40027900
C	-5.50072700	-1.55681000	0.00738000
C	-3.08291900	1.77249400	-1.36352700
C	-5.24699600	0.45893700	-1.29828100
C	-1.75281500	0.09692000	3.76573700
H	-3.51575700	0.86710900	2.57614500
C	0.58103500	4.22385900	-3.10324700
H	1.24000600	2.73247000	-4.52539600
H	-0.07645800	5.49278400	-1.47829400
C	5.16409700	0.03461900	1.59164100
H	4.35317600	-1.65769200	2.66651100
H	5.68942500	1.77414100	0.41912500
H	0.47801900	0.04212000	3.75434400
H	-0.21462600	1.16353500	4.94161200
H	-2.09903000	3.12587100	2.23942100
H	-2.10507300	2.70555200	3.98646000
C	-4.38465700	-2.53683500	2.73214200
C	-3.59693700	-3.90863800	0.74866100
H	-2.58185000	-2.23674300	1.62596300
C	-6.03499600	-0.60395300	-0.85668700
H	-6.12653000	-2.38410200	0.34866200
C	-3.16902300	2.00519000	-2.87782700
C	-3.46198200	3.04712000	-0.59376300
H	-2.03148400	1.55978200	- 1.13078000

H	-5.67650400	1.20008700	-1.97496800
H	-1.71135800	-0.96434500	3.48339800
H	-2.34289400	0.16641300	4.69086700
H	0.50895700	5.01596500	-3.85174300
H	6.18715800	-0.14524900	1.92716100
H	-3.92775900	-3.25488900	3.43140500
H	-5.43540600	-2.83391300	2.58972700
H	-4.38043600	-1.54546300	3.20992400
H	-4.61573200	-4.27245600	0.54276200
H	-3.10897800	-4.64256900	1.40946300
H	-3.05659500	-3.89590600	-0.21142200
H	-7.07199200	-0.68880600	-1.18907000
H	-4.16647600	2.35794300	-3.18221800
H	-2.44068700	2.77291900	-3.18244300
H	-2.95656500	1.08587900	-3.44417100
H	-3.37667200	2.89978300	0.49207200
H	-4.50203500	3.33938700	-0.80841600
H	-2.80573400	3.88355800	-0.88141300
C	3.31946500	-1.00992600	-2.01251400
O	2.11379300	-1.19231500	-1.94315900
C	4.34785100	-1.85120900	-1.39192900
C	6.33945400	-3.37762000	-0.16668600
C	4.00520100	-3.01513400	-0.68051500
C	5.69423300	-1.46352500	-1.48918700
C	6.68881000	-2.22373800	-0.87566800
C	4.99816300	-3.77509000	-0.07131500
H	2.95706800	-3.31057200	-0.62016100
H	5.95470700	-0.55712000	-2.04199000
H	7.73571900	-1.92262100	-0.95075700
H	4.73637100	-4.68264400	0.47684900
H	7.11780800	-3.97731200	0.31097500
H	3.71710100	-0.12849200	-2.57133000

Si/Sb-PC

Si	-0.71425800	-1.21932200	-0.37126300
C	-1.11822200	-1.62700400	-2.13202500
C	-0.00661800	-2.60967100	0.66114500
H	-0.21562000	-2.00889200	-2.63108700
H	-1.90898000	-2.39318500	-2.17052700
H	-1.47214200	-0.73894600	-2.67258400
Sb	0.84678300	0.78706100	0.01750800
N	-2.02459700	-0.37841500	0.47874400
H	-0.68182000	-3.47883200	0.62378000
H	0.08917800	-2.29736000	1.71207200
H	0.98132600	-2.91970100	0.29081600
C	0.79634200	2.45497900	-1.30418700
C	2.83801300	0.56120700	0.71983900
C	-0.49650300	1.22068700	1.56841800
C	-3.38716000	-0.47173800	0.01237700
C	-1.68885200	0.56185000	1.44732800
C	1.12991300	2.29890000	-2.65667900
C	0.33144200	3.68313100	-0.81549300
C	3.18346000	-0.54129400	1.51205600
C	3.80909200	1.49097500	0.32848900
C	-0.50810900	1.91739700	2.92070800
C	-4.21004000	-1.51648300	0.48250400
C	-3.85343300	0.47449600	-0.93054600
C	-2.50767200	0.88052600	2.68669700
C	1.00703500	3.39156100	-3.52005900
H	1.46509800	1.32926300	-3.03136800
C	0.21753600	4.76942600	-1.68717600
H	0.04239300	3.79221500	0.23252100
C	4.50946700	-0.71049300	1.91518100
H	2.43253500	-1.27523900	1.81119200
C	5.13334100	1.31595200	0.74221900
H	3.54140900	2.34842500	-0.29410500
C	-0.44201900	0.79158000	4.00194000
C	-2.00442600	2.30472200	3.00627700
H	0.22435400	2.72306200	3.05660700
C	-3.70669300	-2.54472600	1.48352100
C	-5.52199100	-1.59536600	- 0.00506500

C	-2.97374400	1.61302100	-1.42922800
C	-5.17308700	0.35761400	-1.38334600
C	-1.81057800	0.06603500	3.82948100
H	-3.58813200	0.71968900	2.59440900
C	0.55424600	4.62326600	-3.03667800
H	1.26004900	3.27762500	-4.57659300
H	-0.14115600	5.73055100	-1.31203400
C	5.48272300	0.21646300	1.53065800
H	4.78464500	-1.57478100	2.52292600
H	5.89329800	2.04244400	0.44566700
H	0.42055000	0.12878600	3.84163300
H	-0.34341300	1.22630400	5.00784800
H	-2.29873100	3.04775600	2.25246000
H	-2.30768200	2.65265200	4.00522100
C	-4.56082700	-2.57503900	2.75880000
C	-3.60523400	-3.93776200	0.84292800
H	-2.69365700	-2.23935700	1.77962800
C	-6.00168700	-0.66743000	-0.92688000
H	-6.17880800	-2.39452000	0.34486800
C	-2.99063000	1.77168700	-2.95520100
C	-3.34701800	2.93366600	-0.73926200
H	-1.93811700	1.38461000	-1.14342900
H	-5.55956900	1.07770600	-2.10713700
H	-1.71064200	-0.99711700	3.56786300
H	-2.41604600	0.12163000	4.74569700
H	0.45824100	5.47298500	-3.71616500
H	6.51921000	0.07853000	1.84527700
H	-4.13444600	-3.27688600	3.49278600
H	-5.59190300	-2.90012700	2.54982700
H	-4.61230500	-1.58079900	3.22808100
H	-4.59696500	-4.31747600	0.55113100
H	-3.16356900	-4.66217000	1.54570400
H	-2.98480100	-3.91942900	-0.06773400
H	-7.02759700	-0.74326500	-1.29403800
H	-3.96776700	2.12433700	-3.31943500
H	-2.23583100	2.51127200	-3.26490800
H	-2.77124400	0.82252400	- 3.46809400

H	-3.29344500	2.84110200	0.35450100
H	-4.37462500	3.23289500	-0.99938800
H	-2.66545400	3.73983200	-1.05174700
C	3.38117400	-0.73110000	-2.14495500
O	2.15896800	-0.78925300	-2.17654700
C	4.25545100	-1.74155900	-1.54500600
C	5.93584200	-3.60476900	-0.32340100
C	3.72260100	-2.93643100	-1.02711800
C	5.63402100	-1.49295600	-1.45563400
C	6.47312500	-2.42316300	-0.84239000
C	4.56023000	-3.86424200	-0.41889500
H	2.65136500	-3.11849100	-1.12537700
H	6.04133500	-0.56253000	-1.85882900
H	7.54539500	-2.23093800	-0.76946200
H	4.15298500	-4.79656400	-0.02188900
H	6.59298300	-4.33591200	0.15323900
H	3.90711300	0.15478200	-2.57275500

Si/Bi-PC

Si	-0.76436300	-1.43079700	-0.30305700
C	-1.18277500	-2.03240900	-2.00394000
C	0.09129100	-2.61039300	0.86448500
H	-0.26384500	-2.30557300	-2.54487800
H	-1.83868200	-2.91594200	-1.94780000
H	-1.70696400	-1.24956400	-2.56949000
Bi	0.90783400	0.69470900	-0.25467600
N	-2.01673500	-0.50093000	0.47564500
H	-0.53909300	-3.50728100	0.98059100
H	0.20791600	-2.14274900	1.85322900
H	1.07899600	-2.92140600	0.49562400
C	0.80087800	2.61375700	-1.40312200
C	2.97535000	0.61825200	0.58371200
C	-0.44766000	1.12558400	1.45966700

C	-3.38061300	-0.55059300	0.00526000
C	-1.63571300	0.46620200	1.41936600
C	1.25817200	2.68049100	-2.72271700
C	0.21149700	3.71412900	-0.77446500
C	3.34669500	-0.41777900	1.44605800
C	3.89950900	1.58157100	0.17157000
C	-0.39888200	1.85462000	2.79357000
C	-4.23376400	-1.56204100	0.49707400
C	-3.81807300	0.39218800	-0.95275800
C	-2.39371500	0.78954900	2.69673500
C	1.12463600	3.88655100	-3.42040100
H	1.70434900	1.80596400	-3.20073700
C	0.08888500	4.91384800	-1.48314700
H	-0.16359400	3.64124400	0.24909600
C	4.66470100	-0.48374300	1.90563000
H	2.62878900	-1.17813800	1.75987000
C	5.21685300	1.50710300	0.63957200
H	3.60539200	2.38933900	-0.50376200
C	-0.25813100	0.75016400	3.89114600
C	-1.89370400	2.22699000	2.95598200
H	0.33200100	2.66910400	2.87424300
C	-3.76228400	-2.57272400	1.53236500
C	-5.54220800	-1.62112300	-0.00089800
C	-2.91440100	1.50636000	-1.46149000
C	-5.13662300	0.29580100	-1.41487100
C	-1.62783600	0.01067800	3.81810400
H	-3.47595000	0.61496200	2.66522300
C	0.54325300	4.99839400	-2.80302300
H	1.47421700	3.95379600	-4.45334800
H	-0.36722100	5.78234000	-1.00221800
C	5.59785600	0.47674800	1.50295500
H	4.96379600	-1.29308100	2.57499700
H	5.94421800	2.26106100	0.32942800
H	0.60056300	0.09259000	3.69193800
H	-0.10164700	1.20664900	4.87988200
H	-2.24085100	2.94578600	2.20050200
H		-2.14432900	2.59776000
			3.96149000

C	-4.68742600	-2.62799800	2.75573100
C	-3.58145200	-3.96393200	0.90461300
H	-2.77804500	-2.23783300	1.88835300
C	-5.99080700	-0.70299600	-0.94869500
H	-6.22206300	-2.39478000	0.36153800
C	-2.83874000	1.57320900	-2.99248800
C	-3.33646600	2.85963800	-0.87005100
H	-1.89810300	1.30379200	-1.09969800
H	-5.50109200	1.01237000	-2.15364800
H	-1.53434300	-1.05888800	3.57911800
H	-2.17767200	0.08544800	4.76755200
H	0.44132200	5.93588500	-3.35406200
H	6.62700800	0.42080200	1.86414800
H	-4.27334000	-3.30364100	3.52049300
H	-5.68992900	-3.00099800	2.49475300
H	-4.80761800	-1.63222100	3.20906000
H	-4.53975200	-4.36212100	0.53584900
H	-3.18087600	-4.67949900	1.64029500
H	-2.89239800	-3.93522500	0.04483300
H	-7.01440700	-0.76398300	-1.32493500
H	-3.80224400	1.86489000	-3.43796600
H	-2.08997600	2.31956800	-3.30065000
H	-2.55274900	0.60400800	-3.43039700
H	-3.33303600	2.83041100	0.22937200
H	-4.35368300	3.12972400	-1.19466600
H	-2.65052000	3.65513800	-1.19782800
C	3.61729400	-0.52833700	-2.39485400
O	2.42298700	-0.35490300	-2.59209400
C	4.17552800	-1.65947600	-1.64457400
C	5.22804800	-3.75572400	-0.13160200
C	3.34495900	-2.71887700	-1.23587700
C	5.53579600	-1.66436800	-1.30253700
C	6.05974700	-2.70988300	-0.54087300
C	3.86956500	-3.76389200	-0.48387300
H	2.29548600	-2.70339000	-1.53480000
H	6.17566600	-0.83793500	-1.62138000
H	7.11663900	-2.71189900	- 0.26681700

H	3.23275700	-4.59591100	-0.17441400
H	5.63985500	-4.57789600	0.45840500
H	4.36249000	0.21015100	-2.77269300

C/P-TS

C	-1.15550600	-1.62537300	-0.52631300
C	-1.98044700	-2.40960500	-1.50016700
C	-0.14620000	-2.39552900	0.28861200
H	-1.33373300	-3.08837900	-2.06447200
H	-2.71504300	-3.01542700	-0.95251500
H	-2.51518700	-1.75588500	-2.19701300
P	1.62657100	0.50230900	0.07271000
N	-1.73152700	-0.53703200	0.04606400
H	-0.14531000	-3.44565500	-0.02404400
H	-0.41747600	-2.33569100	1.35241100
H	0.88169500	-2.03596200	0.18857700
C	1.84822200	2.25561500	-0.40731200
C	3.06186300	0.03739500	1.08598100
C	0.21183200	0.59132600	1.19556800
C	-3.08953300	-0.14449900	-0.32757400
C	-1.09619600	0.25630300	1.02237100
C	1.32463900	2.69583400	-1.63460300
C	2.47124800	3.18622700	0.44496100
C	2.92473700	-0.99847900	2.02611000
C	4.34028000	0.56650100	0.83393800
C	0.28325000	1.34462800	2.53317900
C	-4.18198900	-0.87231500	0.20043700
C	-3.26534700	0.95691000	-1.18717600
C	-1.87769900	0.84369100	2.19364400
C	1.42860800	4.03808600	-2.00701900
H	0.81476000	2.00281400	-2.30317800
C	2.57368900	4.52569600	0.06744500
H	2.88836100	2.86557300	1.40064700

C	4.03573900	-1.47233200	2.72472600
H	1.94463300	-1.43763600	2.21587400
C	5.44921700	0.08814700	1.53357800
H	4.47370300	1.35658400	0.09276200
C	-0.01896100	0.33521500	3.68085900
C	-1.05199400	2.11583400	2.47008100
H	1.19437700	1.93440200	2.68001100
C	-4.04286100	-1.98861200	1.23123400
C	-5.46708500	-0.49915100	-0.21223900
C	-2.11003100	1.81098700	-1.68486700
C	-4.57460200	1.28604600	-1.56647500
C	-1.50835300	-0.03178200	3.43459400
H	-2.95003900	0.96609600	2.01475400
C	2.05391100	4.95451000	-1.15871400
H	1.01779100	4.36528600	-2.96486100
H	3.06386700	5.23880900	0.73409300
C	5.30005700	-0.92824800	2.48211200
H	3.91347800	-2.27029100	3.46029600
H	6.43585800	0.51336000	1.33721000
H	0.65044000	-0.53330500	3.66124200
H	0.11738200	0.82927300	4.65386400
H	-1.08681100	2.84023300	1.64495300
H	-1.31751600	2.61222400	3.41551300
C	-4.62330900	-1.55460500	2.58968000
C	-4.71353100	-3.30031600	0.78834800
H	-2.97097300	-2.18780600	1.38021000
C	-5.66511400	0.56002700	-1.09619500
H	-6.33096500	-1.04386600	0.17306500
C	-1.95136100	1.72001700	-3.20880700
C	-2.27110900	3.26481200	-1.21263500
H	-1.18758600	1.41634100	-1.24567300
H	-4.73932200	2.12885100	-2.24030200
H	-1.66683800	-1.10259700	3.24487100
H	-2.14378800	0.24343400	4.28857800
H	2.13803500	6.00320400	-1.45196900
H	6.16947100	-1.29799600	3.02993000
H	-4.43214700	-2.32488500	3.35316900

H	-5.71326200	-1.41567400	2.52141100
H	-4.19110900	-0.60944700	2.94279800
H	-5.80724200	-3.18935300	0.73700700
H	-4.49984100	-4.10122700	1.51281800
H	-4.37670900	-3.63916700	-0.20216300
H	-6.67693500	0.82830500	-1.40780400
H	-2.86580900	2.03989800	-3.73205000
H	-1.13482200	2.37689900	-3.55053100
H	-1.71093700	0.69179900	-3.51557800
H	-2.42491700	3.31736400	-0.12386600
H	-3.13331300	3.75374300	-1.69212700
H	-1.37341700	3.85186300	-1.45797800
C	1.21268100	-0.66847000	-1.94592000
O	-0.05239400	-0.82722200	-1.99563300
C	2.17771100	-1.81065300	-1.94644600
C	3.99341900	-3.94932600	-2.05702000
C	1.72766500	-3.11262800	-2.21294400
C	3.55473600	-1.58616300	-1.78029600
C	4.45534100	-2.64876000	-1.82111900
C	2.62978900	-4.17617600	-2.26777000
H	0.66852500	-3.27836400	-2.40697800
H	3.92506300	-0.57319000	-1.61199100
H	5.52189500	-2.46351900	-1.67338600
H	2.26887800	-5.18422700	-2.48598100
H	4.69887400	-4.78264700	-2.09270400
H	1.61081700	0.21347800	-2.48203600

Si/P-TS

Si	-0.37561700	-1.47430600	-0.60312200
C	-1.27382100	-2.51162800	-1.87499600
C	0.51036100	-2.34342700	0.80155100
H	-0.55454500	-3.18023300	-2.36972700
H	-2.08889300	-3.10763200	-1.45177900

H	-1.71908400	-1.86002100	-2.64398800
P	1.13958200	0.99488400	0.15321100
N	-1.64471800	-0.43003900	0.11282000
H	0.16689800	-3.39140300	0.81930500
H	0.22529100	-1.87789900	1.75499100
H	1.60588200	-2.34005000	0.72796800
C	1.23948200	2.55831000	-0.80057000
C	2.66527700	0.90703000	1.15781100
C	-0.22580900	1.24680100	1.24906700
C	-3.01624400	-0.69865600	-0.27570800
C	-1.40254500	0.59342300	1.01801700
C	0.65725100	2.56324600	-2.08012600
C	1.73936000	3.75946900	-0.26900500
C	2.65111500	0.16894800	2.35415000
C	3.87563800	1.47983800	0.72903700
C	-0.47466000	2.25723900	2.36125000
C	-3.64037300	-1.88557400	0.18117100
C	-3.69153500	0.19391800	-1.13733500
C	-2.42266600	1.17689500	1.98891200
C	0.56932400	3.74947200	-2.81410700
H	0.25577700	1.63626000	-2.49827900
C	1.65714800	4.94091200	-1.00766800
H	2.19239300	3.77107500	0.72423000
C	3.81058400	0.02922100	3.11742100
H	1.72022100	-0.28608000	2.69593400
C	5.03354900	1.34633300	1.50170700
H	3.91176200	2.06041400	-0.19525600
C	-0.67066300	1.45341400	3.67982500
C	-1.93579400	2.64647100	2.04017000
H	0.25978200	3.07029600	2.42154400
C	-3.08508600	-2.71766700	1.33226700
C	-4.87887400	-2.23790600	-0.36859600
C	-3.12221600	1.54994700	-1.53170900
C	-4.95140400	-0.18149600	-1.62465800
C	-1.99600800	0.68014500	3.41064000
H	-3.47220000	0.99243300	1.73637900
C	1.06993400	4.93877400	- 2.27813600

H	0.11011900	3.74433900	-3.80524500
H	2.04779300	5.87057300	-0.58800100
C	5.00458100	0.62562400	2.69859800
H	3.77739200	-0.53577400	4.05164800
H	5.95998800	1.82426800	1.17407300
H	0.18048300	0.79142600	3.88615200
H	-0.77061700	2.13735700	4.53572800
H	-2.03184100	3.16902300	1.07850900
H	-2.42232700	3.23564600	2.83271700
C	-3.99775600	-2.52290000	2.55797200
C	-2.91831700	-4.21271700	1.02241600
H	-2.09787700	-2.31575300	1.59682500
C	-5.52337800	-1.40537200	-1.28183600
H	-5.35593900	-3.17189900	-0.06235400
C	-2.86887200	1.63823400	-3.04264800
C	-4.04359300	2.68777800	-1.05727700
H	-2.15419700	1.68095300	-1.02954300
H	-5.49052800	0.49418500	-2.29214900
H	-1.87434000	-0.41170400	3.43971900
H	-2.77333300	0.94395200	4.14229700
H	1.00354300	5.86701800	-2.84979800
H	5.90568400	0.53720900	3.30936800
H	-3.58755300	-3.03716800	3.44154600
H	-5.00212300	-2.93153700	2.36420100
H	-4.11590000	-1.45663400	2.80026800
H	-3.87767100	-4.68227000	0.75537400
H	-2.53332400	-4.74276900	1.90776000
H	-2.21854900	-4.39543700	0.19336000
H	-6.48736700	-1.69792600	-1.70335400
H	-3.80587900	1.53283100	-3.61158900
H	-2.42492500	2.61129400	-3.30385300
H	-2.18452100	0.84369600	-3.38005400
H	-4.22809300	2.63393400	0.02584000
H	-5.02258400	2.65098000	-1.56056200
H	-3.59333600	3.66853800	-1.27795700
C	2.27661400	-1.02538900	-1.79541500
O	1.07448600	-1.38735100	- 1.81673200

C	3.34720400	-1.96101000	-1.62040100
C	5.40530800	-3.77012700	-1.12299400
C	3.06767000	-3.34774600	-1.54319500
C	4.67038200	-1.49232900	-1.44931300
C	5.69270700	-2.40022600	-1.19325700
C	4.09496000	-4.24514800	-1.30020600
H	2.04136400	-3.68891300	-1.68235500
H	4.87621700	-0.42058800	-1.48773000
H	6.71546800	-2.04997400	-1.04463000
H	3.88817800	-5.31552700	-1.24551300
H	6.21123200	-4.48142500	-0.92733300
H	2.52111200	0.04427800	-1.91198400

Ge/P-TS

Ge	-0.60428400	-1.53732300	-0.54229000
C	-1.70478400	-2.58204300	-1.75627800
C	0.40867900	-2.48858400	0.82560100
H	-1.08055800	-3.32345700	-2.27456200
H	-2.50083700	-3.09428800	-1.20279200
H	-2.16825000	-1.91684400	-2.49685400
P	1.34706400	0.69546300	0.33320900
N	-1.71388300	-0.25435400	0.21088000
H	0.18329700	-3.56269900	0.75188100
H	0.04745800	-2.10028400	1.78840000
H	1.48908900	-2.32584000	0.76237000
C	1.78324100	2.29682900	-0.45992100
C	2.78937800	0.28932000	1.38215800
C	-0.02134500	1.13018100	1.39443900
C	-3.06280500	-0.18067600	-0.30358600
C	-1.29033200	0.70385800	1.11860400
C	1.26940600	2.53860400	-1.74587400
C	2.50829200	3.31235000	0.18706800
C	2.62582600	-0.36541500	2.61395400

C	4.09269500	0.50995700	0.90174000
C	-0.14147200	2.16409900	2.51465700
C	-4.05966900	-1.01963800	0.24531200
C	-3.34237300	0.70871600	-1.36418500
C	-2.23079500	1.45233800	2.05639100
C	1.46805200	3.77202300	-2.37217900
H	0.68806900	1.76574100	-2.25167700
C	2.70695500	4.54360600	-0.44089600
H	2.91845400	3.14006600	1.18435400
C	3.73672000	-0.78563700	3.34890300
H	1.62177800	-0.53978700	3.00417400
C	5.20187700	0.09604900	1.64119200
H	4.24293300	1.02695300	-0.04820800
C	-0.53615800	1.40627200	3.81752900
C	-1.49720500	2.80951400	2.14669700
H	0.71934400	2.83592900	2.61870000
C	-3.81220000	-1.89733700	1.46641300
C	-5.33796000	-0.98022600	-0.32718300
C	-2.29003000	1.65984800	-1.91568400
C	-4.63678700	0.71268400	-1.89985200
C	-1.95973900	0.87277300	3.48428300
H	-3.28345300	1.45977700	1.75365900
C	2.18732500	4.77650300	-1.71945600
H	1.05971600	3.94814300	-3.37032100
H	3.26637200	5.32966700	0.07183500
C	5.02839500	-0.55602400	2.86584900
H	3.59222400	-1.28580700	4.30946000
H	6.20828000	0.29071000	1.26202900
H	0.17470500	0.60757900	4.06597100
H	-0.55935400	2.10048600	4.67078500
H	-1.46640500	3.34725200	1.18868700
H	-1.90390600	3.46723600	2.93054100
C	-4.65284400	-1.41134300	2.66013000
C	-4.07832800	-3.38730600	1.20390200
H	-2.75288800	-1.78876900	1.74273500
C	-5.62443700	-0.13180800	-1.39552000
H	-6.12678500	-1.61813800	0.07684300

C	-1.96284500	1.36335500	-3.38644600
C	-2.70478100	3.12608400	-1.71945500
H	-1.36957000	1.51199400	-1.33788800
H	-4.87611500	1.38919000	-2.72306600
H	-2.02238400	-0.22424300	3.49760100
H	-2.71314500	1.25102200	4.19053500
H	2.34386100	5.74208400	-2.20554000
H	5.89679600	-0.87519500	3.44615300
H	-4.39064500	-1.97086800	3.57182100
H	-5.72751100	-1.56225100	2.47329900
H	-4.49701100	-0.34185300	2.85847800
H	-5.12612200	-3.56559800	0.91670100
H	-3.88035600	-3.97803000	2.11185600
H	-3.44336500	-3.78885700	0.40024900
H	-6.62718000	-0.11926200	-1.82832100
H	-2.85154200	1.46982800	-4.02764800
H	-1.20201700	2.06693600	-3.76114400
H	-1.57129700	0.34287200	-3.51420000
H	-2.95733300	3.33067700	-0.66828300
H	-3.58379900	3.38467400	-2.33064900
H	-1.88213100	3.79851100	-2.00970300
C	1.71259400	-0.88455900	-2.51035800
O	0.50033600	-0.95313600	-2.24268700
C	2.73945300	-1.78575000	-2.03992400
C	4.76039300	-3.43556600	-1.05155900
C	2.43285900	-3.09298400	-1.60078500
C	4.07571400	-1.33202700	-2.01999700
C	5.07708000	-2.14787400	-1.50101600
C	3.44287100	-3.91534800	-1.11931100
H	1.41115900	-3.46655000	-1.68175800
H	4.31173900	-0.32837300	-2.38273700
H	6.10679600	-1.78860100	-1.45013000
H	3.21452400	-4.93418900	-0.79861100
H	5.54933000	-4.08113400	-0.65817200
H	2.03814900	-0.04737300	-3.15850400

Sn/P-TS

Sn	-0.68224700	-1.67052500	-0.63843000
C	-2.06410300	-2.52269500	-2.03629800
C	0.50718500	-2.68994300	0.83082000
H	-1.50452400	-3.15217200	-2.73998500
H	-2.82959600	-3.10639200	-1.51120800
H	-2.54529900	-1.69070400	-2.56757800
P	1.41080900	0.77947000	0.22437200
N	-1.74231800	-0.14745900	0.29052200
H	0.40637600	-3.77540500	0.69826000
H	0.09806400	-2.38273200	1.80312800
H	1.55764000	-2.38986800	0.75481200
C	1.67269200	2.42258400	-0.56340400
C	2.91716500	0.47856600	1.21876400
C	0.09396700	1.11937900	1.38978200
C	-3.10694800	-0.01274200	-0.14182300
C	-1.20897300	0.75070800	1.18564700
C	1.16361600	2.61051100	-1.85895400
C	2.24456100	3.51759600	0.10808600
C	2.84997600	-0.37922400	2.33074000
C	4.17138700	0.97779800	0.82814000
C	0.09569100	2.06227300	2.59545100
C	-4.10084600	-0.84273100	0.42834700
C	-3.41231000	0.90531100	-1.17250700
C	-2.04802100	1.47372900	2.23814800
C	1.22012400	3.86475100	-2.47333600
H	0.69375000	1.77761900	-2.38577400
C	2.30348400	4.76892300	-0.50751000
H	2.64791500	3.39224500	1.11455700
C	4.00540300	-0.73267900	3.02887600
H	1.88258000	-0.76332200	2.65875000
C	5.32606400	0.62928500	1.53350600
H	4.24836200	1.65705700	-0.02253900
C	-0.24090200	1.21987800	3.86141300
C	-1.25058300	2.78880400	2.37063500

H	0.98971800	2.68919300	2.69383800
C	-3.81124700	-1.76129600	1.60892300
C	-5.40180400	-0.76210000	-0.08560400
C	-2.35317800	1.82414400	-1.76538200
C	-4.72839700	0.95135800	-1.64983100
C	-1.71060100	0.78030600	3.59795200
H	-3.11720800	1.54268500	2.00879300
C	1.79110800	4.94577100	-1.79793700
H	0.81774600	3.99623700	-3.48049400
H	2.74901500	5.61341100	0.02331200
C	5.24906700	-0.23075700	2.63133000
H	3.93365000	-1.39463900	3.89496600
H	6.29112100	1.03876900	1.22531200
H	0.44593600	0.37259900	3.98681200
H	-0.16560300	1.84081700	4.76664700
H	-1.26000200	3.39294000	1.45216300
H	-1.57119300	3.40425300	3.22562500
C	-4.62532100	-1.34046400	2.84372700
C	-4.04720000	-3.24377700	1.28331800
H	-2.74796800	-1.64049300	1.86381400
C	-5.71394500	0.11849800	-1.12054700
H	-6.18718300	-1.39222200	0.33754200
C	-2.07448600	1.48968500	-3.23892300
C	-2.72192400	3.30371000	-1.58293200
H	-1.42098800	1.66190800	-1.21051900
H	-4.98676900	1.64923600	-2.44927400
H	-1.83193300	-0.31052200	3.54201300
H	-2.39177800	1.14366000	4.38131000
H	1.83848500	5.92705700	-2.27525700
H	6.15184600	-0.49981800	3.18391000
H	-4.33300900	-1.93731100	3.72201300
H	-5.70395600	-1.49211200	2.68135100
H	-4.47029200	-0.27884000	3.08478400
H	-5.09197000	-3.43207200	0.99071000
H	-3.83002600	-3.87240400	2.16103900
H	-3.40777700	-3.59097600	0.45689900
H	-6.73377700	0.16402000	- 1.50902800

H	-2.98513500	1.57408700	-3.85202500
H	-1.32897800	2.18265000	-3.65961800
H	-1.68423800	0.46603800	-3.35609100
H	-2.92635000	3.53288200	-0.52585800
H	-3.61666300	3.57698800	-2.16435900
H	-1.89272900	3.94702900	-1.91686400
C	1.85794100	-0.87816500	-2.31090800
O	0.65623300	-1.23562600	-2.36265700
C	2.94741800	-1.70254200	-1.84380100
C	5.06887800	-3.21556600	-0.84300800
C	2.76590700	-3.07633200	-1.56343900
C	4.21369700	-1.10951600	-1.65340000
C	5.26497600	-1.86177400	-1.13807400
C	3.82406600	-3.82678200	-1.06969800
H	1.79992000	-3.54272800	-1.76469800
H	4.35454300	-0.05375600	-1.89274000
H	6.23674700	-1.39703300	-0.96208600
H	3.69367100	-4.89135100	-0.86312200
H	5.89606000	-3.80806700	-0.44466200
H	2.12690100	0.11608900	-2.71280700

Pb/P-TS

Pb	-0.74027000	-1.65694000	-0.40357200
C	-2.20962300	-2.34940800	-1.93486100
C	0.57523700	-2.26325700	1.30355600
H	-1.64106900	-2.94992000	-2.65363800
H	-3.00804000	-2.90969600	-1.43950400
H	-2.58649200	-1.41880200	-2.37594900
P	1.69495700	0.98037800	0.08392600
N	-1.60851100	0.21451400	0.34197500
H	0.25900400	-3.26624600	1.61909300
H	0.36164000	-1.49684000	2.05783200
H	1.61873600	-2.23744800	0.97372500

C	1.88940700	2.47760000	-0.97112700
C	3.20511100	0.86581000	1.10284600
C	0.36843100	1.49146200	1.18301400
C	-3.01144100	0.23009700	0.07999500
C	-0.96516700	1.17960100	1.06352200
C	1.17961900	2.49073300	-2.18586200
C	2.59526700	3.62841400	-0.58118000
C	3.13163500	0.25405000	2.36628100
C	4.47057600	1.21241800	0.59535000
C	0.45694800	2.62227700	2.21818400
C	-3.82347400	-0.77860700	0.66400900
C	-3.55116000	1.14667200	-0.85479500
C	-1.72064700	2.10936300	2.01758700
C	1.17910800	3.63045000	-2.99482800
H	0.60898300	1.61042000	-2.49419200
C	2.59787600	4.76325900	-1.39585000
H	3.14518500	3.64214000	0.36157700
C	4.28687700	0.00517600	3.10847700
H	2.15790200	-0.02224800	2.77354500
C	5.62562600	0.96919300	1.34349200
H	4.55728700	1.68965900	-0.38319100
C	0.11946100	2.03322100	3.61756900
C	-0.85383800	3.38025200	1.90691900
H	1.38589300	3.20451000	2.18201200
C	-3.34652200	-1.61240700	1.85129800
C	-5.13858700	-0.92823400	0.20564800
C	-2.73375100	2.30077100	-1.41758500
C	-4.88297700	0.97674100	-1.25520800
C	-1.37382700	1.62385100	3.45998500
H	-2.79403600	2.19561600	1.81460400
C	1.89094500	4.76739700	-2.60268300
H	0.62529500	3.62843600	-3.93655300
H	3.15238800	5.65189300	-1.08496600
C	5.53885700	0.36405100	2.60047600
H	4.20787000	-0.46534100	4.09127100
H	6.59980600	1.26027600	0.94341700
H	0.77210000	1.19161200	3.88302300

H	0.24247000	2.80122800	4.39619100
H	-0.86143300	3.82307100	0.90092700
H	-1.11257100	4.14821500	2.65280500
C	-4.12152700	-1.19271600	3.11249900
C	-3.43800100	-3.13108800	1.64052300
H	-2.29177500	-1.35724000	2.03825600
C	-5.66191500	-0.07035600	-0.76053500
H	-5.77041300	-1.71534500	0.62454500
C	-2.55834600	2.18893700	-2.93819900
C	-3.35379500	3.65156600	-1.02245900
H	-1.72950700	2.25797200	-0.97536900
H	-5.31656000	1.66976400	-1.97947100
H	-1.54124000	0.54298600	3.57562700
H	-2.01685000	2.13347300	4.19257600
H	1.89650700	5.65686700	-3.23687300
H	6.44246000	0.17740600	3.18473500
H	-3.73422500	-1.71308800	4.00254400
H	-5.19123400	-1.43499100	3.01539100
H	-4.03768600	-0.10922100	3.28087200
H	-4.46945600	-3.45185000	1.42889900
H	-3.10552000	-3.66728600	2.54288100
H	-2.81667900	-3.48431300	0.79977300
H	-6.68746500	-0.20326400	-1.11184700
H	-3.52629700	2.23255100	-3.46207700
H	-1.93741600	3.01710900	-3.31346600
H	-2.06712000	1.24229300	-3.21548400
H	-3.46221100	3.74010700	0.06892600
H	-4.35331600	3.78315600	-1.46668400
H	-2.72168200	4.48383300	-1.36977000
C	1.87632500	-0.96609200	-2.04149100
O	0.64112400	-1.12137400	-2.20810200
C	2.76126200	-2.02674200	-1.56758700
C	4.49009700	-4.09800900	-0.81413200
C	2.28145400	-3.34897900	-1.44360300
C	4.12157900	-1.75980500	-1.31666900
C	4.97805500	-2.79156500	-0.93603200
C	3.13919000	-4.37650300	- 1.06743600

H	1.24187400	-3.57138100	-1.69434600
H	4.50130400	-0.74170700	-1.41622500
H	6.03341600	-2.58389000	-0.74711800
H	2.76749300	-5.40095200	-0.99305100
H	5.16768800	-4.90975700	-0.53834900
H	2.35727500	-0.05854900	-2.44656500

Si/N-TS

Si	0.05434700	-0.87856400	-0.54514800
C	-0.32573400	-1.50566500	-2.26704300
C	0.87274400	-2.05467200	0.65299800
H	0.53377600	-2.02921700	-2.70569400
H	-1.18396600	-2.19066900	-2.20739400
H	-0.61967500	-0.68878100	-2.94280900
N	0.59018400	1.14797200	0.52840800
N	-1.57806600	-0.51053600	0.07427000
H	0.70768700	-3.06771400	0.25164900
H	0.38673400	-2.00452500	1.63548400
H	1.94902200	-1.90199200	0.78079300
C	0.35343400	2.33169100	-0.33061000
C	1.93071500	1.13168400	1.09976100
C	-0.50169200	1.05702500	1.49873500
C	-2.81603000	-0.97904200	-0.49496000
C	-1.57982400	0.31599900	1.17289200
C	0.25440400	2.21436200	-1.71692300
C	0.21911800	3.59151700	0.27184900
C	2.20507200	0.32036500	2.20696800
C	2.96072700	1.91192200	0.55444000
C	-0.80121000	1.75080500	2.82647300
C	-3.27197500	-2.27767800	-0.17084200
C	-3.55461900	-0.13866900	-1.35755700
C	-2.62297100	0.51975400	2.25584700
C	0.00001900	3.34793400	-2.49858800

H	0.38938200	1.25254400	-2.20423100	
C	-0.03353300	4.71670000	-0.50987800	
H	0.32493300	3.69534500	1.35070500	
C	3.49396800	0.25896800	2.73619000	
H	1.40581700	-0.26061700	2.65776400	
C	4.24916100	1.84991200	1.09375100	
H	2.75756800	2.58297800	-0.27824200	
C	-0.87019100	0.66439700	3.95175100	
C	-2.32234700	1.99661100	2.62477400	
H	-0.18197900	2.61718000	3.08601100	
C	-2.53546500	-3.17366300	0.81330600	
C	-4.45410400	-2.73664900	-0.76642800	
C	-3.12326100	1.28699200	-1.65912200	
C	-4.73681200	-0.63825800	-1.91982400	
C	-2.08340300	-0.21470300	3.52669600	
H	-3.64899300	0.25961800	1.96985200	
C	-0.14921500	4.59898700	-1.90073200	
H	-0.08118100	3.24136500	-3.58246100	
H	-0.13538600	5.69300600	-0.02962300	
C	4.52699600	1.01859700	2.17926700	
H	3.68663800	-0.38173500	3.59958300	
H	5.03773200	2.47059500	0.66181600	
H	0.06096200	0.09358900	4.05461000	
H	-1.05483600	1.15244100	4.92038500	
H	-2.53507200	2.69605400	1.80421300	
H	-2.83810100	2.32457700	3.54047500	
C	-3.43035200	-3.57434300	1.99578100	
C	-1.93871800	-4.40952400	0.12293400	
H	-1.70511000	-2.58851600	1.22656100	
C	-5.17981200	-1.92925600	-1.63959800	
H	-4.81755300	-3.74003600	-0.53451800	
C	-3.00025600	1.55301600	-3.16504600	
C	-4.06807300	2.30055900	-0.99298200	
H	-2.13029000	1.43485400	-1.21888700	
H	-5.32166400	-0.00421600	-2.58928600	
H	-1.80614000	-1.25489200	3.30436100	
H		-2.85794300	-0.24287800	4.30684400

H	-0.34721700	5.48175100	-2.51194100
H	5.53313500	0.97537000	2.60049900
H	-2.85304100	-4.14453500	2.74092500
H	-4.27140200	-4.20769700	1.67366900
H	-3.85150100	-2.68812400	2.49434600
H	-2.72897700	-5.05855800	-0.28590100
H	-1.34941200	-5.00969000	0.83458900
H	-1.28194300	-4.12935000	-0.71557100
H	-6.09974700	-2.30350600	-2.09436200
H	-3.96720400	1.44291500	-3.68026000
H	-2.64566200	2.57933800	-3.34414100
H	-2.29095900	0.85713100	-3.64129800
H	-4.15352400	2.11675100	0.08843700
H	-5.08213700	2.24327800	-1.42044500
H	-3.69671000	3.32764400	-1.13754400
C	3.08725100	-0.09753800	-1.58142400
O	1.88423700	-0.33004400	-1.42846600
C	4.16060300	-1.04886400	-1.36181800
C	6.27483400	-2.82286800	-0.95463500
C	3.89948300	-2.41822800	-1.14598000
C	5.48975500	-0.58148400	-1.38845300
C	6.54325500	-1.46642100	-1.17490200
C	4.95556100	-3.29976300	-0.94711000
H	2.87095400	-2.77761400	-1.16390200
H	5.68550300	0.47897300	-1.56566300
H	7.57409300	-1.10714500	-1.18654800
H	4.76062600	-4.36312500	-0.79325300
H	7.10170100	-3.51961700	-0.79741900
H	3.38648600	0.90259300	-1.95086400

Si/As-TS

Si	-0.49513200	-1.67049900	-0.48281300
C	-1.29226900	-2.66229100	-1.84801500

C	0.29524700	-2.44679000	1.03069900
H	-0.58648300	-3.41054700	-2.23552900
H	-2.22054300	-3.15627100	-1.54170400
H	-1.55344400	-1.97549900	-2.67122800
As	1.03288200	1.11037700	-0.04916300
N	-1.74967400	-0.55599100	0.09782700
H	-0.05671600	-3.49035400	1.08730000
H	-0.04009900	-1.92596200	1.93742000
H	1.39255700	-2.46007900	1.01287000
C	1.13103200	2.92185500	-0.76668700
C	2.62200500	0.95054200	1.07628600
C	-0.40161700	1.22026800	1.18726300
C	-3.10841000	-0.79842200	-0.35428300
C	-1.53568900	0.49232800	0.99251600
C	0.53497000	3.11369700	-2.02294600
C	1.71082400	4.00999200	-0.09946900
C	2.56490700	0.15463000	2.23090800
C	3.85224900	1.50690900	0.69072900
C	-0.67559700	2.18146800	2.33762600
C	-3.78556700	-1.95444000	0.10782300
C	-3.71974200	0.08886500	-1.26718900
C	-2.56392900	0.99120900	2.00436600
C	0.50941700	4.38311900	-2.60546200
H	0.08628800	2.26750500	-2.54985000
C	1.69205400	5.27712100	-0.68997100
H	2.18318800	3.87165600	0.87529200
C	3.71116100	-0.06913700	2.99708500
H	1.61436000	-0.28145700	2.54140400
C	4.99745700	1.28874700	1.46467000
H	3.91771000	2.13484700	-0.20138100
C	-0.77880000	1.33266000	3.64139000
C	-2.16915600	2.48592700	2.07905000
H	0.00668600	3.03834900	2.40007200
C	-3.27976700	-2.79540700	1.27557300
C	-5.01766000	-2.27813600	-0.47285200
C	-3.11033100	1.43233400	-1.64544900
C	-4.96805000	-0.26532400	- 1.79886600

C	-2.06743300	0.49042900	3.40078500
H	-3.60653400	0.74649800	1.77314200
C	1.09135500	5.46528200	-1.93940600
H	0.04273700	4.52438300	-3.58314700
H	2.14844700	6.12346600	-0.17182100
C	4.93012600	0.50153400	2.61828700
H	3.64832400	-0.68065100	3.90023200
H	5.94496400	1.74758400	1.17206600
H	0.11569300	0.71751100	3.80364000
H	-0.88823600	1.99010500	4.51661500
H	-2.33252500	3.02533000	1.13669600
H	-2.66075800	3.02309300	2.90469100
C	-4.22454300	-2.62041400	2.47812100
C	-3.09754600	-4.28532500	0.94759300
H	-2.30445300	-2.39561200	1.57988500
C	-5.59684300	-1.45499300	-1.43723400
H	-5.54066100	-3.18227900	-0.15317600
C	-2.82136600	1.54071000	-3.14827600
C	-4.02348400	2.57913300	-1.17408800
H	-2.15312900	1.53870500	-1.11900200
H	-5.45544100	0.40364200	-2.51109900
H	-1.88616400	-0.59404800	3.40456800
H	-2.83291300	0.69623900	4.16311400
H	1.08061600	6.45705800	-2.39650000
H	5.82272100	0.34108300	3.22693300
H	-3.83127500	-3.14676600	3.36194900
H	-5.22288400	-3.02957300	2.25851100
H	-4.34827100	-1.55846100	2.73571400
H	-4.04518000	-4.75001800	0.63450500
H	-2.74478700	-4.83084000	1.83682700
H	-2.36745800	-4.45179600	0.14178300
H	-6.55488200	-1.72717500	-1.88504900
H	-3.74298300	1.44980600	-3.74388500
H	-2.37106800	2.51818000	-3.38188400
H	-2.12836700	0.75224600	-3.48219800
H	-4.25319200	2.49512600	-0.10189600
H	-4.98198500	2.57840100	- 1.71677600

H	-3.54231100	3.55491400	-1.34599600
C	2.33430500	-1.39649700	-1.54296600
O	1.14758300	-1.77395900	-1.46494300
C	3.43805000	-2.31203800	-1.49079400
C	5.59336200	-4.04976300	-1.20948400
C	3.21464800	-3.70811400	-1.43941600
C	4.75018500	-1.79567200	-1.40209400
C	5.82337100	-2.66874500	-1.25370200
C	4.29199900	-4.57055100	-1.30574500
H	2.19329300	-4.08514500	-1.50840500
H	4.90961000	-0.71504900	-1.41744100
H	6.83974700	-2.28109100	-1.16731800
H	4.13131900	-5.64953900	-1.27127300
H	6.43760600	-4.73356100	-1.09560600
H	2.54514000	-0.31599400	-1.61477900

Si/Sb-TS

Si	0.64748100	1.68828400	-0.52492000
C	1.42208200	2.55929400	-1.97965800
C	-0.10119700	2.53381900	0.97261800
H	0.76831900	3.36298200	-2.34435100
H	2.41361500	2.96250100	-1.74316500
H	1.55994100	1.82701400	-2.79358900
Sb	-0.92987900	-1.12088800	-0.21020700
N	1.90770200	0.61424100	0.10259600
H	0.24328600	3.58174700	0.95283000
H	0.27363600	2.06568400	1.89202300
H	-1.19765800	2.54123200	0.99222100
C	-1.16339500	-3.21739000	-0.63292000
C	-2.69570600	-0.73386500	0.97591700
C	0.55522000	-1.09299300	1.27855400
C	3.25601000	0.76229300	-0.40544500
C	1.68638100	-0.36450100	1.07043900

C	-0.61488200	-3.67668200	-1.84015700
C	-1.83906500	-4.10879500	0.21180500
C	-2.61385200	0.13160300	2.07758500
C	-3.94728900	-1.24796600	0.60189200
C	0.79222400	-1.91808700	2.53778300
C	4.01975300	1.87842500	0.01336800
C	3.76834000	-0.18123800	-1.32076400
C	2.68004100	-0.73695100	2.16538300
C	-0.73379000	-5.02207500	-2.19950400
H	-0.09654100	-2.98514600	-2.51101600
C	-1.95797600	-5.45402000	-0.15353600
H	-2.28138400	-3.76063200	1.14855900
C	-3.76239900	0.47869700	2.79524700
H	-1.64548600	0.52516000	2.39195700
C	-5.09522400	-0.90628300	1.32610000
H	-4.03329100	-1.93697000	-0.24341700
C	0.82144100	-0.92389200	3.74061800
C	2.30199200	-2.21960100	2.38441800
H	0.12245000	-2.77692800	2.67064400
C	3.55772500	2.81570200	1.12347600
C	5.27170300	2.08023700	-0.57952800
C	3.02581700	-1.46475000	-1.66809100
C	5.03169900	0.05969700	-1.87881100
C	2.11500500	-0.09708500	3.47536300
H	3.72821000	-0.50098200	1.94925100
C	-1.40718500	-5.91012900	-1.35603700
H	-0.30793800	-5.37338700	-3.14265700
H	-2.48600500	-6.15018300	0.50266300
C	-5.00534900	-0.03960600	2.42020700
H	-3.68327800	1.14523500	3.65775900
H	-6.06288100	-1.32761700	1.04198400
H	-0.08524300	-0.30538400	3.78261500
H	0.88751300	-1.47477200	4.69061200
H	2.52063300	-2.85400200	1.51493400
H	2.75917100	-2.65482300	3.28644900
C	4.48104800	2.69682800	2.34749600
C		3.43576500	4.28031700 0.67623400

H	2.56363100	2.48182400	1.44603800
C	5.76796200	1.19117100	-1.53260100
H	5.87348500	2.94251600	-0.28385000
C	2.71419800	-1.58558800	-3.16527100
C	3.81412400	-2.68542200	-1.16116600
H	2.06636000	-1.45546800	-1.13529400
H	5.44615900	-0.65194500	-2.59603900
H	1.92840300	0.98026200	3.35765300
H	2.84384200	-0.21227500	4.29089700
H	-1.50767600	-6.96043700	-1.63929100
H	-5.90115900	0.22151000	2.98848200
H	4.09364300	3.30091300	3.18303800
H	5.49694400	3.05387500	2.11798800
H	4.56155100	1.65435200	2.68826000
H	4.40522800	4.68408800	0.34545100
H	3.08647300	4.90768700	1.51143400
H	2.72664300	4.40401400	-0.15602000
H	6.74288000	1.37085400	-1.99113300
H	3.63263300	-1.59839900	-3.77243600
H	2.17402700	-2.52472900	-3.36784400
H	2.09071000	-0.74812500	-3.51731500
H	4.06956400	-2.58029300	-0.09632800
H	4.75800000	-2.81086900	-1.71502700
H	3.22539900	-3.60859300	-1.28404600
C	-2.30396000	1.63779800	-1.54635100
O	-1.11318100	1.97730300	-1.46367400
C	-3.39677400	2.57081600	-1.45752100
C	-5.52917500	4.32151300	-1.09544200
C	-3.15747700	3.96128900	-1.37819500
C	-4.71082000	2.06595100	-1.35880100
C	-5.77342500	2.94492700	-1.17004400
C	-4.22450000	4.83093500	-1.20386700
H	-2.13322800	4.32975900	-1.45698900
H	-4.88054500	0.98746400	-1.39717600
H	-6.79162800	2.56348800	-1.07478500
H	-4.05245000	5.90742400	-1.14648500
H	-6.36434000	5.01037300	- 0.94774200

H	-2.55150100	0.56487300	-1.65182000
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Si/Bi-TS

Si	0.81726600	1.76257500	-0.41052500
C	1.41306000	2.58880300	-1.96401600
C	0.03185400	2.59276000	1.06549800
H	0.74110300	3.40778300	-2.25153000
H	2.44017000	2.95841300	-1.84377000
H	1.42578400	1.84232400	-2.77653900
Bi	-0.82175400	-1.02170600	-0.26311100
N	2.08245900	0.69998300	0.15117200
H	0.30389200	3.66039900	1.00277400
H	0.45806100	2.17250500	1.98582000
H	-1.06059100	2.52466200	1.10317800
C	-1.11393600	-3.23479000	-0.60633500
C	-2.61538200	-0.62058500	1.06271900
C	0.74056700	-1.00929400	1.32483400
C	3.40526200	0.82584600	-0.42085200
C	1.87070400	-0.28352300	1.12576900
C	-0.61607900	-3.74682700	-1.81185100
C	-1.81501100	-4.06140100	0.27870300
C	-2.48535200	0.20709400	2.18636800
C	-3.88126100	-1.10868700	0.70863800
C	0.97400200	-1.82808600	2.58778500
C	4.19705700	1.93571000	-0.04077500
C	3.85906400	-0.12558200	-1.35822300
C	2.86365700	-0.64394200	2.22359700
C	-0.81470500	-5.09384000	-2.13230200
H	-0.07916400	-3.10231500	-2.51480700
C	-2.01055700	-5.40888700	-0.04816000
H	-2.21959300	-3.66528900	1.21376100
C	-3.60915500	0.54958700	2.94599300
H	-1.50303200	0.57614900	2.48666700

C	-5.00395600	-0.77038600	1.47410600
H	-4.00241300	-1.77154600	-0.15342600
C	0.99696400	-0.82643700	3.78656800
C	2.48747500	-2.12664200	2.44516500
H	0.30619600	-2.68766000	2.72468800
C	3.77940100	2.89819100	1.06559900
C	5.43055200	2.11115600	-0.67939400
C	3.06149700	-1.37765200	-1.69673900
C	5.10484700	0.09051400	-1.96287400
C	2.29310300	-0.00111100	3.52882700
H	3.91208900	-0.40600700	2.00822800
C	-1.51366300	-5.92323600	-1.25058500
H	-0.43114400	-5.49102800	-3.07564500
H	-2.55899500	-6.05927600	0.63788800
C	-4.86995600	0.06277800	2.58932900
H	-3.49640100	1.18957400	3.82484800
H	-5.98597200	-1.16688800	1.20369300
H	0.09012800	-0.20783200	3.82042300
H	1.05569000	-1.37422400	4.73879900
H	2.71468600	-2.76276500	1.57887500
H	2.93795600	-2.55919500	3.35189500
C	4.75129600	2.81947300	2.25404400
C	3.62656100	4.34645700	0.57621300
H	2.80141900	2.56937700	1.44091000
C	5.87600000	1.20694400	-1.64332300
H	6.05764300	2.96452700	-0.41221900
C	2.67650400	-1.44819800	-3.18042600
C	3.82377400	-2.63755200	-1.25271100
H	2.12912000	-1.34818800	-1.11920600
H	5.47637800	-0.62637900	-2.69802600
H	2.10843100	1.07652300	3.40767400
H	3.01590100	-0.11506400	4.34994700
H	-1.67695000	-6.97324300	-1.50453000
H	-5.74609000	0.32339700	3.18757400
H	4.39630600	3.45053200	3.08393000
H	5.75721500	3.16865300	1.97419300
H	4.84492400	1.78816400	2.62503000

H	4.57844100	4.74567200	0.19305500
H	3.30379000	4.99925900	1.40241900
H	2.88464100	4.43522000	-0.23213400
H	6.83760400	1.36577200	-2.13633600
H	3.56447400	-1.48017500	-3.83060000
H	2.09008000	-2.35999500	-3.37998800
H	2.07119900	-0.57842100	-3.48294600
H	4.12057100	-2.56991700	-0.19537200
H	4.74119800	-2.78140400	-1.84509600
H	3.19715600	-3.53520800	-1.37702800
C	-2.40367400	1.83054200	-1.41417500
O	-1.21789600	2.16075500	-1.36340800
C	-3.51140400	2.76354500	-1.34781600
C	-5.66299300	4.51428400	-1.11310700
C	-3.28443300	4.15559300	-1.34133700
C	-4.82024500	2.25534400	-1.23559100
C	-5.89387900	3.13395400	-1.11207400
C	-4.36093200	5.02597700	-1.23028000
H	-2.26175000	4.52665000	-1.42961500
H	-4.98098000	1.17459000	-1.22074300
H	-6.91037100	2.74866800	-1.01278600
H	-4.19726900	6.10543300	-1.23274300
H	-6.50593400	5.20303400	-1.02041100
H	-2.67550400	0.75696200	-1.48703800

C/P-Prod

C	-0.72170000	-0.64683800	0.98844000
H	-1.32526700	0.26122200	1.11518800
C	0.74066700	-0.40256900	0.58043000
C	1.21576200	-1.59169700	0.05929900
C	-0.69529500	-1.58329600	2.22941700
H	-1.70897200	-1.72056100	2.63409600
H	-0.06902400	-1.17270400	3.03335000

C	-0.13598200	-2.90599900	1.63047500
H	0.80869100	-3.22529500	2.09054800
H	-0.84825000	-3.73613100	1.73982100
C	0.03810700	-2.56709700	0.11080200
H	0.13674100	-3.43746800	-0.54419100
C	-1.15736200	-1.62834900	-0.11639900
H	-1.17407600	-1.18132500	-1.11996900
H	-2.12613900	-2.10972700	0.08333400
N	2.45256300	-2.00244300	-0.33680100
P	1.41631900	1.20472200	0.71616900
C	0.96081100	1.94091500	2.30818100
C	0.22277300	2.94401800	4.81508700
C	1.56173200	1.43746700	3.47665500
C	-0.02362300	2.93622200	2.40525100
C	-0.38812700	3.43442300	3.65860700
C	1.19656800	1.94298800	4.72357600
H	2.30906400	0.64298500	3.42130800
H	-0.50913200	3.32098800	1.50767400
H	-1.15492700	4.20876900	3.72943200
H	1.66902500	1.55245000	5.62729700
H	-0.06308100	3.33796900	5.79271000
C	0.80650100	2.26738000	-0.61549000
C	-0.04109600	3.86259100	-2.74977500
C	1.07760900	3.64872000	-0.61286600
C	0.11450000	1.69242800	-1.69102200
C	-0.31011300	2.49173200	-2.75424800
C	0.65237600	4.43837300	-1.67940200
H	1.62792900	4.10717500	0.20891300
H	-0.08540000	0.62222700	-1.69473500
H	-0.85387000	2.04082200	-3.58683700
H	0.86930000	5.50840400	-1.67701100
H	-0.37275600	4.48637300	-3.58275500
C	2.53712000	-3.02377200	-1.36397500
C	2.80502300	-4.93106700	-3.37551500
C	2.40368000	-2.62495600	-2.71194000
C	2.76608400	-4.37009200	-1.00747100
C	2.90242900	-5.30937300	- 2.03795700

C	2.54755100	-3.60249800	-3.70563700
H	3.08384400	-6.35665000	-1.78831200
H	2.45671800	-3.31823500	-4.75595700
H	2.92002900	-5.67795200	-4.16408800
C	2.09000700	-1.18943400	-3.11542800
H	2.03379600	-0.58413000	-2.20264600
C	3.19133300	-0.56888300	-3.98750300
H	4.16761200	-0.58837400	-3.48096500
H	2.94993400	0.48235500	-4.21213300
H	3.30004500	-1.09750400	-4.94734900
C	0.72552600	-1.11298400	-3.81801700
H	-0.07900700	-1.50597000	-3.17722100
H	0.71902000	-1.69919000	-4.74983800
H	0.48391400	-0.07219600	-4.08149700
C	2.83594400	-4.83615200	0.43964400
H	2.64476700	-3.96005900	1.07365200
C	4.22156900	-5.38960300	0.80767000
H	5.02134300	-4.65414300	0.63294500
H	4.46389500	-6.28465300	0.21396700
H	4.25307300	-5.67758400	1.87022900
C	1.74337700	-5.87243400	0.74897700
H	0.74343700	-5.50276800	0.47946900
H	1.73858400	-6.11815500	1.82246500
H	1.91135400	-6.80928800	0.19566900
C	3.68332500	-1.29522700	0.09296800
C	3.86247800	-1.48344400	1.60287700
H	4.69909100	-0.88121200	1.98422600
H	4.10253200	-2.53674900	1.79118500
H	2.94967300	-1.24406000	2.16453100
C	4.91386600	-1.80887400	-0.64572500
H	5.78724800	-1.26233700	-0.26561200
H	4.82646700	-1.62182300	-1.72117400
H	5.06555100	-2.88197200	-0.49063900
C	3.28931200	1.09701900	0.60818600
O	3.59796000	0.08927400	-0.30641000
C	3.88058700	2.41619300	0.18964000
C	4.14089500	2.68407900	-1.15981500

C	4.09757400	3.41070300	1.15359500
C	4.61105800	3.94204300	-1.54084000
H	3.97123300	1.90465400	-1.90318300
C	4.55743600	4.67159200	0.76725000
H	3.90111000	3.20215600	2.20856600
C	4.81222800	4.93930400	-0.58164200
H	4.81752600	4.14677200	-2.59359500
H	4.72802900	5.44266800	1.52163000
H	5.17766200	5.92334500	-0.88338300
H	3.62386500	0.86390300	1.62808000

Si/P-Prod

C	-0.64867400	-0.56277800	1.09584400
H	-1.21069000	0.36158800	1.27712400
C	0.79345000	-0.35958100	0.58301600
C	1.17638400	-1.55996200	0.00720400
C	-0.57276600	-1.51935800	2.31806900
H	-1.56256900	-1.62704300	2.78596800
H	0.11764200	-1.14665000	3.08618300
C	-0.10252300	-2.84967100	1.66476500
H	0.86184000	-3.20406700	2.05124000
H	-0.83169800	-3.65845000	1.81505000
C	-0.02651600	-2.49371100	0.14071900
H	-0.00350200	-3.35931000	-0.52875200
C	-1.19958100	-1.50886500	0.01284900
H	-1.27281300	-1.04134200	-0.97864800
H	-2.16928300	-1.95663200	0.27659400
N	2.36885400	-1.99767400	-0.49626300
P	1.47367400	1.25749200	0.70619900
C	0.91457300	1.98519700	2.26867100
C	0.07707700	3.00198500	4.73711800
C	1.40275800	1.42882100	3.46480500
C	-0.00817100	3.03955300	2.31616100
C	-0.42273400	3.54482400	3.55127600
C	0.98828600	1.94066600	4.69345200
H	2.10197300	0.58971200	3.44177300
H	-0.40870400	3.46454200	1.39537900
H	-1.14170300	4.36596200	3.58443400
H	1.37239500	1.50837300	5.61965900
H	-0.24775400	3.40157100	5.70017600

C	0.92710300	2.29019300	-0.67537700
C	0.14563600	3.83480300	-2.87231800
C	1.18662700	3.67437300	-0.69094200
C	0.27726200	1.68849100	-1.76320600
C	-0.11246700	2.46180800	-2.85801600
C	0.79323400	4.43797000	-1.78900700
H	1.69444300	4.15751100	0.14332000
H	0.07920200	0.61796100	-1.74854200
H	-0.62275700	1.99010300	-3.70007700
H	0.99842200	5.51026300	-1.79899000
H	-0.16062300	4.43881300	-3.72924700
C	2.37487200	-3.09222600	-1.45195900
C	2.51526300	-5.13798500	-3.34183800
C	2.16992200	-2.78738700	-2.81602100
C	2.64403900	-4.40960400	-1.02255700
C	2.71148300	-5.41976900	-1.99187900
C	2.24202100	-3.83291800	-3.74575800
H	2.91918100	-6.44610800	-1.68273400
H	2.08477000	-3.62115300	-4.80519300
H	2.57294800	-5.93913700	-4.08185700
C	1.84756500	-1.37902600	-3.29703600
H	1.96609300	-0.69424100	-2.44611300
C	2.80190400	-0.89501200	-4.39784500
H	3.85292300	-0.95364500	-4.07712200
H	2.58453800	0.15337900	-4.65573700
H	2.70140100	-1.48975300	-5.31880600
C	0.38593700	-1.29918500	-3.76663000
H	-0.31162400	-1.58737600	-2.96576700
H	0.20650800	-1.97583200	-4.61652500
H	0.13596500	-0.27944400	-4.09681200
C	2.85197700	-4.76855600	0.44124200
H	2.69265200	-3.85510000	1.03013300
C	4.28517500	-5.25410200	0.70953200
H	5.03537800	-4.51619200	0.38725600
H	4.49585600	-6.19044600	0.17003500
H	4.43608800	-5.44799100	1.78328700
C	1.82613000	-5.80683800	0.92176100
H	0.79547600	-5.48150600	0.71861200
H	1.92481500	-5.97406800	2.00583500
H	1.97306800	-6.77704300	0.42274200
Si	3.94807400	-1.28032800	-0.06850800
C	4.30589200	-1.63049600	1.73306700
H	5.11032000	-0.98167800	2.11542500
H	4.63514100	-2.67240500	1.85551000
H	3.41186200	-1.49050100	2.36081900

C	5.23809000	-1.84052300	-1.27020200
H	6.21452300	-1.42066700	-0.98183800
H	4.99614900	-1.49085600	-2.28415200
H	5.32145000	-2.93588100	-1.30167800
C	3.35699600	1.26067800	0.73990500
C	3.89952000	2.65383700	0.56084800
C	4.74962600	5.29492900	0.19035200
C	3.91312200	3.54685800	1.64227700
C	4.32716300	3.08271100	-0.70122500
C	4.75627000	4.39894900	-0.88255600
C	4.33077600	4.86584600	1.45446800
H	3.59170500	3.21468400	2.63192500
H	4.31697300	2.37814600	-1.53305600
H	5.09312100	4.72816400	-1.86796100
H	4.34024200	5.55776700	2.29937000
H	5.08197400	6.32527200	0.04587200
O	3.78286800	0.39009300	-0.26071400
H	3.61241700	0.89705300	1.74981900

Ge/P-Prod

C	-0.53393800	-0.85281400	1.39314600
H	-1.10398400	0.02819800	1.70976000
C	0.86232600	-0.55377400	0.80274900
C	1.22535200	-1.68962800	0.09149500
C	-0.35767100	-1.92857800	2.50208900
H	-1.30967600	-2.10211300	3.02549400
H	0.38468700	-1.63147400	3.25543100
C	0.08219700	-3.17753100	1.68846300
H	1.07260700	-3.55251200	1.97683400
H	-0.62769400	-4.00924400	1.80214400
C	0.05473600	-2.66659600	0.21026600
H	0.05065700	-3.45863400	-0.54548200
C	-1.14089700	-1.69869500	0.25691500
H	-1.27670700	-1.12899700	-0.67265200
H	-2.08561100	-2.19252200	0.53068100
N	2.38536900	-2.02902000	-0.53195800
P	1.44100300	1.10739700	0.69702700

C	0.74730800	2.05987000	2.06451400
C	-0.02265300	3.59932800	4.26668600
C	0.74057500	1.49370700	3.35084100
C	0.37676700	3.40148300	1.88641100
C	-0.01276900	4.16452400	2.98873900
C	0.35535600	2.26404500	4.44766900
H	1.03686800	0.45336800	3.49445700
H	0.40374300	3.85419000	0.89475700
H	-0.30306100	5.20761500	2.84792200
H	0.34758600	1.82189800	5.44607700
H	-0.32613500	4.20036900	5.12664700
C	0.88399300	1.85783200	-0.85740800
C	-0.10250300	2.94509000	-3.23888800
C	1.76680400	2.18262100	-1.89698900
C	-0.49955000	2.05558400	-1.02426800
C	-0.98751200	2.59965100	-2.21109700
C	1.26860900	2.73219300	-3.08107700
H	2.83153100	1.99550200	-1.79028200
H	-1.19581900	1.79514900	-0.22412200
H	-2.06098700	2.75718000	-2.33433900
H	1.95987500	2.99502700	-3.88443400
H	-0.48563800	3.37655200	-4.16609800
C	2.37971800	-3.02872600	-1.57935500
C	2.45780800	-4.89565000	-3.64739300
C	2.11375500	-2.60558800	-2.90130100
C	2.70119300	-4.37095800	-1.28312200
C	2.73405900	-5.29076900	-2.34034900
C	2.15029200	-3.56412500	-3.92188500
H	2.97769600	-6.33517700	-2.13546000
H	1.93966400	-3.26336900	-4.94969800
H	2.48523000	-5.62833000	-4.45691600
C	1.77223900	-1.15849300	-3.22407100
H	2.04775500	-0.54935600	-2.35283100
C	2.55964700	-0.61543400	-4.42319900
H	3.64504400	-0.74429200	-4.28885000
H	2.35554900	0.45790000	-4.55385300
H	2.27896400	-1.11618900	- 5.36253400

C	0.25952400	-0.99045000	-3.43547100
H	-0.30782900	-1.35584400	-2.56771400
H	-0.07920400	-1.55908800	-4.31623800
H	0.00316200	0.06816100	-3.58975600
C	3.01210100	-4.84342100	0.12960300
H	2.84522100	-3.99299600	0.80529800
C	4.48193600	-5.27002500	0.27275100
H	5.17420700	-4.46387700	-0.01533000
H	4.70886900	-6.13698600	-0.36689100
H	4.70569700	-5.55579200	1.31282700
C	2.07051700	-5.97261400	0.57498100
H	1.01474600	-5.68792400	0.45791700
H	2.24208600	-6.22411000	1.63338900
H	2.23546700	-6.88849700	-0.01312500
Ge	4.07700600	-1.30493100	-0.09278700
C	4.46462300	-1.76245800	1.76049500
H	5.21723200	-1.07727700	2.17737300
H	4.85879500	-2.78684400	1.80454700
H	3.54763900	-1.71215600	2.36446700
C	5.31948700	-1.73302400	-1.50704500
H	6.32931800	-1.40810600	-1.21915700
H	5.01338000	-1.20193700	-2.41866300
H	5.32314100	-2.81152000	-1.71020500
C	3.31593900	1.22804500	0.85899400
C	3.83761900	2.64759100	0.92239100
C	4.80254100	5.28110200	1.05383000
C	3.64764200	3.41743800	2.08072900
C	4.54693200	3.19674300	-0.15346300
C	5.02400100	4.50768900	-0.08835800
C	4.12065000	4.72872900	2.14191700
H	3.13759400	2.99110000	2.94590000
H	4.74951800	2.58163000	-1.02996600
H	5.57945200	4.92352000	-0.93192000
H	3.96516600	5.31703900	3.04877500
H	5.17553500	6.30639600	1.10341800
O	3.88038300	0.49903800	-0.18506300
H	3.47869800	0.75533400	1.84695300

Sn/P-Prod

C	-0.51320000	-0.77703000	1.38033500
H	-1.04898800	0.12089000	1.70757500
C	0.90171500	-0.52613300	0.80525500
C	1.21520400	-1.66766000	0.07266100
C	-0.39357500	-1.87756800	2.47170800
H	-1.35652700	-2.01904400	2.98481600
H	0.35482800	-1.62517800	3.23536900
C	-0.00166300	-3.13098300	1.63971900
H	0.97152900	-3.55154300	1.92545600
H	-0.74598700	-3.93443200	1.73684000
C	0.00065400	-2.59438900	0.17225100
H	-0.03342800	-3.37366300	-0.59591700
C	-1.14864000	-1.57377100	0.22438300
H	-1.24608500	-0.98253900	-0.69692600
H	-2.11868000	-2.02697500	0.48011600
N	2.34731300	-2.05101700	-0.56301300
P	1.50672000	1.12689200	0.69464800
C	0.80493000	2.09016900	2.05269100
C	0.03738300	3.64507400	4.24613800
C	0.75570800	1.52100600	3.33647100
C	0.48146900	3.44370300	1.87439400
C	0.09199900	4.21421700	2.97125400
C	0.37166700	2.29867200	4.42866500
H	1.01823500	0.47202400	3.48171900
H	0.54759800	3.90101500	0.88668600
H	-0.16105200	5.26668500	2.82878000
H	0.33061000	1.85310700	5.42475000
H	-0.26572700	4.25181800	5.10220000
C	0.95909600	1.86401600	-0.87168800
C	-0.01076900	2.88878600	-3.28871500
C	1.83728200	2.08006700	-1.94383700
C	-0.41315000	2.13670400	- 1.02444400

C	-0.89281100	2.64804700	-2.22928500
C	1.34816300	2.60194900	-3.14413900
H	2.88918600	1.82313700	-1.84432100
H	-1.10668100	1.95939800	-0.19985200
H	-1.95741200	2.86368600	-2.34110000
H	2.03658300	2.78393400	-3.97190000
H	-0.38670200	3.29687200	-4.22939200
C	2.29556500	-3.07511500	-1.57726800
C	2.28741800	-5.00896100	-3.58954000
C	1.95243500	-2.69984300	-2.89620100
C	2.65155600	-4.40529100	-1.26011400
C	2.64219900	-5.35804300	-2.28778600
C	1.94599800	-3.69074000	-3.88682300
H	2.91207900	-6.39221000	-2.06441200
H	1.67476600	-3.42433000	-4.91040000
H	2.28005400	-5.76684900	-4.37588800
C	1.60014700	-1.26460100	-3.25671700
H	1.78585000	-0.64298100	-2.37178700
C	2.49197900	-0.72623300	-4.38407100
H	3.55893800	-0.79567000	-4.12020200
H	2.25710700	0.32932200	-4.58566800
H	2.34474900	-1.28134100	-5.32330300
C	0.11076900	-1.12196200	-3.60412000
H	-0.52630200	-1.50468900	-2.79300300
H	-0.14213600	-1.68301700	-4.51786500
H	-0.14619600	-0.06465900	-3.77029600
C	3.05236600	-4.82201100	0.14786900
H	2.87380000	-3.96172500	0.80935200
C	4.54859400	-5.16815200	0.22153200
H	5.18226000	-4.34042100	-0.13721400
H	4.78482000	-6.04210700	-0.40495200
H	4.84844900	-5.40536600	1.25460300
C	2.19363100	-5.98019100	0.67591700
H	1.12126300	-5.74381800	0.61356400
H	2.43713500	-6.19319100	1.72863200
H	2.36612000	-6.90460100	0.10360500
Sn	4.28522100	-1.35816600	- 0.11177200

C	4.61269200	-1.81079200	1.96376300
H	5.28804100	-1.06647500	2.40753200
H	5.05605100	-2.81088900	2.04986200
H	3.64014700	-1.79211300	2.47409500
C	5.51469700	-1.80150900	-1.80007400
H	6.49419100	-2.17593000	-1.47593100
H	5.63741200	-0.87121900	-2.37108100
H	5.00081000	-2.55674000	-2.40899600
C	3.38669000	1.30156300	0.87866700
C	3.81567300	2.74646400	1.01922300
C	4.58371700	5.43315700	1.29742800
C	3.68743500	3.39965400	2.25469600
C	4.36077400	3.44345800	-0.06663300
C	4.73996100	4.78040800	0.07183000
C	4.06338300	4.73605100	2.39159800
H	3.29216000	2.86168800	3.11856600
H	4.51239100	2.92721000	-1.01345700
H	5.16729100	5.31248900	-0.78097300
H	3.95684900	5.23154500	3.35895800
H	4.88097300	6.47869300	1.40414800
O	4.01141800	0.65221500	-0.17632800
H	3.54573600	0.80425300	1.85737100

Pb/P-Prod

C	-0.47717800	-0.76971600	1.40686000
H	-0.99869000	0.13132200	1.74733300
C	0.93254100	-0.53061500	0.81324100
C	1.21966800	-1.67152100	0.06167300
C	-0.35557900	-1.87888700	2.48833400
H	-1.31185500	-2.01339400	3.01585400
H	0.40811600	-1.64082000	3.24174400
C	0.00778800	-3.13089100	1.64084100
H	0.97986600	-3.56540600	1.90876300

H	-0.74448500	-3.92616000	1.74492900
C	-0.00655600	-2.58441700	0.17749000
H	-0.06238900	-3.35832300	-0.59530300
C	-1.14147600	-1.55008000	0.25604200
H	-1.24716900	-0.95023200	-0.65858900
H	-2.11303400	-1.99318400	0.52418400
N	2.32783300	-2.05900900	-0.59686700
P	1.54814400	1.11626300	0.68248400
C	0.83879100	2.09993900	2.02409500
C	0.06897400	3.69028100	4.19261300
C	0.77307600	1.54813600	3.31456500
C	0.53134300	3.45460800	1.82763400
C	0.14096200	4.24281700	2.91135100
C	0.38775500	2.34301800	4.39397300
H	1.02382800	0.49856200	3.47529400
H	0.61261300	3.89973000	0.83546100
H	-0.09860300	5.29627200	2.75367500
H	0.33358800	1.90992100	5.39497200
H	-0.23502600	4.31063800	5.03855700
C	1.01064900	1.83917000	-0.89621600
C	0.06038100	2.84687700	-3.32891100
C	1.89501600	2.03466300	-1.96748300
C	-0.35811700	2.12270500	-1.05834100
C	-0.82808900	2.62590100	-2.27051100
C	1.41582400	2.54816800	-3.17555100
H	2.94407900	1.76835300	-1.85614300
H	-1.05638800	1.96076900	-0.23452200
H	-1.89012400	2.85062200	-2.38902700
H	2.10929400	2.71503100	-4.00236500
H	-0.30784700	3.24864900	-4.27536900
C	2.28130900	-3.08894700	-1.59492700
C	2.31304700	-5.04002400	-3.59639600
C	1.95584600	-2.72736600	-2.92421000
C	2.64479900	-4.41623800	-1.26757300
C	2.65413200	-5.37670700	-2.28785800
C	1.96802500	-3.72561200	-3.90715100
H	2.92810300	-6.40748700	- 2.05356400

H	1.70817300	-3.46860300	-4.93588400
H	2.31973200	-5.80361700	-4.37719600
C	1.59390700	-1.29712800	-3.29368300
H	1.84166000	-0.66199900	-2.43337000
C	2.40594500	-0.78247300	-4.48946500
H	3.48915500	-0.86395700	-4.30783100
H	2.17071800	0.27480400	-4.68069200
H	2.17996900	-1.33934400	-5.41182600
C	0.08494700	-1.15312600	-3.54416800
H	-0.49854300	-1.51137800	-2.68373300
H	-0.22827400	-1.73738900	-4.42426100
H	-0.17845700	-0.09905400	-3.72010000
C	3.03552000	-4.82045800	0.14689100
H	2.84607400	-3.95562600	0.79933100
C	4.53250600	-5.15993500	0.23732000
H	5.16801900	-4.33336600	-0.12399900
H	4.77927800	-6.03714000	-0.38035900
H	4.82573700	-5.38753700	1.27457700
C	2.17872100	-5.97906600	0.67703000
H	1.10611200	-5.74779800	0.60351700
H	2.41388000	-6.18304500	1.73348400
H	2.36038000	-6.90672400	0.11289500
Pb	4.40799100	-1.40257400	-0.12528100
C	4.55590500	-1.81925800	2.07136600
H	5.20621800	-1.06235400	2.52588200
H	4.97040100	-2.82708300	2.18479200
H	3.52914200	-1.76046500	2.45159600
C	5.50347300	-1.75555100	-2.02947800
H	6.47658600	-2.20632000	-1.80494200
H	5.60683300	-0.76689700	-2.49212700
H	4.86660000	-2.42417600	-2.62059300
C	3.43212600	1.31855300	0.87853900
C	3.81173000	2.77174100	1.07522900
C	4.46980300	5.47502800	1.45868600
C	3.72744000	3.35218400	2.34970300
C	4.25622300	3.55203500	0.00023000
C	4.58037500	4.89704000	0.19111200

C	4.04920900	4.69598200	2.54039300
H	3.40177400	2.75108000	3.20129200
H	4.36935600	3.09698700	-0.98239300
H	4.92799900	5.49498800	-0.65427700
H	3.97638100	5.13398600	3.53814700
H	4.72382300	6.52703300	1.60611700
O	4.08664900	0.72438900	-0.18192900
H	3.58671700	0.80073100	1.84860500

Si/N-Prod

C	-0.53190100	-0.47404100	1.25341300
H	-1.10762400	0.41962700	1.51168900
C	0.87360600	-0.21308500	0.68019900
C	1.26806400	-1.37106500	0.05528500
C	-0.43414600	-1.50684300	2.42066000
H	-1.42858800	-1.64831400	2.86862400
H	0.23926400	-1.19397400	3.22720400
C	0.05392200	-2.79115800	1.70070600
H	1.03808000	-3.13073300	2.04907000
H	-0.64704100	-3.62796800	1.83163200
C	0.08979700	-2.34627200	0.20894300
H	0.11778500	-3.16991500	-0.51129400
C	-1.10488200	-1.38075600	0.14613900
H	-1.19763800	-0.86691300	-0.81990400
H	-2.06242900	-1.85249300	0.41336400
N	2.43414500	-1.79977600	-0.55047600
N	1.41713000	1.18659200	0.60114400
C	0.94474600	2.03722000	1.73995500
C	0.33661000	3.64602700	3.93873300
C	0.95321700	1.49267400	3.02315500
C	0.67251300	3.39254900	1.54968200
C	0.36274800	4.18992000	2.65292700
C	0.63903200	2.29499800	4.12120300

H	1.20940600	0.44663100	3.17257100
H	0.72246700	3.84019700	0.56001400
H	0.15020300	5.24954700	2.49955900
H	0.63545600	1.85788500	5.12163500
H	0.08966700	4.27469300	4.79641200
C	0.93111500	1.71911900	-0.72331100
C	-0.11177300	2.67347000	-3.14388500
C	1.77080500	1.88944700	-1.82228300
C	-0.43896900	1.99427600	-0.84321700
C	-0.95463900	2.46666400	-2.04703500
C	1.24415600	2.38137300	-3.02284900
H	2.81817000	1.62234200	-1.76956100
H	-1.10603600	1.86315800	0.00533400
H	-2.02224800	2.68210800	-2.12228400
H	1.91569900	2.52764600	-3.87074400
H	-0.51377100	3.05496900	-4.08435600
C	2.38210700	-2.90489300	-1.49398500
C	2.37687300	-4.98515100	-3.36145800
C	2.00734600	-2.63896500	-2.83088200
C	2.74145800	-4.20836200	-1.08254800
C	2.73862700	-5.23238100	-2.04002600
C	2.00775900	-3.69875700	-3.74684200
H	3.01732100	-6.24472400	-1.74107800
H	1.71629400	-3.51145700	-4.78215600
H	2.37778900	-5.79768000	-4.09125500
C	1.58066800	-1.25674200	-3.29602400
H	1.74187800	-0.56151600	-2.46437200
C	2.42077800	-0.75978800	-4.48042700
H	3.49467800	-0.74330800	-4.23812500
H	2.11816200	0.25898900	-4.76532900
H	2.29253100	-1.39820100	-5.36788500
C	0.08162200	-1.22492800	-3.63272600
H	-0.52488400	-1.59662600	-2.79413500
H	-0.14406400	-1.85354500	-4.50862900
H	-0.24095700	-0.19725800	-3.85931700
C	3.11043400	-4.55091700	0.35309700
H	2.97802000	-3.64216100	0.95556400

C	4.57903400	-4.98887700	0.47025100
H	5.26679800	-4.23815100	0.05200300
H	4.75640400	-5.92914100	-0.07425800
H	4.85448100	-5.15810700	1.52325900
C	2.17683300	-5.62298900	0.93752300
H	1.11987500	-5.33856800	0.83371600
H	2.38725900	-5.77606300	2.00773200
H	2.31178000	-6.59165900	0.43239600
Si	4.00930100	-1.09688600	-0.17624400
C	4.58360100	-1.51419500	1.55262700
H	5.32954300	-0.77888400	1.89554700
H	5.05752100	-2.50517700	1.57454000
H	3.75152100	-1.53052300	2.27338000
C	5.22049500	-1.42537100	-1.53281200
H	6.18477900	-0.94531400	-1.30457700
H	4.84666700	-1.02948500	-2.48829800
H	5.38941000	-2.50472000	-1.65950100
C	3.08159100	1.23067200	0.83464700
C	3.59872200	2.62464300	1.06292600
C	4.61752700	5.18423500	1.61098300
C	3.81271700	3.04206800	2.38570800
C	3.94127000	3.49118100	0.01454500
C	4.43831900	4.76562900	0.28932800
C	4.31408500	4.31348300	2.66041100
H	3.57466100	2.37004500	3.21173300
H	3.83179500	3.17782100	-1.02055100
H	4.69635300	5.43288400	-0.53573500
H	4.47006100	4.62280800	3.69586600
H	5.00745800	6.18251100	1.82133000
O	3.70102100	0.58268400	-0.17420300
H	3.09619300	0.67432900	1.78109300

Si/As-Prod

C	-0.56546600	-1.01870200	1.42161000
H	-1.17514900	-0.16032000	1.72980900
C	0.79680200	-0.66959400	0.80213600
C	1.22341500	-1.78420900	0.11416300
C	-0.31276100	-2.06220100	2.54890400
H	-1.24427500	-2.27460800	3.09419400
H	0.42657000	-1.70902500	3.28119600
C	0.17955700	-3.30292700	1.75200100
H	1.19093100	-3.62244400	2.03474700
H	-0.48658300	-4.16616400	1.89128200
C	0.10871800	-2.82223600	0.26456500
H	0.13531900	-3.62507900	-0.47876200
C	-1.13987100	-1.92218000	0.31076900
H	-1.32119200	-1.38226200	-0.62885200
H	-2.05104800	-2.46189400	0.60991800
N	2.41541300	-2.06377200	-0.50791600
As	1.41790500	1.10269300	0.73878300
C	0.64729300	2.08178600	2.19457000
C	-0.25823300	3.56317900	4.37525000
C	0.60933000	1.49369000	3.46774000
C	0.24107600	3.41050900	2.00977400
C	-0.21539600	4.14664000	3.10549600
C	0.15408600	2.23849100	4.55685600
H	0.92851000	0.45943100	3.61102700
H	0.28513300	3.87188400	1.02179100
H	-0.53610200	5.18113300	2.96617700
H	0.11885900	1.78371000	5.54904500
H	-0.61542200	4.14298600	5.22907700
C	0.82665800	1.93105800	-0.89503100
C	-0.13433900	3.08654400	-3.24319400
C	1.72865100	2.33799400	-1.88476700
C	-0.55630400	2.08446300	-1.08095700
C	-1.03280000	2.66538100	-2.25652200
C	1.24038100	2.92001700	-3.05795200
H	2.79955000	2.20472700	-1.75038100
H	-1.26185300	1.75919400	-0.31271300
H	-2.10774900	2.78949100	- 2.40321900

H	1.94124900	3.24558600	-3.82940800
H	-0.50956700	3.54345600	-4.16138600
C	2.41359100	-3.01608600	-1.60619800
C	2.47462200	-4.78156800	-3.76082400
C	2.16629000	-2.52469000	-2.90714900
C	2.70268200	-4.37748300	-1.37113300
C	2.72826900	-5.24504100	-2.47191400
C	2.19510500	-3.43280400	-3.97324400
H	2.94861400	-6.30293800	-2.31574500
H	2.00010500	-3.07893700	-4.98706800
H	2.49685800	-5.47454700	-4.60475500
C	1.84955400	-1.05805200	-3.16265700
H	2.14545100	-0.49213800	-2.26904400
C	2.63592500	-0.47515700	-4.34346100
H	3.71942100	-0.63290100	-4.22632100
H	2.45316000	0.60732700	-4.42038500
H	2.33494500	-0.92401700	-5.30247700
C	0.33809700	-0.85552100	-3.34981200
H	-0.22345800	-1.22321100	-2.47901500
H	-0.02369900	-1.40285300	-4.23474500
H	0.10023800	0.20979300	-3.48384400
C	2.98096900	-4.92888000	0.02011900
H	2.82243700	-4.11091200	0.73540100
C	4.43740400	-5.39746500	0.16785100
H	5.15287500	-4.59023000	-0.04856100
H	4.66071900	-6.22729000	-0.52057500
H	4.62810200	-5.75399400	1.19249500
C	2.00968900	-6.05959500	0.39307900
H	0.96107500	-5.75171100	0.27182500
H	2.15737400	-6.36429700	1.44098100
H	2.16932200	-6.94960200	-0.23487600
Si	3.99294800	-1.37230600	-0.03933000
C	4.35802800	-1.85486700	1.72725900
H	5.17922100	-1.25267800	2.14759900
H	4.66150800	-2.91153800	1.77077700
H	3.47164000	-1.73725500	2.37002500
C	5.26015300	-1.81580500	- 1.31382400

H	6.24024900	-1.41587800	-1.00998200
H	4.98883600	-1.37078000	-2.28271700
H	5.35049700	-2.90083200	-1.45647300
C	3.41771900	1.15554400	0.88902000
C	3.97395300	2.55328500	0.81761300
C	4.99433700	5.16215700	0.69501000
C	3.71765800	3.46319600	1.85535900
C	4.76698500	2.95015300	-0.26661700
C	5.27372500	4.25039900	-0.32620000
C	4.22032600	4.76313500	1.78913900
H	3.13132200	3.15646800	2.72364900
H	4.99945700	2.22696000	-1.04911900
H	5.89606700	4.55017700	-1.17225100
H	4.01532700	5.46424800	2.60101200
H	5.39056000	6.17865800	0.64625200
O	3.89837800	0.32310300	-0.10834500
H	3.57529900	0.74332200	1.90217900

Si/Sb-Prod

C	-0.81602200	-1.07680400	1.06697400
H	-1.44609600	-0.20128700	1.27288500
C	0.62104500	-0.76860700	0.63153400
C	1.12276700	-1.89815700	0.03783600
C	-0.73372400	-2.09873200	2.23837400
H	-1.73286100	-2.28761000	2.65830400
H	-0.09622500	-1.72933700	3.05382700
C	-0.15930000	-3.36365700	1.53795400
H	0.80178800	-3.69091900	1.95680200
H	-0.85197500	-4.21469400	1.60476800
C	-0.02274300	-2.91345900	0.04525200
H	0.08793500	-3.72925100	-0.67537200
C	-1.24910800	-1.99485400	-0.09627100
H	-1.28997800	-1.47891300	-1.06642500

H	-2.20292000	-2.51259000	0.08574200
N	2.38801400	-2.22017200	-0.40326500
Sb	1.41811800	1.13511100	0.86608100
C	0.67057700	1.97721600	2.66594100
C	-0.26889400	3.06248500	5.05529600
C	0.92944800	1.31961200	3.87785200
C	-0.05321400	3.17651100	2.64420100
C	-0.52274900	3.71536000	3.84574300
C	0.45538700	1.86580300	5.07243400
H	1.49035000	0.38116800	3.89953800
H	-0.26053500	3.68716100	1.70123700
H	-1.09168600	4.64757500	3.83479300
H	0.65014000	1.35564300	6.01825300
H	-0.63888700	3.48708100	5.99101600
C	0.67777400	2.31755000	-0.73289900
C	-0.28844800	3.82425400	-2.86976300
C	1.04941900	3.66513700	-0.85526700
C	-0.16795100	1.72039300	-1.67661800
C	-0.65282300	2.48052300	-2.74435500
C	0.56130300	4.41384400	-1.92837100
H	1.72254400	4.13406800	-0.13558200
H	-0.44177100	0.66772600	-1.58588400
H	-1.31532600	2.01977500	-3.48024700
H	0.85237100	5.46145800	-2.03049100
H	-0.66712600	4.41505500	-3.70669300
C	2.49475900	-3.12709300	-1.53334300
C	2.87094000	-4.78570600	-3.73816900
C	2.39889800	-2.57873000	-2.83084800
C	2.74560900	-4.50111400	-1.32305400
C	2.93456100	-5.31304000	-2.44962700
C	2.59654100	-3.43215500	-3.92456500
H	3.13244000	-6.37857300	-2.31592200
H	2.53719900	-3.03094600	-4.93844000
H	3.02774100	-5.43536600	-4.60203100
C	2.09668500	-1.10338300	-3.06813400
H	1.89520300	-0.63896000	-2.09450000
C	3.29635100	-0.36173800	- 3.67629500

H	4.18255600	-0.43404200	-3.02851400
H	3.05921900	0.70624900	-3.80731900
H	3.56566900	-0.76913300	-4.66326600
C	0.83575900	-0.92264300	-3.92542800
H	-0.03458500	-1.41306600	-3.46151100
H	0.96196000	-1.35290100	-4.93085600
H	0.60604200	0.14631400	-4.04921500
C	2.77622500	-5.12820300	0.06576800
H	2.58615000	-4.32579800	0.79247800
C	4.13656500	-5.75485700	0.40921300
H	4.95174800	-5.01767100	0.38443700
H	4.39655000	-6.56050100	-0.29477000
H	4.11254100	-6.19332100	1.41912200
C	1.66046900	-6.17481300	0.22744000
H	0.67316300	-5.76604700	-0.02939900
H	1.61984500	-6.53787600	1.26628300
H	1.83725200	-7.04610400	-0.42206700
Si	3.91700100	-1.57653400	0.23982300
C	3.93261300	-1.83411400	2.09046600
H	4.75837700	-1.28940300	2.57480800
H	4.06819200	-2.90572400	2.30547700
H	2.98428500	-1.52348600	2.55633000
C	5.34714000	-2.27353800	-0.70666000
H	6.28032800	-1.84256600	-0.31101500
H	5.26635600	-2.00446400	-1.76966400
H	5.40822500	-3.36672400	-0.64342800
C	3.66130800	1.12689200	0.76332500
C	4.05924300	2.47953000	0.26600800
C	4.63789300	5.05687500	-0.66431800
C	4.12111700	3.55715600	1.16436700
C	4.29261300	2.69746000	-1.09805800
C	4.58650700	3.98287100	-1.55753100
C	4.40586900	4.84159300	0.69925900
H	3.94418200	3.39053600	2.23103800
H	4.24022000	1.85604100	-1.78919800
H	4.77281600	4.14733600	-2.62097300
H	4.45852600	5.67511300	1.40292700

H	4.86704600	6.06109300	-1.02726500
O	4.00817900	0.09607000	-0.07315100
H	3.96678800	0.97313300	1.81196000

Si/Bi-Prod

C	-0.19905600	-2.22881600	1.99599400
H	0.79826400	-2.32212700	2.44511300
C	-0.29618000	-1.25761900	0.81522600
C	-1.61335400	-0.93432700	0.66139200
C	-0.84343400	-3.57511200	1.54928300
H	-0.70842200	-4.34663500	2.32231700
H	-0.39938000	-3.95522500	0.61820800
C	-2.33955800	-3.18858600	1.37935200
H	-2.71146000	-3.35371000	0.35999200
H	-2.98547100	-3.76121700	2.06052000
C	-2.36236200	-1.67713400	1.77681700
H	-3.35586300	-1.27763400	2.00541200
C	-1.31183300	-1.65917700	2.90119400
H	-1.08799500	-0.64928000	3.27191700
H	-1.56892700	-2.31526700	3.74703300
N	-2.30508700	-0.18738300	-0.29233800
Bi	1.53539800	-0.60377700	-0.26380900
C	3.06267100	-2.26838800	-0.16180800
C	5.03417900	-4.24506300	-0.20958900
C	4.32478700	-1.98164200	-0.69955000
C	2.77553600	-3.54216800	0.33809200
C	3.76970400	-4.52823000	0.31506900
C	5.31231000	-2.97229500	-0.71631800
H	4.55291500	-0.99448200	-1.11267400
H	1.79325500	-3.78187800	0.74623300
H	3.55044900	-5.52362700	0.70874100
H	6.29813400	-2.74916900	-1.13179500
H	5.80409100	-5.02011500	-0.22873600

C	-3.57528200	0.40439500	0.10083200
C	-5.99833200	1.64763400	0.69649400
C	-3.56614900	1.65380000	0.75703100
C	-4.78414700	-0.24669200	-0.23445300
C	-5.98799100	0.40326900	0.06922100
C	-4.79655800	2.25941600	1.04633500
H	-6.93536100	-0.07685700	-0.18419600
H	-4.81431600	3.22789800	1.55057900
H	-6.94781100	2.13825000	0.92172900
C	-2.27403200	2.34800100	1.16671600
H	-1.43499700	1.72738500	0.82597100
C	-2.12164200	3.72263600	0.49954000
H	-2.10697200	3.63783900	-0.59779000
H	-1.18164500	4.20149600	0.81711300
H	-2.94240700	4.40315500	0.77336000
C	-2.17316500	2.45697300	2.69595800
H	-2.23306100	1.46605200	3.17099300
H	-2.98502100	3.07461700	3.11048400
H	-1.21984400	2.92324500	2.98869400
C	-4.82533500	-1.63558100	-0.86056300
H	-3.78714600	-1.98163100	-0.96387500
C	-5.46012800	-1.64545900	-2.25992000
H	-4.90330100	-1.02129500	-2.97401100
H	-6.49643300	-1.27427500	-2.23378200
H	-5.48530300	-2.67022900	-2.66227400
C	-5.55656100	-2.62879000	0.05889300
H	-5.15069900	-2.61348900	1.08002000
H	-5.46566400	-3.65473400	-0.33066600
H	-6.62998200	-2.39277300	0.12435500
Si	-1.78913200	0.21386700	-1.92209100
C	-1.22186000	-1.30479600	-2.84325900
H	-0.63355100	-1.06596800	-3.74328000
H	-2.12141000	-1.84813900	-3.17642200
H	-0.64220200	-1.99233500	-2.20984100
C	-3.02764500	1.28073900	-2.79059200
H	-2.64006600	1.54519300	-3.78752200
H	-3.19346800	2.20795500	- 2.22341300

H	-3.99864700	0.78466600	-2.91132400
C	0.82574600	1.16766200	-2.12241300
C	1.76883400	2.22538000	-1.80087500
C	3.64260200	4.18687400	-1.12545500
C	3.05281300	2.20791300	-2.38457100
C	1.43507800	3.23224000	-0.87345300
C	2.37148100	4.20864600	-0.54269100
C	3.98220100	3.18592600	-2.04884900
H	3.31566500	1.42036200	-3.09772200
H	0.44361000	3.23646600	-0.42414500
H	2.11347300	4.98633600	0.17933900
H	4.97375500	3.17664200	-2.50598500
H	4.37629100	4.95148500	-0.85992200
O	-0.43288600	1.31051300	-1.77543000
C	2.30316400	0.85862500	1.26551300
C	3.63764700	1.27799800	1.23560000
C	1.39536900	1.45003000	2.15178600
C	4.06331800	2.29334300	2.09673900
H	4.35642800	0.82325300	0.54978900
C	1.82846600	2.46116800	3.01578600
H	0.35487800	1.11983000	2.17662800
C	3.15954900	2.88717500	2.98383800
H	5.10583700	2.61980700	2.07655000
H	1.12485300	2.91392100	3.71884500
H	3.49614900	3.67793700	3.65812700
H	1.05214800	0.52541900	-2.98349700
