

Theoretical Investigation on the Effect of Ligand on Bis-silylation of C(sp)-C(sp) by Ni complexes

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Table S1. Energies calculated at B3LYP/BSI (6-31g*, SDD) level in gas phase, and correction energies calculated at ω B97X-D/BSII (6-311g, SDD) in toluene of reaction pathways. (unit: a.u.)**

	<i>E+ZPE</i>	<i>E</i>	<i>H</i>	<i>G</i>	<i>G_{toluene}</i>
Ni1a	-794.675688	-794.659152	-794.658208	-794.717528	-794.708708
Ni1b	-794.635311	-794.617763	-794.616819	-794.681146	-794.665765
Ni2a	-1863.740699	-1863.697611	-1863.696667	-1863.820056	-1863.753804
Ni3a	-1329.199968	-1329.170051	-1329.169107	-1329.261049	-1329.221768
SIPr(01)	-846.372946	-846.352716	-846.351772	-846.422485	-846.379478
SIPr(03)	-846.263642	-846.243521	-846.242577	-846.314001	-846.265844
COD	-311.845714	-311.838086	-311.837142	-311.877514	-311.868569
R1	-1179.639117	-1179.618144	-1179.617199	-1179.688619	-1179.66247
INT1a	-1662.437887	-1662.406974	-1662.406029	-1662.499658	-1662.480203
INT1b	-1662.416953	-1662.385628	-1662.384683	-1662.480569	-1662.462475
INT1c	-2196.980957	-2196.936321	-2196.935377	-2197.062466	-2197.015828
TS1a	-1662.418635	-1662.388955	-1662.388011	-1662.477147	-1662.467915
TS1c	-2196.95698	-2196.91358	-2196.91264	-2197.03232	-2197.005594
INT2a	-1662.43845	-1662.407616	-1662.406672	-1662.49871	-1662.485624
INT2b	-1662.416751	-1662.38433	-1662.383386	-1662.48424	-1662.46715
INT2c	-2196.957237	-2196.913454	-2196.91251	-2197.032921	-2197.008045
INT3a	-1506.504107	-1506.475424	-1506.47448	-1506.562193	-1506.534595
INT3b	-1506.467866	-1506.437985	-1506.437041	-1506.529503	-1506.50258
INT3c	-1698.188469	-1698.157022	-1698.156077	-1698.250888	-1698.209428
INT3d	-1698.190888	-1698.159337	-1698.158393	-1698.253524	-1698.211529
INT3e	-1889.875098	-1889.840777	-1889.839832	-1889.941781	-1889.884158
TS2a	-1506.481983	-1506.454565	-1506.45362	-1506.538205	-1506.508445
TS2b	-1506.452242	-1506.423892	-1506.422948	-1506.511959	-1506.479042
TS2c	-1698.165662	-1698.135198	-1698.134254	-1698.226371	-1698.185428
TS2d	-1698.170207	-1698.139656	-1698.138712	-1698.232074	-1698.185422
TS2e	-1889.851991	-1889.818563	-1889.817619	-1889.917234	-1889.860061
R2a	-155.894337	-155.88856	-155.887616	-155.922	-155.909483
R2b	-539.269068	-539.258852	-539.257908	-539.306218	-539.249874

R2c	-347.581994	-347.574522	-347.573578	-347.614384	-347.581116
INT4a	-1818.365682	-1818.330193	-1818.329249	-1818.430198	-1818.423831
INT4c	-2352.89192	-2352.84382	-2352.842876	-2352.971237	-2352.947544
TS3a	-1818.341259	-1818.305842	-1818.304897	-1818.406502	-1818.397159
Pro	-1335.566664	-1335.54082	-1335.539875	-1335.622107	-1335.594008

Figure S1. Reaction mechanism of Bis-silylation of C(sp)-C(sp) bond catalyzed by Ni-complex.

[Ni] = Ni1a/COD as ligand/multiplicity=1

Ni1b/COD as ligand/multiplicity=3

Ni2a/SIPr as ligand/multiplicity=1

Ni2b/SIPr as ligand/multiplicity=3

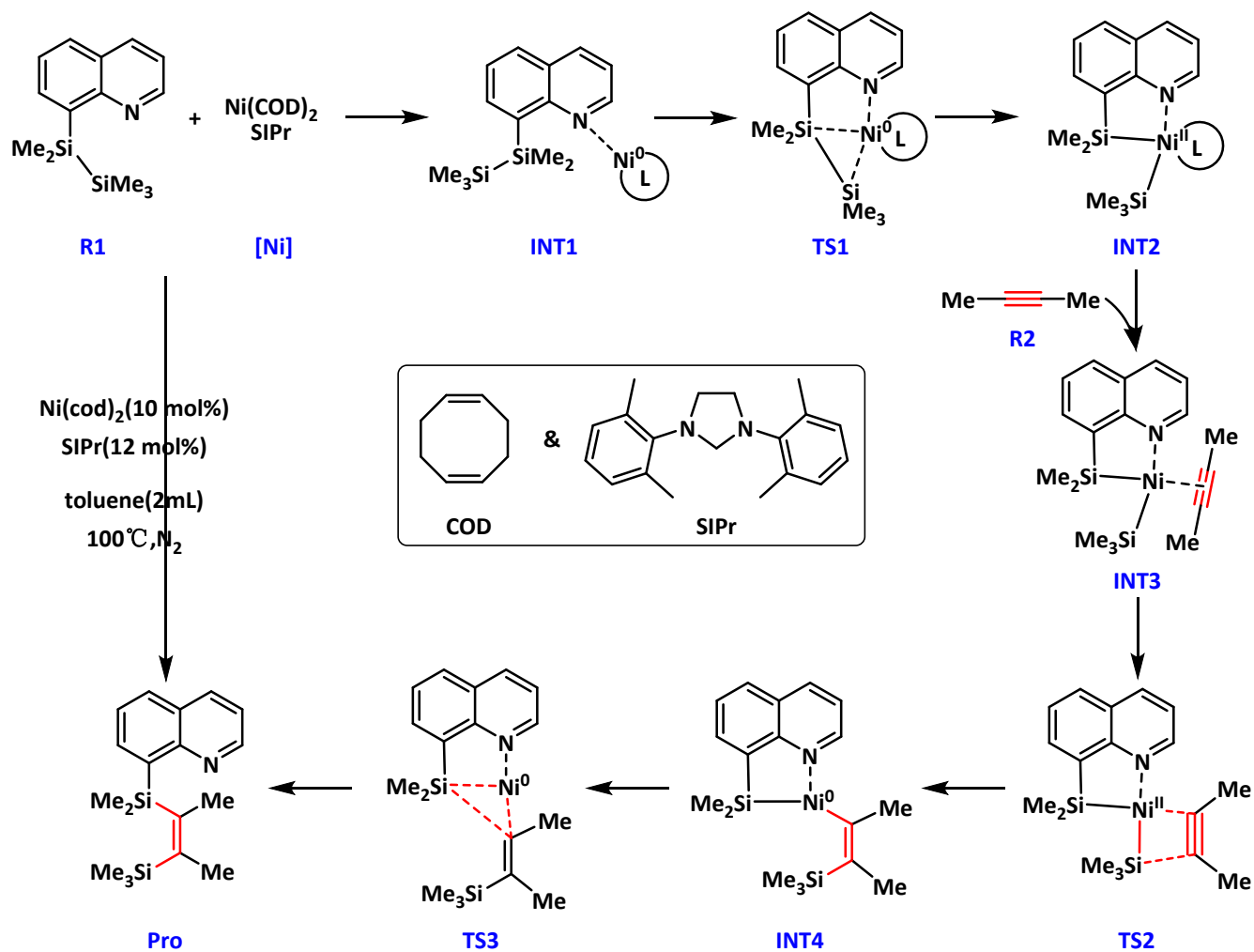


Figure S2. Energies surface of Bis-silylation of C(sp)-C(sp) bond catalyzed by Ni-complex in gas phase.

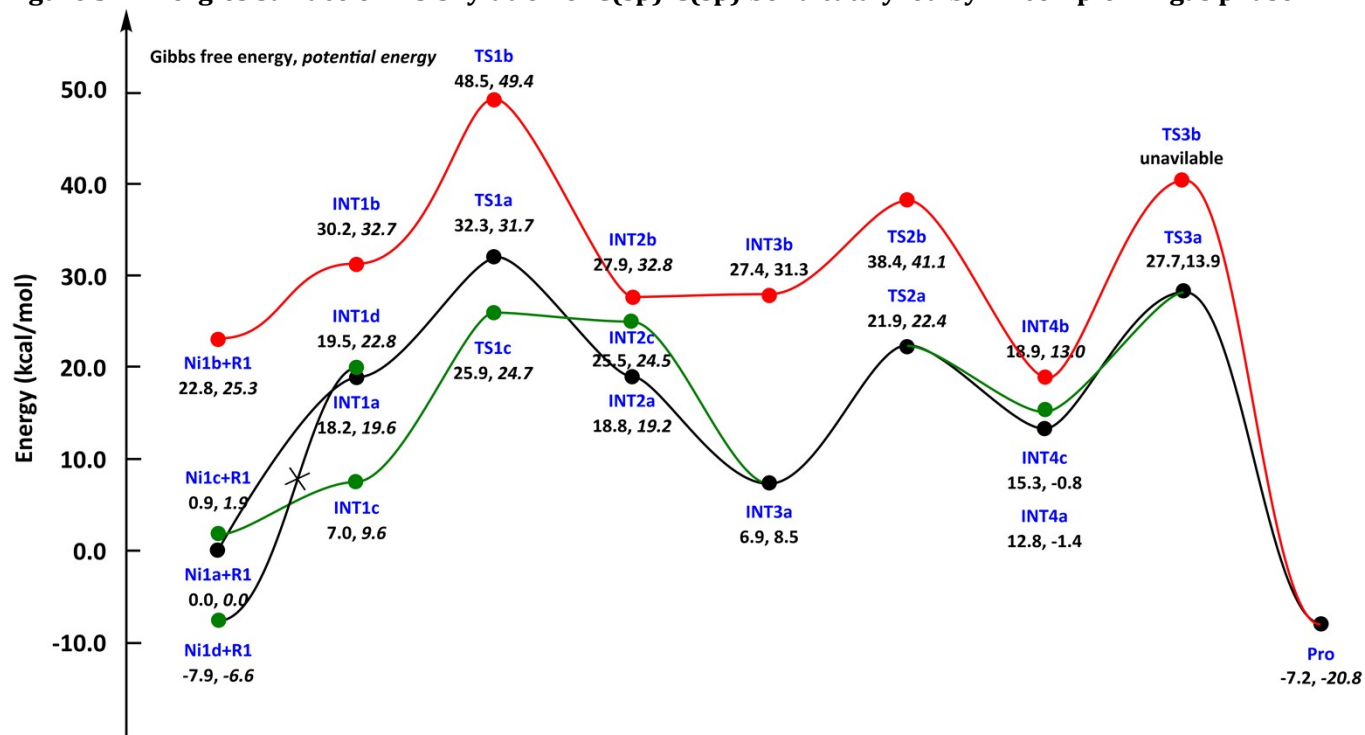
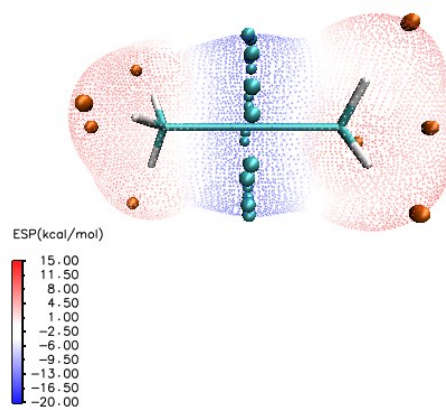
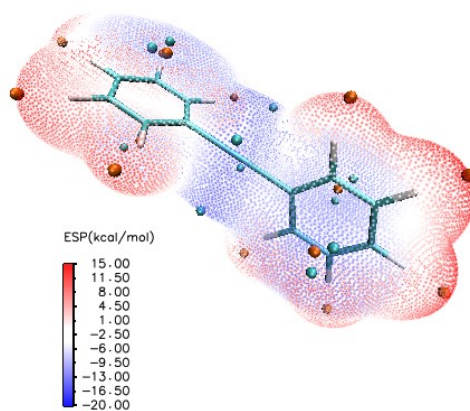


Figure S3. Restrained electrostatic potential (RESP) surface in R2a, R2b and R2c.

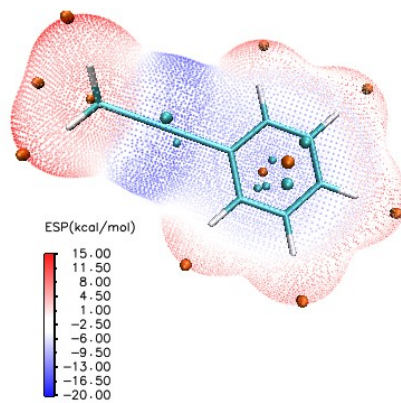
R2a



R2b



R2c



S6

Cartesian coordinates of all stationary points optimized at ω B97X-D/BSI (6-311g, SDD) level.****Ni1a**

C	-2.02865000	1.75063600	1.17102500
C	-1.39364100	0.96413600	0.20249600
C	-0.12837600	1.41229300	-0.27852500
C	0.38544800	2.68368200	0.11893300
C	-0.30809200	3.43775100	1.08580000
C	-1.48996200	2.96428100	1.63058500
H	-2.98741100	1.43456600	1.57197000
C	1.58951600	3.16236700	-0.51205600
H	0.09814100	4.39915900	1.39452800
H	-2.01752100	3.54228700	2.38469600
C	2.18352800	2.43250900	-1.49722500
C	1.66913600	1.12536900	-1.83625200
H	1.97718100	4.13764800	-0.22549100
H	3.04707800	2.81513100	-2.03662000
H	1.88622100	0.71254000	-2.82334100
N	0.57604500	0.60059400	-1.16934400
Si	-2.33928500	-0.45839000	-0.65400000
Si	-4.51113300	-0.73593600	0.27574800
C	-2.53921400	0.00564700	-2.49052300
H	-3.05657100	0.96443200	-2.61158100
H	-1.55478900	0.09042800	-2.96306800
H	-3.11477400	-0.75732100	-3.02941600
C	-1.50206700	-2.16820700	-0.58720800
H	-0.50673300	-2.12779300	-1.04057900
H	-1.40694200	-2.55188200	0.43547900
H	-2.10503600	-2.89048200	-1.15229000
C	-5.36045200	-2.17232300	-0.64930800
H	-4.80823800	-3.11273000	-0.53453200
H	-6.37460700	-2.33531900	-0.26207500
H	-5.44665900	-1.96770200	-1.72329200
C	-4.45850300	-1.20189400	2.12501000
H	-4.00276800	-0.41812100	2.74129900
H	-5.47213100	-1.37768600	2.50825000
H	-3.88244300	-2.12141200	2.28571400
C	-5.60724700	0.80873400	0.06080000
H	-6.61170900	0.63065100	0.46632800
H	-5.19282400	1.68696300	0.56857800
H	-5.72032000	1.06713200	-0.99893100
C	3.79393500	-2.69897900	-0.00370700
C	2.39499900	-2.92618600	0.63401300
C	4.62889600	0.19841900	1.02699800
C	1.69701500	-1.65534400	1.07294600
C	3.72415800	-0.45587100	2.10601100
C	2.27314200	-0.56664100	1.67611000
H	4.03062200	-3.56296700	-0.63560100
H	2.48786500	-3.63207400	1.47391700
H	4.53249400	1.28855100	1.10069100
H	3.78029700	0.14799200	3.01930300
H	4.56353700	-2.67893600	0.77432400
H	1.74574500	-3.41809700	-0.10017000
H	5.68405800	-0.02818000	1.24849500
H	0.61269500	-1.67040400	1.01043100
H	4.10918800	-1.44412800	2.37365700
H	1.60625900	0.22288300	2.02169700
C	3.87960800	-1.43415000	-0.84617100
C	4.28254100	-0.18912500	-0.39638800
Ni	2.19433400	-0.22688300	-0.48451600
H	3.84690900	-1.58129500	-1.92600000
H	4.57107100	0.54265600	-1.14918400

Ni1b

C	-2.13161800	1.74644200	1.15738200
C	-1.43975300	1.00368300	0.18800500
C	-0.20096500	1.52899500	-0.28772600
C	0.24662700	2.82087600	0.15447400
C	-0.49838800	3.51568300	1.12482400
C	-1.66984800	2.97762700	1.63993800
H	-3.07035300	1.36499000	1.54952100
C	1.43939900	3.37909000	-0.42915700
H	-0.14167200	4.48721600	1.46117400
H	-2.23730700	3.51639900	2.39403100
C	2.09548600	2.69214400	-1.42131000
C	1.64556500	1.40159300	-1.79062900
H	1.76950900	4.36433900	-0.10995400
H	2.95191800	3.12225300	-1.93490300
H	2.00113500	0.94673300	-2.71496800
N	0.54939600	0.78951300	-1.19785000
Si	-2.21688900	-0.58897800	-0.51142100
Si	-4.50510700	-0.78969400	0.09932200
C	-2.15840200	-0.60041000	-2.41415400
H	-2.69262100	0.26091800	-2.83304100
H	-1.12292200	-0.55323600	-2.76332500
H	-2.62497800	-1.50965200	-2.81377600
C	-1.30817400	-2.13167700	0.14378800
H	-0.24287800	-2.07751800	-0.10435900
H	-1.39692700	-2.21345800	1.23392500
H	-1.71757900	-3.05034000	-0.29528300
C	-5.21705900	-2.30927200	-0.80849000
H	-4.68044400	-3.22839900	-0.54392300
H	-6.27300500	-2.45639400	-0.54702400
H	-5.15939800	-2.19361700	-1.89724600
C	-4.75989500	-1.08253600	1.96755800
H	-4.42271800	-0.23566400	2.57666700
H	-5.82297400	-1.24502800	2.18849500
H	-4.21381000	-1.97024600	2.30950300
C	-5.52220800	0.73223000	-0.42970300
H	-6.58257200	0.60056800	-0.17803400
H	-5.17285700	1.64887300	0.05890500
H	-5.45667900	0.89317100	-1.51262700
C	2.75808300	-2.62957700	1.28023900
C	2.21507200	-1.48195000	2.17373200
C	4.91995300	-1.16625100	-0.53285300
C	2.44209200	-0.08580600	1.62276700
C	4.86502600	-0.41181800	0.82156200
C	3.58447200	0.38316100	1.01260800
H	2.20727600	-3.54541200	1.52313500
H	2.64549900	-1.56826400	3.18517100
H	5.28025600	-0.47737400	-1.30566600
H	5.72069200	0.27143700	0.87589300
H	3.80500500	-2.83787800	1.52495300
H	1.13445700	-1.61442400	2.29396000
H	5.66936300	-1.97334600	-0.47214000
H	1.68202100	0.64833800	1.88840500
H	4.99046800	-1.11513000	1.65053200
H	3.63432500	1.45023400	0.80519100
C	2.62569700	-2.35533800	-0.21196000
C	3.58252400	-1.71527900	-0.99710200
Ni	2.12070300	-0.30192200	-0.51097400

H 1.85072500 -2.91226200 -0.73668200

Ni2a

Ni -0.00002300 0.00064800 0.00010500
C -0.44232800 0.62284100 4.11069800
C 0.46273300 -0.62038200 4.10868800
C 0.00481200 0.00090300 1.85191000
H -1.44287100 0.40758700 4.51035600
H -0.02320200 1.45189100 4.69116900
H 0.04646900 -1.44929600 4.69136800
H 1.46518100 -0.40504500 4.50346100
N -0.51381200 0.95957900 2.67718900
N 0.52755400 -0.95733000 2.67492800
C 1.25532700 -2.10821600 2.23034400
C 2.63148400 -1.99922200 1.95053300
C 0.58269500 -3.34165400 2.13878900
C 3.32636900 -3.15494600 1.57469900
C 1.31364500 -4.47375700 1.76035000
C 2.67644200 -4.38459700 1.48176500
H 4.38877300 -3.08427300 1.35350900
H 0.80458000 -5.43156700 1.68295400
H 3.23196400 -5.27306700 1.19230900
C -1.24508600 2.10957800 2.23594700
C -2.62285600 1.99953400 1.96466500
C -0.57377500 3.34335100 2.13932600
C -3.32078600 3.15467100 1.59275300
C -1.30781600 4.47488600 1.76509900
C -2.67229300 4.38476300 1.49530200
H -4.38448500 3.08322300 1.37815900
H -0.79980700 5.43295900 1.68404500
H -3.23025500 5.27275600 1.20909500
C 0.91091200 3.43890500 2.39647600
H 1.17572200 3.12642000 3.41439000
H 1.46675100 2.79243700 1.70755000
H 1.26199500 4.46718500 2.26336800
C -3.32572100 0.66539200 2.03186000
H -2.90497400 -0.02888600 1.29406800
H -3.22109700 0.19209900 3.01564900
H -4.39518600 0.77940500 1.82847300
C 3.33598900 -0.66571400 2.01371700
H 2.91369000 0.02826400 1.27652000
H 3.23493600 -0.19109100 2.99723200
H 4.40467600 -0.78115900 1.80705600
C -0.90035500 -3.43633200 2.40568600
H -1.15801400 -3.12569000 3.42599500
H -1.46035200 -2.78811000 1.72180900
H -1.25322800 -4.46406800 2.27313700
C -0.00421200 -0.00020200 -1.85167000
N -0.96413400 -0.52167000 -2.67355800
N 0.95194100 0.52108000 -2.67794600
C -0.63057800 -0.45352500 -4.10800500
C -2.11397900 -1.25064700 -2.22836000
C 0.61296000 0.45120200 -4.11095500
C 2.10397800 1.24964300 -2.23762900
H -1.46069500 -0.03532000 -4.68758100
H -0.41680200 -1.45505200 -4.50593800
C -3.34785300 -0.57899000 -2.13519000
C -2.00384300 -2.62705100 -1.95027200
H 0.39746000 1.45226400 -4.50909300
H 1.44095100 0.03248400 -4.69324600
C 3.33710800 0.57651500 -2.14518600
C 1.99632700 2.62694500 -1.96290700
C -4.47932800 -1.31127400 -1.75738900

H 3.48943500 -1.83886400 -2.07765400
C -3.44361700 0.90431600 -2.40026700
C -3.15894600 -3.32327600 -1.57513200
C -0.66964200 -3.33023000 -2.01351300
C 4.47038200 1.30833800 -1.77187800
C 3.43018600 -0.90789400 -2.40508400
C 3.15319000 3.32263100 -1.59219600
C 0.66288800 3.33165800 -2.02524100
C -4.38908800 -2.67439800 -1.48091500
H -5.43748600 -0.80300800 -1.67903200
H -2.79506500 1.46383000 -1.71631100
H -3.13408800 1.16318600 -3.42059500
H -4.47140700 1.25654000 -2.26632100
H -3.08742700 -4.38590200 -1.35528900
H -0.19369400 -3.22639100 -2.99610700
H 0.02303400 -2.90914100 -1.27433800
H -0.78448900 -4.39951600 -1.80963200
C 4.38265800 2.67234600 -1.49898100
H 5.42795600 0.79889000 -1.69397200
H 2.78495400 -1.46419100 -1.71531500
H 3.11483700 -1.17061100 -3.42264600
H 4.45839700 -1.26039300 -2.27524100
H 3.08360600 4.38593700 -1.37506800
H 0.18602500 3.22801000 -3.00740200
H -0.02952900 2.91159200 -1.28525000
H 0.77914300 4.40089800 -1.82190200
H -5.27705800 -3.23103800 -1.19208100
H 5.27202200 3.22851900 -1.21355800

Ni3a

C 1.37699400 3.52433400 -0.67499500
C 1.77630800 3.11561800 0.77164500
C -1.77578800 3.11688800 -0.77165000
C 0.73808100 2.27471500 1.48506400
C -1.37624200 3.52523100 0.67502300
C -0.63116100 2.42912300 1.41566900
H 2.29171200 3.77305500 -1.22736400
H 2.02023600 4.02225000 1.34978000
H -2.70163900 2.52979400 -0.72868700
H -2.29081100 3.77448100 1.22740200
H 0.78193200 4.44264500 -0.65551500
H 2.70174000 2.52787300 0.72860700
H -2.01905900 4.02371300 -1.34976000
H 1.13367200 1.60791600 2.25025700
H -0.78061500 4.44317600 0.65564100
H -1.23242800 1.83505700 2.10329800
C 0.63119900 2.42876800 -1.41573200
C -0.73813200 2.27528400 -1.48506200
Ni -0.00033600 0.93875900 0.00001800
H 1.23206400 1.83431500 -2.10337100
H -1.13417900 1.60863000 -2.25014900
C -0.00004500 -0.94045900 -0.00000400
N -1.09101800 -1.77706600 -0.03930800
N 1.09099200 -1.77697500 0.03936800
C -0.76047300 -3.20413800 0.10948300
C -2.44471200 -1.31733600 0.01891700
C 0.76055800 -3.20407700 -0.10940400
C 2.44465700 -1.31717600 -0.01889100
H -1.29439000 -3.81480100 -0.62682600
H -1.03092300 -3.57140800 1.11006500
C -3.15418300 -1.14953500 -1.18624500
C -3.05114700 -1.06570400 1.26556200
H 1.03105000 -3.57133300 -1.10998200

H	1.29452200	-3.81468600	0.62691700
C	3.15419000	-1.14936900	1.18623600
C	-4.48378300	-0.71627100	-1.12592700
C	-2.49174100	-1.41956600	-2.51643900
C	-4.38304900	-0.63416000	1.28410200
C	-2.28754300	-1.24681100	2.55655400
C	4.38298000	-0.63417900	-1.28418700
C	2.28743400	-1.24695200	-2.55652200
C	4.48379800	-0.71613500	1.12584400
C	2.49186300	-1.41949400	2.51647000
C	-5.09662800	-0.45975900	0.09960300
H	-5.03980000	-0.57956600	-2.05037700
H	-1.58120300	-0.82126200	-2.62937400
H	-2.19737000	-2.47172600	-2.61952300
H	-3.16878800	-1.18193500	-3.34305900
H	-4.86066600	-0.43254400	2.24007300
H	-2.08977400	-2.30576400	2.76882300
H	-1.31908300	-0.73686700	2.51480800
H	-2.85574300	-0.84601000	3.40194800
C	5.09660500	-0.45970900	-0.09972500
H	4.86057900	-0.43267700	-2.24019200
H	2.08986300	-2.30595700	-2.76873800
H	1.31888300	-0.73718700	-2.51476100
H	2.85552400	-0.84608000	-3.40195500
H	5.03986900	-0.57943800	2.05026200
H	1.58123600	-0.82134300	2.62945900
H	2.19767000	-2.47170500	2.61957600
H	3.16892200	-1.18175600	3.34304900
H	-6.12973400	-0.12333100	0.13137400
H	6.12972700	-0.12333600	-0.13155600

SIPr(01)

C	0.76186400	-0.08785300	1.91299700
C	-0.76185700	0.08784000	1.91300200
C	-0.00000200	0.00002700	-0.35525400
H	1.27878300	0.67275300	2.50449500
H	1.07299600	-1.07421300	2.28142100
H	-1.07298900	1.07419400	2.28144000
H	-1.27877100	-0.67277400	2.50449300
N	1.07758200	0.03899600	0.46350800
N	-1.07758100	-0.03899300	0.46351100
C	-2.42839500	0.04923200	-0.00351200
C	-2.87930400	1.24155800	-0.60541500
C	-3.28661000	-1.05434800	0.16320300
C	-4.20998100	1.30971500	-1.03071200
C	-4.61338400	-0.94126900	-0.26970100
C	-5.07625300	0.23140700	-0.85964400
H	-4.56773000	2.22329200	-1.49942800
H	-5.28199700	-1.79073000	-0.15115100
H	-6.10773800	0.30287100	-1.19468400
C	2.42839400	-0.04923400	-0.00352100
C	3.28660100	1.05434900	0.16320000
C	2.87931100	-1.24156000	-0.60541900
C	4.61337800	0.94127700	-0.26969800
C	4.20999100	-1.30971100	-1.03071000
C	5.07625500	-0.23139700	-0.85964000
H	5.28198700	1.79073900	-0.15114200
H	4.56774800	-2.22328700	-1.49942100
H	6.10774200	-0.30285600	-1.19467400
C	1.95283400	-2.41725200	-0.80404400
H	1.53816100	-2.77199200	0.14828500
H	1.10241500	-2.14065800	-1.43572300
H	2.48307700	-3.25352600	-1.27003200

C	3.05105900	-1.06565800	-1.26556800
C	2.79773800	2.34834100	0.77043700
H	1.77801300	2.57814600	0.44645700
H	2.79103800	2.31248800	1.86855800
H	3.44747200	3.18028100	0.48137500
C	-1.95281900	2.41724400	-0.80404000
H	-1.53814700	2.77198100	0.14829100
H	-1.10239900	2.14064600	-1.43571600
H	-2.48305600	3.25352000	-1.27003000
C	-2.79776100	-2.34835400	0.77042300
H	-1.77801500	-2.57813600	0.44649100
H	-2.79112500	-2.31253900	1.86854600
H	-3.44746800	-3.18029300	0.48129800

SIPr(03)

C	-0.59643800	0.49324600	1.63322400
C	0.59633000	-0.49276200	1.63333000
C	0.00000600	0.00013000	-0.52360700
H	-1.38495400	0.21513200	2.33574000
H	-0.26126600	1.51414800	1.85441500
H	0.26115100	-1.51362400	1.85469100
H	1.38482100	-0.21452400	2.33582500
N	-1.09470000	0.38113800	0.23804100
N	1.09464500	-0.38089700	0.23814500
C	2.44675900	-0.04035800	-0.04000000
C	3.43815600	-0.98749400	0.31824800
C	2.80999100	1.17022400	-0.68320800
C	4.77921900	-0.69839200	0.05441800
C	4.16436400	1.39852900	-0.94744300
C	5.14997300	0.48489700	-0.57973000
H	5.53747500	-1.42804500	0.32941100
H	4.44726200	2.32788700	-1.43672800
H	6.19527100	0.69068100	-0.79297000
C	-2.44676800	0.04038900	-0.04008900
C	-2.80983600	-1.17033100	-0.68312900
C	-3.43828700	0.98746300	0.31798700
C	-4.16417500	-1.39883900	-0.94736400
C	-4.77930800	0.69816100	0.05416500
C	-5.14990300	-0.48527000	-0.57981100
H	-4.44694800	-2.32830300	-1.43651900
H	-5.53765800	1.42776500	0.32902600
H	-6.19517100	-0.69121200	-0.79304700
C	-3.06325600	2.31527200	0.93323300
H	-2.79721000	2.23360500	1.99575400
H	-2.19774600	2.75188900	0.42180100
H	-3.89787700	3.02018000	0.86538500
C	-1.80539500	-2.23468500	-1.05688100
H	-1.07783800	-1.87821000	-1.79587100
H	-1.22194300	-2.57209900	-0.19172700
H	-2.31989500	-3.10805600	-1.47193300
C	3.06295200	-2.31516600	0.93368600
H	2.79682800	-2.23329600	1.99617100
H	2.19744200	-2.75178800	0.42225900
H	3.89751300	-3.02016300	0.86602200
C	1.80569000	2.23465300	-1.05712800
H	1.07810800	1.87817500	-1.79609200
H	1.22225800	2.57225000	-0.19203300
H	2.32031000	3.10790600	-1.47227900

COD

C	-0.87721100	-1.63329000	-0.19409400
C	0.38455600	-1.81236900	0.21320800

C	-0.38455600	1.81236900	-0.21320800
C	1.26363700	-0.80984900	0.92890800
C	0.87721100	1.63329000	0.19409400
C	1.72052400	0.38712500	0.03323000
H	-1.35218600	-2.45778300	-0.72618200
H	0.74931500	-0.40903400	1.81259100
H	-0.85207100	2.77043600	0.01485300
H	1.35218600	2.45778300	0.72618200
H	0.85207100	-2.77043600	-0.01485300
H	2.15230200	-1.33262000	1.30075100
H	2.75837600	0.63799300	0.28060600
H	1.72382100	0.05766200	-1.01438000
C	-1.72052400	-0.38712500	-0.03323000
H	-1.72382100	-0.05766200	1.01438000
H	-2.75837600	-0.63799300	-0.28060600
C	-1.26363700	0.80984900	-0.92890800
H	-0.74931500	0.40903400	-1.81259100
H	-2.15230200	1.33262000	-1.30075100

R1

C	0.34613500	1.77666400	-0.00002600
C	0.56035700	0.40635800	-0.00007100
C	1.92277500	-0.04514800	-0.00007600
C	3.00217900	0.89861700	-0.00002700
C	2.71254100	2.28776900	-0.00001700
C	1.40702300	2.71651500	-0.00001600
H	-0.66926100	2.16310000	-0.00000700
C	4.32664200	0.39249000	0.00000100
H	3.53535100	2.99925600	0.00000900
H	1.18013600	3.77941500	0.00000900
C	4.53396800	-0.96612500	0.00001500
C	3.40337700	-1.81831300	0.00004200
H	5.16235800	1.08904100	0.00001000
H	5.53382600	-1.38960100	0.00002200
H	3.54385800	-2.89908100	0.00001700
N	2.15632800	-1.39250300	-0.00001200
Si	-0.88053600	-0.85316700	-0.00008200
Si	-2.98400100	0.25310100	0.00008600
C	-0.78518500	-1.94385100	-1.55488900
H	-0.83826400	-1.34478600	-2.47155500
H	0.15705800	-2.49989300	-1.56512100
H	-1.61267300	-2.66374500	-1.57905500
C	-0.78502400	-1.94402700	1.55459200
H	0.15722100	-2.50007100	1.56466900
H	-0.83801600	-1.34506800	2.47133200
H	-1.61250700	-2.66392700	1.57875400
C	-4.34612500	-1.08019300	0.00014900
H	-4.28193800	-1.72450700	0.88499300
H	-5.34116700	-0.61702300	0.00023400
H	-4.28206500	-1.72445900	-0.88474000
C	-3.23453200	1.33644800	1.54891900
H	-2.50316400	2.15073000	1.60983800
H	-4.23476300	1.78846400	1.54661200
H	-3.14217200	0.74437900	2.46729200
C	-3.23474900	1.33652400	-1.54866100
H	-4.23498300	1.78853400	-1.54619400
H	-2.50339500	2.15081400	-1.60964300
H	-3.14251300	0.74450000	-2.46707500

INT1a

C	-2.02865000	1.75063600	1.17102500
C	-1.39364100	0.96413600	0.20249600

C	-0.12837600	1.41229300	-0.27852500
C	0.38544800	2.68368200	0.11893300
C	-0.30809200	3.43775100	1.08580000
C	-1.48996200	2.96428100	1.63058500
H	-2.98741100	1.43456600	1.57197000
C	1.58951600	3.16236700	-0.51205600
H	0.09814100	4.39915900	1.39452800
H	-2.01752100	3.54228700	2.38469600
C	2.18352800	2.43250900	-1.49722500
C	1.66913600	1.12536900	-1.83625200
H	1.97718100	4.13764800	-0.22549100
H	3.04707800	2.81513100	-2.03662000
H	1.88622100	0.71254000	-2.82334100
N	0.57604500	0.60059400	-1.16934400
Si	-2.33928500	-0.45839000	-0.65400000
Si	-4.51113300	-0.73593600	0.27574800
C	-2.53921400	0.00564700	-2.49052300
H	-3.05657100	0.96443200	-2.61158100
H	-1.55478900	0.09042800	-2.96306800
H	-3.11477400	-0.75732100	-3.02941600
C	-1.50206700	-2.16820700	-0.58720800
H	-0.50673300	-2.12779300	-1.04057900
H	-1.40694200	-2.55188200	0.43547900
H	-2.10503600	-2.89048200	-1.15229000
C	-5.36045200	-2.17232300	-0.64930800
H	-4.80823800	-3.11273000	-0.53453200
H	-6.37460700	-2.33531900	-0.26207500
H	-5.44665900	-1.96770200	-1.72329200
C	-4.45850300	-1.20189400	2.12501000
H	-4.00276800	-0.41812100	2.74129900
H	-5.47213100	-1.37768600	2.50825000
H	-3.88244300	-2.12141200	2.28571400
C	-5.60724700	0.80873400	0.06080000
H	-6.61170900	0.63065100	0.46632800
H	-5.19282400	1.68696300	0.56857800
H	-5.72032000	1.06713200	-0.99893100
C	3.79393500	-2.69897900	-0.00370700
C	2.39499900	-2.92618600	0.63401300
C	4.62889600	0.19841900	1.02699800
C	1.69701500	-1.65534400	1.07294600
C	3.72415800	-0.45587100	2.10601100
C	2.27314200	-0.56664100	1.67611000
H	4.03062200	-3.56296700	-0.63560100
H	2.48786500	-3.63207400	1.47391700
H	4.53249400	1.28855100	1.10069100
H	3.78029700	0.14799200	3.01930300
H	4.56353700	-2.67893600	0.77432400
H	1.74574500	-3.41809700	-0.10017000
H	5.68405800	-0.02818000	1.24849500
H	0.61269500	-1.67040400	1.01043100
H	4.10918800	-1.44412800	2.37365700
H	1.60625900	0.22288300	2.02169700
C	3.87960800	-1.43415000	-0.84617100
C	4.28254100	-0.18912500	-0.39638800
Ni	2.19433400	-0.22688300	-0.48451600
H	3.84690900	-1.58129500	-1.92600000
H	4.57107100	0.54265600	-1.14918400

INT1b

C	-2.13161800	1.74644200	1.15738200
C	-1.43975300	1.00368300	0.18800500
C	-0.20096500	1.52899500	-0.28772600

C	0.24662700	2.82087600	0.15447400
C	-0.49838800	3.51568300	1.12482400
C	-1.66984800	2.97762700	1.63993800
H	-3.07035300	1.36499000	1.54952100
C	1.43939900	3.37909000	-0.42915700
H	-0.14167200	4.48721600	1.46117400
H	-2.23730700	3.51639900	2.39403100
C	2.09548600	2.69214400	-1.42131000
C	1.64556500	1.40159300	-1.79062900
H	1.76950900	4.36433900	-0.10995400
H	2.95191800	3.12225300	-1.93490300
H	2.00113500	0.94673300	-2.71496800
N	0.54939600	0.78951300	-1.19785000
Si	-2.21688900	-0.58897800	-0.51142100
Si	-4.50510700	-0.78969400	0.09932200
C	-2.15840200	-0.60041000	-2.41415400
H	-2.69262100	0.26091800	-2.83304100
H	-1.12292200	-0.55323600	-2.76332500
H	-2.62497800	-1.50965200	-2.81377600
C	-1.30817400	-2.13167700	0.14378800
H	-0.24287800	-2.07751800	-0.10435900
H	-1.39692700	-2.21345800	1.23392500
H	-1.71757900	-3.05034000	-0.29528300
C	-5.21705900	-2.30927200	-0.80849000
H	-4.68044400	-3.22839900	-0.54392300
H	-6.27300500	-2.45639400	-0.54702400
H	-5.15939800	-2.19361700	-1.89724600
C	-4.75989500	-1.08253600	1.96755800
H	-4.42271800	-0.23566400	2.57666700
H	-5.82297400	-1.24502800	2.18849500
H	-4.21381000	-1.97024600	2.30950300
C	-5.52220800	0.73223000	-0.42970300
H	-6.58257200	0.60056800	-0.17803400
H	-5.17285700	1.64887300	0.05890500
H	-5.45667900	0.89317100	-1.51262700
C	2.75808300	-2.62957700	1.28023900
C	2.21507200	-1.48195000	2.17373200
C	4.91995300	-1.16625100	-0.53285300
C	2.44209200	-0.08580600	1.62276700
C	4.86502600	-0.41181800	0.82156200
C	3.58447200	0.38316100	1.01260800
H	2.20727600	-3.54541200	1.52313500
H	2.64549900	-1.56826400	3.18517100
H	5.28025600	-0.47737400	-1.30566600
H	5.72069200	0.27143700	0.87589300
H	3.80500500	-2.83787800	1.52495300
H	1.13445700	-1.61442400	2.29396000
H	5.66936300	-1.97334600	-0.47214000
H	1.68202100	0.64833800	1.88840500
H	4.99046800	-1.11513000	1.65053200
H	3.63432500	1.45023400	0.80519100
C	2.62569700	-2.35533800	-0.21196000
C	3.58252400	-1.71527900	-0.99710200
Ni	2.12070300	-0.30192200	-0.51097400
H	1.85072500	-2.91226200	-0.73668200
H	3.48943500	-1.83886400	-2.07765400

INT1c

Ni	0.48661300	0.18304000	-0.11096500
Si	-3.44359700	-0.08360900	0.78413200
Si	-3.72283400	2.21644800	1.30024100
C	-5.10098900	-0.99068200	1.06609900
C	-2.18686500	-0.89223300	1.96563700

C	-2.96073800	-0.33843700	-1.03856500
C	2.11168200	-0.60084700	0.34434600
N	-1.04166600	1.09884300	-0.74555000
C	-5.25283300	2.42309200	2.42536000
C	-4.01072300	3.25279600	-0.26871100
C	-2.21683500	2.89931500	2.24082100
H	-5.01214000	-2.06828000	0.87730200
H	-5.42259700	-0.86694000	2.10747900
H	-5.90561900	-0.60445900	0.42910500
H	-2.52770500	-0.81904200	3.00689700
H	-1.20823200	-0.40261900	1.89321600
H	-2.05132300	-1.95404700	1.72693800
C	-1.82498800	0.32251700	-1.59327100
C	-3.74781700	-1.10857100	-1.89679500
N	2.33969700	-1.91288500	0.63472200
N	3.31730700	0.02828100	0.42554200
C	0.05074800	1.75529800	-1.27376700
H	-6.16828600	2.07322700	1.93332400
H	-5.40126200	3.47867200	2.68846600
H	-5.14720200	1.86229000	3.36233600
H	-4.89374100	2.90999100	-0.82137600
H	-4.16562000	4.30984100	-0.01553800
H	-3.14955700	3.18694500	-0.94220600
H	-1.30724100	2.76244000	1.64673200
H	-2.33513100	3.96955900	2.45537000
H	-2.07550500	2.38127800	3.19743000
C	-1.54482600	0.23066100	-2.99268300
C	-3.46458900	-1.22715600	-3.27048300
H	-4.61886400	-1.62729600	-1.50486200
C	3.76924600	-2.23879500	0.80395600
C	1.35836500	-2.95551200	0.54782700
C	4.40928000	-0.84529700	0.89626300
C	3.51748400	1.44068900	0.28077500
C	0.35623700	1.70433000	-2.67938100
H	0.43984400	2.59155500	-0.69244300
C	-2.38196300	-0.55643700	-3.81088600
C	-0.42101800	0.95731400	-3.51415500
H	-4.10545700	-1.83367800	-3.90543700
H	3.93418600	-2.84342400	1.70065900
H	4.13469600	-2.80955200	-0.06055300
C	0.82697400	-3.47974900	1.74224900
C	0.98173900	-3.46139200	-0.71189000
H	5.29836700	-0.74178400	0.26688400
H	4.69160300	-0.58457700	1.92519200
C	3.25238100	2.30011900	1.36379700
C	4.01801200	1.92765000	-0.94165400
H	1.19841900	2.28107900	-3.05282000
H	-2.16262700	-0.62494300	-4.87479200
H	-0.21411600	0.90694700	-4.58119300
C	1.22043200	-2.91557500	3.08724100
C	-0.09758100	-4.52676700	1.65597200
C	1.53696700	-2.88830700	-1.99435800
C	0.05061300	-4.50622100	-0.75285900
C	2.69720300	1.77396900	2.66603200
C	3.49278000	3.66941600	1.19668600
C	4.27345200	0.99737100	-2.10401000
C	4.24855800	3.30263600	-1.06612800
H	0.61705300	-3.36136500	3.88365300
H	2.27407800	-3.11099100	3.32573200
H	1.07834800	-1.83007500	3.11858700
C	-0.48461700	-5.03783000	0.41840600
H	-0.51949600	-4.93738200	2.56988700
H	2.62651100	-2.77489300	-1.95884200
H	1.11774000	-1.89415200	-2.19135400

H	1.29197300	-3.53482200	-2.84266800
H	-0.25367500	-4.90361000	-1.71777800
H	3.33529500	0.99536200	3.10162900
H	1.70523600	1.33113900	2.51621500
H	2.60536100	2.57950100	3.40080400
C	3.98886000	4.16946400	-0.00591900
H	3.28755500	4.34616000	2.02238500
H	3.36393500	0.45062400	-2.37643000
H	5.04343600	0.25002100	-1.87423700
H	4.61234500	1.55814000	-2.98066200
H	4.63184000	3.69283400	-2.00581000
H	-1.20476200	-5.85011200	0.36690300
H	4.17206900	5.23492200	-0.11703700

TS1a

Ni	-0.68752900	0.01819300	-0.12852600
Si	1.37022800	1.55279400	-0.78669200
Si	-0.01826700	2.24439800	1.07939300
C	3.82557900	0.05846900	-0.82569200
C	2.47986600	0.01374100	-0.48275400
C	2.00143000	-1.18883700	0.12323600
C	2.89490900	-2.27741800	0.38957200
C	4.25547000	-2.16972500	0.00247600
C	4.71027600	-1.02340600	-0.60372800
H	4.23120200	0.95866600	-1.27808100
C	2.38988600	-3.43228500	1.03749300
H	4.92407600	-3.00460900	0.19808200
H	5.75147600	-0.93590600	-0.90249200
C	1.06275400	-3.48048300	1.39188200
C	0.23566400	-2.38450000	1.07426800
H	3.06097300	-4.26169100	1.24704000
H	0.63620400	-4.34164300	1.89624800
H	-0.82309700	-2.40879300	1.31451800
N	0.66420800	-1.28522900	0.45756500
C	2.62366700	3.02167200	-0.70065600
H	3.23249000	3.01620100	0.20917800
H	3.30329600	3.01018700	-1.56300300
H	2.09067500	3.98049300	-0.73537500
C	0.83835100	1.70174200	-2.61584700
H	1.73892900	1.82076300	-3.23240200
H	0.27274200	0.85043400	-2.99622500
H	0.22794800	2.60352800	-2.75138600
C	-1.16749900	3.66458700	0.54505700
H	-1.64614400	4.12203800	1.42119200
H	-0.60820200	4.45476900	0.02899600
H	-1.95609100	3.31721500	-0.12956200
C	-0.95861300	0.99816700	2.19942000
H	-0.24663900	0.54579800	2.89889900
H	-1.68808300	1.58166600	2.77737600
H	-1.52665500	0.17898500	1.72914800
C	1.23103400	2.99017300	2.32127200
H	0.69896500	3.29946400	3.23092300
H	1.99797700	2.26475700	2.61861500
H	1.74264600	3.86982600	1.91780700
C	-3.63190200	0.78227800	-0.91339700
C	-4.07867800	0.47316900	0.53117000
C	-2.21722900	-2.15591600	-1.62737500
C	-3.87495800	-0.90448000	1.11422600
C	-3.60865600	-2.34441000	-0.98357800
C	-3.67691400	-2.07797500	0.49957700
H	-3.80606800	1.85897800	-1.04397000
H	-5.14951900	0.72465100	0.61386900
H	-1.50994200	-2.85275400	-1.15211400

H	-3.90902000	-3.38610200	-1.15820000
H	-4.32435200	0.30499200	-1.61950900
H	-3.57484200	1.18386600	1.19866100
H	-2.30314500	-2.50678100	-2.66829400
H	-3.91453800	-0.92418700	2.20528600
H	-4.33897000	-1.73142600	-1.51851800
H	-3.55158100	-2.95461200	1.13801300
C	-2.18174100	0.50767100	-1.33940700
C	-1.60377400	-0.75777300	-1.66792400
H	-1.81023100	1.32573000	-1.96047900
H	-0.84211600	-0.72474600	-2.45202200

TS1c

C	-3.44470800	1.61457300	1.64354900
C	-2.33079900	1.42000300	0.83974800
C	-2.56302800	1.05987700	-0.52452600
C	-3.89304800	0.99246500	-1.04881400
C	-4.98974500	1.20362900	-0.17367700
C	-4.76786400	1.49031700	1.15375000
H	-3.31006600	1.89804500	2.68582800
C	-4.06044800	0.72464200	-2.43168300
H	-6.00004600	1.13975100	-0.57144900
H	-5.60784000	1.65083000	1.82533200
C	-2.95114100	0.52694600	-3.21937300
C	-1.67521000	0.55077000	-2.61386800
H	-5.06347000	0.68434400	-2.85037700
H	-3.03486500	0.33508500	-4.28489400
H	-0.78789600	0.35680700	-3.21144600
N	-1.47074300	0.78719900	-1.32602800
Si	-0.52234200	1.79473300	1.42087400
Si	1.24867000	2.56022100	-0.61654900
C	-0.68432700	3.65564400	1.89846400
H	-1.13713800	4.25833300	1.10626000
H	-1.33251600	3.73311400	2.78253800
H	0.27752200	4.11211000	2.16200900
C	-0.22219800	1.04830100	3.16425400
H	-1.09382300	1.20921300	3.81491900
H	0.00319400	-0.01984100	3.14721300
H	0.62523400	1.56392700	3.63454900
C	2.74693400	3.27808300	0.33020200
H	3.48217000	2.50199200	0.56619700
H	3.24956100	4.04131700	-0.28054900
H	2.45013500	3.75670100	1.27102600
C	1.93658600	1.71997200	-2.22084600
H	2.15734000	0.65161600	-2.12345400
H	1.23524100	1.85412500	-3.05312900
H	2.88089400	2.21322500	-2.49140300
C	0.32792200	4.09200100	-1.31352500
H	0.93001900	4.52884300	-2.12259500
H	-0.64974500	3.83026700	-1.73580200
H	0.17373100	4.87465800	-0.56451100
Ni	0.31555700	0.56455300	-0.21091300
C	0.90156000	-1.22729100	0.27385400
N	0.09061300	-2.25839300	0.69088300
N	2.17737600	-1.71109600	0.36123200
C	0.81785200	-3.50923400	1.00029100
C	-1.31224300	-2.38846900	0.40259300
C	2.28032900	-3.06338900	0.94691600
C	3.40391200	-1.02061800	0.08099600
H	0.58597600	-4.27667700	0.25062300
H	0.52437900	-3.90109000	1.97980700
C	-2.24621400	-2.38651000	1.45407700

C	-1.71666600	-2.65484500	-0.92631700
H	2.73830600	-3.00977800	1.94320000
C	4.01866800	-0.24704500	1.08367400
C	4.03014800	-1.24147200	-1.16180500
C	-3.59896000	-2.59784800	1.14942500
C	-1.85233800	-2.17889800	2.89723700
C	-3.07482300	-2.85138300	-1.18688400
C	-0.71378000	-2.75914400	-2.05077700
C	5.27130500	0.31728600	0.81365700
C	3.33755000	-0.00435000	2.40656900
C	5.27874200	-0.65287900	-1.39448100
C	3.38433600	-2.09785500	-2.22623200
C	-4.01589500	-2.81810300	-0.15748100
H	-4.32655200	-2.58887700	1.95766300
H	-2.29495900	-2.95456100	3.53374800
H	-0.77027400	-2.19407600	3.03501100
H	-2.21387700	-1.21104900	3.26205600
H	-3.39405400	-3.04548300	-2.20774900
H	-1.22146700	-2.94103800	-3.00299100
H	-0.12107700	-1.84404400	-2.14171900
H	-0.00768800	-3.58448300	-1.89222600
C	5.89876200	0.11926400	-0.41471300
H	5.75416800	0.91895500	1.57959400
H	2.40033700	0.53936600	2.25172700
H	3.08696000	-0.93958900	2.92190400
H	3.97746300	0.58326700	3.07207200
H	5.76672300	-0.80846500	-2.35348400
H	2.36267000	-1.77076700	-2.44395900
H	3.96081800	-2.05704400	-3.15547800
H	3.32387900	-3.15135300	-1.92298900
H	-5.06858600	-2.97766000	-0.37564000
H	6.87054800	0.56593000	-0.60775600

INT2a

C	-3.85311200	-0.43718100	-1.29901700
C	-2.56283700	-0.19871700	-0.85253800
C	-2.33494600	0.99495900	-0.10497700
C	-3.40562500	1.89969100	0.18009200
C	-4.70291900	1.60557600	-0.31543900
C	-4.92052700	0.45915000	-1.04397700
H	-4.06751600	-1.34294200	-1.86186600
C	-3.12772700	3.05109600	0.95835600
H	-5.51512100	2.29691300	-0.10431500
H	-5.91463100	0.23201500	-1.41994200
C	-1.84852500	3.26439300	1.41470300
C	-0.84097300	2.33495100	1.07786900
H	-3.93004500	3.74881700	1.18630600
H	-1.59439600	4.13010500	2.01787700
H	0.17808400	2.49350600	1.41465500
N	-1.05309400	1.24652000	0.34879000
Si	-1.06258400	-1.35399100	-1.15112300
Si	-0.05492900	-1.76259300	1.43042900
C	-1.72829700	-3.14402000	-1.23004100
H	-2.18577000	-3.49948100	-0.30261600
H	-2.48148500	-3.21937000	-2.02604000
H	-0.91829600	-3.83547700	-1.49138700
C	-0.48401600	-1.05907800	-2.95691500
H	-1.31478200	-1.26155900	-3.64691100
H	-0.14555100	-0.03192500	-3.12706000
H	0.33893400	-1.73509200	-3.21879800
C	0.64902500	-3.53534400	1.34487500
H	1.64644300	-3.56613000	0.89269100
H	0.73145300	-3.95180200	2.35822700

H	2.90675100	-3.71338600	0.32720200
H	0.00344000	-4.20548300	0.76750800
C	0.97191300	-0.82720700	2.76792600
H	0.53184000	0.14906700	3.00250300
H	0.95346000	-1.42590300	3.69043800
H	2.02089900	-0.67147600	2.49694100
C	-1.78208400	-1.90101100	2.24587400
H	-1.68831700	-2.41076200	3.21457200
H	-2.20609300	-0.90768400	2.43529400
H	-2.51142200	-2.45960300	1.65020800
C	3.36900700	-1.17064600	-0.11308600
C	4.59149600	-0.37014200	0.40746900
C	2.65149700	2.02076900	0.08231900
C	5.29598700	0.45620000	-0.64075700
C	3.91494700	2.63636300	-0.56923400
C	5.00853100	1.70256500	-1.03544200
H	2.96107700	-1.72377500	0.73963600
H	5.30335100	-1.10023200	0.81536200
H	2.88578500	1.62536000	1.07453100
H	4.34291100	3.38179900	0.12202500
H	3.74488400	-1.93987900	-0.80165600
H	4.29551500	0.25291800	1.25604600
H	1.95696200	2.85605200	0.25045200
H	6.12804700	-0.03975600	-1.14233100
H	3.58821500	3.21694700	-1.44446300
H	5.64833100	2.13097800	-1.80865700
C	2.27520700	-0.40037700	-0.86189100
C	1.97486200	0.97953000	-0.79035100
Ni	0.42733300	-0.10738500	-0.06463800
H	2.04787600	-0.85620100	-1.82445200
H	1.55215300	1.41423400	-1.70165100

INT2b

C	3.62733300	1.52566500	0.87427900
C	2.41188100	1.03950100	0.41483000
C	2.45403300	0.09291000	-0.65650200
C	3.70210200	-0.29207100	-1.24991700
C	4.90763100	0.25064100	-0.73532300
C	4.86922000	1.13654700	0.31628800
H	3.63742600	2.24339200	1.69205900
C	3.68603300	-1.20651400	-2.33167300
H	5.85197800	-0.04685500	-1.18470300
H	5.79197800	1.55043400	0.71491600
C	2.48694200	-1.70904700	-2.78130500
C	1.30405100	-1.31157000	-2.12616100
H	4.62571400	-1.50171200	-2.79274100
H	2.43364200	-2.41112200	-3.60707200
H	0.34901200	-1.72692800	-2.43761700
N	1.27035400	-0.45787100	-1.11192400
Si	0.69879000	1.59757300	1.10590500
Si	-0.47716100	-1.95347500	1.52706500
C	0.86779200	1.72400900	3.00621400
H	1.07807900	0.75385900	3.46860400
H	1.66182900	2.42110900	3.30774600
H	-0.07092400	2.09541000	3.43732400
C	0.55528100	3.42744400	0.52253500
H	1.39256200	4.03124900	0.89993500
H	0.55478300	3.50968700	-0.57132800
H	-0.37165000	3.88555100	0.89118700
C	-1.66277700	-1.76498700	3.02193600
H	-2.70503300	-1.64638900	2.69925800
H	-1.61682600	-2.64336900	3.68126400
H	-1.40599300	-0.88390500	3.62249100

C	-0.96025600	-3.61785800	0.68268600
H	-0.89096500	-4.45130000	1.39640000
H	-1.98511400	-3.60860000	0.29051900
C	1.26359700	-2.28912600	2.25377700
H	1.24746900	-3.16018900	2.92385800
H	1.99134500	-2.49619100	1.45909900
H	1.64266400	-1.43520400	2.82645400
C	-4.72823900	-0.13368300	-0.55522300
C	-3.73609800	-1.23258400	-0.99259100
C	-2.90879400	2.52925700	-1.00189700
C	-2.43490500	-0.81199000	-1.63690000
C	-2.87142800	1.65359600	-2.27477200
C	-2.06388500	0.37430200	-2.16842800
H	-5.60008100	-0.64070000	-0.12369900
H	-4.25011900	-1.91382800	-1.68988700
H	-1.89143900	2.88849800	-0.80461100
H	-2.42845700	2.26352700	-3.07135800
H	-5.10487200	0.40221000	-1.43022100
H	-3.48780700	-1.84904300	-0.11904700
H	-3.49811000	3.43290100	-1.22664900
H	-1.73987100	-1.64495900	-1.75397900
H	-3.88914200	1.43225000	-2.60686200
H	-1.08337800	0.40943600	-2.64318800
C	-4.16948200	0.82065200	0.47631300
C	-3.42087700	1.91404000	0.27779500
Ni	-0.48211200	-0.10601400	0.04045200
H	-4.39539200	0.56458700	1.51124900
H	-3.12498200	2.46786100	1.16927000

INT2c

C	-3.34169700	1.69131400	1.75012100
C	-2.26625100	1.45950800	0.90491000
C	-2.56260500	1.09303700	-0.44504200
C	-3.91522300	1.05002800	-0.91296000
C	-4.97001700	1.29421600	0.00408900
C	-4.68674800	1.59260700	1.31707800
H	-3.15717700	1.98199200	2.78277000
C	-4.14678400	0.77336000	-2.28461400
H	-5.99716100	1.24710200	-0.35062100
H	-5.49427300	1.77969800	2.02086900
C	-3.07644100	0.54716000	-3.11676700
C	-1.77602500	0.55224000	-2.56505300
H	-5.16747000	0.75056900	-2.65981300
H	-3.20869600	0.34827700	-4.17607100
H	-0.91902400	0.34071400	-3.20024500
N	-1.51171700	0.79334100	-1.28983000
Si	-0.42432000	1.76704800	1.41931400
Si	1.25347700	2.55104000	-0.71757200
C	-0.49803200	3.63090200	1.91482700
H	-0.92424400	4.26520300	1.13186600
H	-1.13286700	3.73885800	2.80548300
H	0.48956200	4.03321500	2.17305600
C	-0.12127600	1.00944800	3.16080500
H	-0.97829700	1.19862000	3.82325000
H	0.06731600	-0.06651700	3.14387100
H	0.74723500	1.49759900	3.62169800
C	2.80984400	3.30535700	0.08885600
H	3.52366200	2.52634300	0.37498900
H	3.31407800	3.98414200	-0.61338700
H	2.56532900	3.88747200	0.98538600
C	1.81307700	1.48814900	-2.23751900
H	1.41835600	0.45459900	-2.22828600
H	1.45709900	1.95193000	-3.16621000

H	-0.28941600	-3.85036200	-0.15520700
H	2.90354100	1.39576100	-2.27081400
C	0.30419100	4.03825000	-1.46168000
H	0.89771600	4.48032500	-2.27411400
H	-0.66234900	3.73680000	-1.88200200
H	0.12044100	4.82889600	-0.72715900
Ni	0.36490400	0.57388400	-0.26431700
C	0.87997800	-1.22396600	0.27025500
N	0.05466100	-2.24582500	0.67726300
N	2.15188500	-1.70699900	0.40662600
C	0.77010700	-3.49587400	1.01814200
C	-1.34281900	-2.37728800	0.36266400
C	2.23490300	-3.05321700	1.00788900
C	3.38226200	-1.02609200	0.11700200
H	0.56021900	-4.26832100	0.26701400
H	0.44560600	-3.88079700	1.99041600
C	-2.29759100	-2.35947100	1.39567600
C	-1.72041800	-2.66497400	-0.96887800
H	2.87878500	-3.70909400	0.41247900
H	2.66012700	-2.99352700	2.01783000
C	4.02755900	-0.28270500	1.12383900
C	3.98199300	-1.22509200	-1.14266200
C	-3.64236400	-2.58611200	1.06873300
C	-1.93530100	-2.10204000	2.83867400
C	-3.07231200	-2.87552700	-1.25243400
C	-0.69657900	-2.76972900	-2.07398100
C	5.27386000	0.28721700	0.83609800
C	3.39807400	-0.09550300	2.48123900
C	5.22747800	-0.63569700	-1.39099500
C	3.31551500	-2.06309500	-2.20831800
C	-4.03265200	-2.83313500	-0.24205500
H	-4.38553300	-2.56771200	1.86234200
H	-2.51821100	-2.74932200	3.50370300
H	-0.87481500	-2.26674500	3.03762900
H	-2.15660200	-1.06433200	3.11110200
H	-3.37036400	-3.08810000	-2.27605900
H	-1.18113400	-3.00445200	-3.02673400
H	-0.13968800	-1.83469000	-2.18789600
H	0.04085700	-3.55793200	-1.87621800
C	5.87099300	0.11719000	-0.41119800
H	5.77665200	0.86954400	1.60419200
H	2.37712500	0.28161800	2.38538100
H	3.34951500	-1.03736800	3.04375700
H	3.97571200	0.61405400	3.08175300
H	5.69524500	-0.77712400	-2.36221000
H	2.32830700	-1.67079700	-2.47149800
H	3.92458400	-2.08521300	-3.11723200
H	3.17057100	-3.10064800	-1.88159500
H	-5.07956300	-3.00638200	-0.47706800
H	6.83831100	0.56735500	-0.61798600

INT3a

C	-2.77640000	-1.88096000	-0.80261600
C	-1.70910400	-1.01872900	-0.60901500
C	-1.99731000	0.28171900	-0.09921000
C	-3.33996200	0.67993900	0.18943600
C	-4.39208800	-0.24559400	-0.03886600
C	-4.11344000	-1.50257300	-0.52421200
H	-2.59418300	-2.88474200	-1.17984500
C	-3.56084900	1.98343700	0.69947900
H	-5.41368500	0.05565900	0.17971500
H	-4.91904700	-2.21192500	-0.69461000
C	-2.48887000	2.82160000	0.89933600

C	-1.19239700	2.35852300	0.58837400
H	-4.57498600	2.30431300	0.92563000

H	-2.61599400	3.82690200	1.28776700
H	-0.33042100	3.00160800	0.73135200
N	-0.93908900	1.14439500	0.11465900
Si	0.12989700	-1.41024900	-0.96892100
Si	1.40145900	-0.82097600	1.55237300
C	0.38308900	-3.28782100	-0.72982200
H	0.20757600	-3.64441400	0.28907300
H	-0.29558800	-3.83490700	-1.39838600
H	1.40433300	-3.56958500	-1.01285400
C	0.41644500	-1.16715400	-2.84775000
H	-0.19822600	-1.87104900	-3.42597300
H	0.17202900	-0.14974800	-3.16876700
H	1.46827000	-1.35108200	-3.09752100
C	2.81838300	-2.09906300	1.54537100
H	3.71457700	-1.70090500	1.05630900
H	3.09083000	-2.35141200	2.57938100
H	2.54949400	-3.03114200	1.03865600
C	2.02486400	0.62284500	2.65547100
H	1.26644900	1.40583800	2.77279900
H	2.26618500	0.23892100	3.65764200
H	2.92399500	1.08968100	2.23975600
C	-0.04090300	-1.57619100	2.55837400
H	0.31217500	-1.82599800	3.56836000
H	-0.86304400	-0.85838900	2.66484700
H	-0.45747900	-2.48862500	2.11981100
Ni	0.96455900	0.53066000	-0.23093700
C	1.93357100	2.00728100	-0.97308700
C	2.67088300	0.96065200	-0.90794700
C	1.80776300	3.43569800	-1.37052500
H	0.85017700	3.63874400	-1.86575800
H	1.85776800	4.09426200	-0.49257500
H	2.61160400	3.74380500	-2.05383900
C	3.99586400	0.33426900	-1.15996200
H	3.89425200	-0.64683900	-1.63771900
H	4.62237500	0.96616200	-1.80449700
H	4.54032300	0.17550500	-0.22042100

INT3b

C	3.13575200	-1.43293100	0.28329300
C	1.91132100	-0.78853600	0.37769100
C	1.86006300	0.57804600	-0.03568500
C	3.03877600	1.26159900	-0.47704500
C	4.26242300	0.54590900	-0.54316400
C	4.30505200	-0.78053900	-0.17912300
H	3.21515200	-2.47639800	0.58100100
C	2.93273100	2.63037700	-0.82851200
H	5.15654700	1.06238900	-0.88387100
H	5.24115700	-1.33043700	-0.23355800
C	1.71339600	3.26310300	-0.74060800
C	0.59101000	2.51522600	-0.32918600
H	3.81902300	3.16545500	-1.16159200
H	1.59528700	4.31150300	-0.99519300
H	-0.39061000	2.97831600	-0.27492300
N	0.64427800	1.23097300	-0.00200200
Si	0.29611200	-1.57545300	1.06139100
Si	-1.51878700	-0.91080100	-1.68187000
C	0.28287700	-3.42516400	0.58120600
H	0.22297000	-3.59820500	-0.49738400
H	1.18017200	-3.93750700	0.95538400
H	-0.58259900	-3.91830200	1.04212800

C	0.55623100	-1.62106900	2.96885900
H	1.41715600	-2.25263600	3.22982300
H	0.73674300	-0.62211600	3.38102500
H	-0.32524900	-2.03737700	3.47311100
C	-2.70290700	-2.40565400	-1.53249800
H	-3.63813400	-2.11839400	-1.03539400
H	-2.96300800	-2.80261400	-2.52387200
H	-2.25905500	-3.21997000	-0.94969300
C	-2.40343600	0.32218800	-2.86600800
H	-1.82477900	1.24379000	-3.00622100
H	-2.53135500	-0.14017000	-3.85584200
H	-3.39756500	0.60406700	-2.50220400
C	0.01020900	-1.45934500	-2.69447500
H	-0.31164400	-1.87697100	-3.65895400
H	0.66050200	-0.60174100	-2.90760400
H	0.62326900	-2.21405400	-2.19236600
Ni	-1.11615500	0.15329100	0.39594700
C	-2.13606100	1.17069700	1.94420900
C	-2.66042300	1.51381600	0.86574200
C	-1.87165700	1.09865800	3.39521600
H	-1.94848100	0.07064600	3.76251400
H	-0.86259500	1.45393300	3.63131100
H	-2.59013200	1.71841500	3.95034800
C	-3.61774400	2.21850600	-0.01652700
H	-4.32094000	1.51238300	-0.47088000
H	-4.19720900	2.95814200	0.55316100
H	-3.11044900	2.73710800	-0.83634700

INT3c

C	-3.38543900	-1.92236400	-1.14240000
C	-2.37185700	-1.05149300	-0.77544700
C	-2.74916200	0.26022900	-0.36212100
C	-4.12232000	0.65885100	-0.33480000
C	-5.11413300	-0.27564100	-0.73280500
C	-4.75058200	-1.54225900	-1.12823800
H	-3.13785500	-2.93513500	-1.45254000
C	-4.43479100	1.97119000	0.09836400
H	-6.15839900	0.02644200	-0.71460100
H	-5.51060400	-2.25863500	-1.42879100
C	-3.41939900	2.81796900	0.47698800
C	-2.08737400	2.35547600	0.41852700
H	-5.47362100	2.29141200	0.12666800
H	-3.61715100	3.82945800	0.81661800
H	-1.26756900	3.00446800	0.70694600
N	-1.74960200	1.13442400	0.02134400
Si	-0.49908200	-1.44895400	-0.78302200
Si	0.26401800	-0.73679900	1.90803300
C	-0.30047400	-3.30800000	-0.39779300
H	-0.64767600	-3.59798200	0.59790200
H	-0.86322700	-3.89645600	-1.13525600
H	0.75023300	-3.60846200	-0.48699900
C	0.09630500	-1.29138100	-2.59638200
H	-0.41685400	-2.02754800	-3.23065700
H	-0.10140900	-0.29279800	-2.99898100
H	1.17503500	-1.47017000	-2.66977500
C	1.64071800	-2.00241800	2.26657300
H	2.61882200	-1.62244300	1.95307500
H	1.68547600	-2.18719300	3.34870400
H	1.48128100	-2.96722300	1.77441600
C	0.66627500	0.77341500	3.02213300

H	-0.08585800	1.56620500	2.93612600
H	1.64103100	1.20494600	2.77221800
H	-1.20905100	-1.66161100	3.70182000
H	-2.17135000	-0.69949100	2.57061300
H	-1.71269200	-2.35385100	2.15400300
Ni	0.18678500	0.53533500	0.00727000
C	1.21056700	2.02523400	-0.59311300
C	1.97001700	1.00063600	-0.40599600
C	1.10402700	3.43685900	-1.04774400
H	0.12532000	3.65600700	-1.49171400
H	1.23650200	4.12892400	-0.20391300
H	1.87474300	3.68204500	-1.79186000
C	3.33391800	0.49759800	-0.46541500
C	4.41730200	1.39992400	-0.44245200
C	3.61722800	-0.87598300	-0.56547300
C	5.73070100	0.94227900	-0.51896500
H	4.21483400	2.46411500	-0.35826700
C	4.93199800	-1.33244600	-0.64962600
H	2.79068900	-1.57929400	-0.57555700
C	5.99466500	-0.42633300	-0.62505800
H	6.55146700	1.65496800	-0.49627600
H	5.12780800	-2.39866500	-0.73123000
H	7.01957900	-0.78261400	-0.68578800

INT3d

C	-3.59505100	1.35871300	-1.20739900
C	-2.37169000	0.84964800	-0.80192900
C	-1.55906500	1.67380000	0.03151100
C	-1.99142800	2.97762700	0.42694300
C	-3.25193300	3.44675100	-0.02768400
C	-4.03769100	2.65087100	-0.82920000
H	-4.24699000	0.75554400	-1.83538400
C	-1.14173800	3.74353500	1.26339300
H	-3.58250400	4.43860300	0.27082100
H	-5.00397000	3.00973100	-1.17366300
C	0.06454300	3.21900500	1.66483800
C	0.42727600	1.92637300	1.22903300
H	-1.45380400	4.73735800	1.57561300
H	0.74468200	3.77456400	2.30215000
H	1.38202800	1.49783900	1.51475700
N	-0.34211600	1.17285200	0.45216700
Si	-1.66533000	-0.87003200	-1.25775300
Si	-1.07252300	-1.98500300	1.34424500
C	-3.13361800	-2.06570500	-1.49170500
H	-3.73165600	-2.22891600	-0.59078500
H	-3.80075800	-1.67394200	-2.27163000
H	-2.77619100	-3.04239200	-1.83906800
C	-0.90566800	-0.74161000	-3.01033500
H	-1.68173600	-0.48877000	-3.74609000
H	-0.12252700	0.02141900	-3.05876200
H	-0.45715000	-1.69773600	-3.30528100
C	-1.37810000	-3.83865600	1.01754600
H	-0.47031600	-4.33148300	0.65251700
H	-1.67039400	-4.33370000	1.95374600
H	-2.17175100	-4.01958100	0.28603400
C	0.19779200	-1.91660400	2.78131100
H	0.44433100	-0.88629500	3.06286700
H	-0.22694900	-2.41242300	3.66639800
H	1.13287900	-2.42245200	2.51891100
C	-2.67004400	-1.26067300	2.10807000
H	-2.94519500	-1.84740200	2.99538400
H	-2.51291400	-0.22565900	2.43516900
H	-3.53075400	-1.26271700	1.43186200

H	0.69062100	0.44940800	4.07302700
C	-1.36185500	-1.43611300	2.63740100
Ni	0.21067500	-0.70963900	-0.04489500
C	2.10183300	-0.72338400	-0.38274200
C	1.58288100	-1.88891300	-0.55387600
C	3.29353800	0.10402300	-0.36868400
C	4.49868200	-0.37788200	0.18404800
C	3.28192900	1.41020100	-0.89664900
C	5.64417100	0.41539500	0.20204100
H	4.52210200	-1.38090400	0.60114100
C	4.43378900	2.19541500	-0.88965100
H	2.35869100	1.79354300	-1.32240600
C	5.61954300	1.70462300	-0.33723300
H	6.56184400	0.02382900	0.63424000
H	4.40491900	3.19604300	-1.31410300
H	6.51509300	2.32014400	-0.32594700
C	1.81188000	-3.30192500	-0.95625300
H	2.78743500	-3.42460900	-1.44563200
H	1.79187100	-3.96579100	-0.08214500
H	1.03456300	-3.65719600	-1.64205200

INT3e

C	-3.92425100	-1.44215300	-1.46307700
C	-2.75867200	-0.91380200	-0.93143100
C	-2.84993200	0.34357000	-0.26379200
C	-4.09909300	1.03004100	-0.15244100
C	-5.25688300	0.44122300	-0.72540100
C	-5.16937700	-0.77201000	-1.36828200
H	-3.89598300	-2.40387700	-1.97056400
C	-4.12743500	2.26932900	0.53433700
H	-6.20712300	0.96309500	-0.64310500
H	-6.05688400	-1.22365600	-1.80347800
C	-2.96483500	2.77489300	1.06690000
C	-1.76728100	2.04439800	0.91155600
H	-5.06880900	2.80520300	0.63039800
H	-2.94418600	3.72095800	1.59778400
H	-0.83391200	2.43088600	1.30596700
N	-1.69780600	0.87777200	0.28141200
Si	-1.02671100	-1.72265200	-1.01325800
Si	-0.29048100	-1.71442900	1.78476600
C	-1.25676400	-3.61641500	-0.99744600
H	-1.71497400	-4.00698100	-0.08448600
H	-1.88923600	-3.91357700	-1.84496400
H	-0.29140700	-4.11942100	-1.13055900
C	-0.30368700	-1.36332600	-2.74865400
H	-0.93125700	-1.82242100	-3.52518700
H	-0.24147400	-0.28865600	-2.94678600
H	0.70764100	-1.77601300	-2.83794700
C	0.73216400	-3.31325300	1.93787200
H	1.79909500	-3.12217000	1.78254300
H	0.61087800	-3.71405300	2.95368600
H	0.42502700	-4.09627800	1.23729100
C	0.36735800	-0.55973200	3.16851700
H	-0.18115600	0.38790500	3.21656000
H	0.25004000	-1.06215100	4.13993400
H	1.42822700	-0.32875100	3.02726200
C	-2.07639900	-2.13216900	2.32924200
H	-2.04596000	-2.58449400	3.33004800
H	-2.69010300	-1.22640400	2.39579100
H	-2.59570100	-2.83275100	1.66736300
Ni	0.04716000	-0.14218100	0.15910200
C	1.43512900	1.14647800	-0.11868800
C	1.90803000	-0.05684400	-0.12788300

C	3.11227700	-0.84890600	-0.32707300
C	3.05509800	-2.22241500	-0.62245400
C	5.54280300	-0.97414300	-0.45962400
H	4.44052400	0.82563900	-0.03094300
C	4.21967200	-2.95868000	-0.83616700
H	2.08474400	-2.70380000	-0.68331300
C	5.46842900	-2.33912000	-0.75320600
H	6.51059400	-0.48307300	-0.39540600
H	4.15202500	-4.01885200	-1.06679000
H	6.37641600	-2.91358100	-0.91633600
C	1.64457200	2.57667200	-0.20332100
C	2.59737600	3.22038900	0.61514600
C	0.88574600	3.37013000	-1.08822700
C	2.78662500	4.59938400	0.54163400
H	3.17975100	2.62606900	1.31385200
C	1.09077600	4.74611900	-1.16914200
H	0.14369500	2.88765400	-1.71822500
C	2.03861700	5.36940600	-0.35303300
H	3.52531000	5.07406800	1.18279800
H	0.50436400	5.33570200	-1.86957700
H	2.19190400	6.44353800	-0.41240100

TS2a

C	-3.27686600	-1.83420100	-0.10841700
C	-2.12211400	-1.07120400	-0.18486100
C	-2.24854900	0.32994600	0.03379900
C	-3.52065900	0.92336000	0.31590700
C	-4.66670600	0.08826900	0.37476400
C	-4.54526500	-1.26649200	0.16608300
H	-3.21832400	-2.90955700	-0.26348400
C	-3.58373400	2.32104500	0.53393100
H	-5.63304700	0.53783000	0.58982900
H	-5.42306300	-1.90590100	0.21376800
C	-2.43097900	3.06751000	0.46630600
C	-1.21288100	2.42011700	0.17487100
H	-4.54278900	2.78546400	0.75133600
H	-2.43518500	4.14071700	0.62673900
H	-0.29136200	2.98454100	0.10356900
N	-1.10376900	1.10967100	-0.03214200
Si	-0.34483100	-1.70833600	-0.56113400
Si	2.36863900	-0.28100000	1.16272000
C	-0.17860300	-3.34106900	0.43123000
H	-0.08891200	-3.17946500	1.51145900
H	-1.05188000	-3.98648700	0.26424800
H	0.70200100	-3.90764900	0.10489500
C	-0.37557600	-2.26725300	-2.39752200
H	-1.12893900	-3.04670600	-2.57685900
H	-0.59432200	-1.42646700	-3.06645500
H	0.60060700	-2.67460400	-2.69119000
C	3.16303800	-2.00386700	1.15067500
H	2.43818800	-2.79846700	0.95886100
H	3.96495200	-2.09065700	0.41093500
H	3.60811000	-2.18639900	2.13826600
C	3.71243900	0.93234900	1.77168400
H	3.30435700	1.94815600	1.84138700
H	4.04953100	0.63929700	2.77553600
H	4.59387300	0.97305800	1.12285800
C	1.09322900	-0.19676100	2.59051500
H	1.63344600	-0.35450500	3.53592000
H	0.61045200	0.78479800	2.64547100
H	0.31035700	-0.95464200	2.50719600
Ni	0.67400500	0.34099900	-0.39094300
C	1.87668100	1.65114600	-1.05366700

C	4.38040000	-0.23639200	-0.25037300
C	2.51141300	0.49857000	-0.89788600
C	2.18016400	2.94183800	-1.73214800
H	1.30289200	3.35908100	-2.24140500
H	2.49748900	3.68784300	-0.98853800
H	2.99699600	2.85630800	-2.46558000
C	3.68301500	-0.15589400	-1.58821400
H	3.45353700	-1.18948500	-1.86948700
H	3.92483900	0.39986200	-2.50336100
H	4.58884800	-0.17539100	-0.96900600

TS2b

C	-3.64950500	1.02355200	-0.49284200
C	-2.32968600	0.70176300	-0.21417500
C	-2.04236100	-0.67112300	0.06291000
C	-3.08207200	-1.65868400	0.06951900
C	-4.41139800	-1.25937900	-0.22472500
C	-4.68726300	0.05924000	-0.50433300
H	-3.91002300	2.05750800	-0.71063600
C	-2.73978900	-2.99919900	0.37453000
H	-5.19881300	-2.00923000	-0.22256600
H	-5.70506800	0.36671900	-0.73078900
C	-1.43301300	-3.32299200	0.65794500
C	-0.46166200	-2.30097500	0.62029700
H	-3.51918400	-3.75777300	0.98406900
H	-1.13544900	-4.33789000	0.30109300
H	0.58089800	-2.52214900	0.83168700
N	-0.73844300	-1.03771200	0.33247600
Si	-0.87204300	1.96885700	-0.16097500
Si	2.48821600	-0.39706300	-1.25693500
C	-1.00078400	2.97608700	-1.78778800
H	-0.88512700	2.33973600	-2.67276600
H	-1.96396500	3.49827600	-1.87423600
H	-0.21165500	3.73807500	-1.82459200
C	-1.32583200	3.21055800	1.22652100
H	-2.28718500	3.70812700	1.03860700
H	-1.38798900	2.71491900	2.20226100
H	-0.55916800	3.99254400	1.30211500
C	3.89796600	0.82663000	-1.61871000
H	3.49675100	1.84174600	-1.72091500
H	4.66526600	0.85319900	-0.83849700
H	4.38956100	0.56643800	-2.56598800
C	3.14463000	-2.18794800	-1.28772500
H	2.35246800	-2.90605900	-1.04128600
H	3.48022400	-2.41854200	-2.30793900
H	3.98608100	-2.37306000	-0.61532500
C	1.32725000	-0.32598000	-2.78555700
H	1.88822800	-0.65455600	-3.67435700
H	0.45905600	-0.98487600	-2.67419300
H	0.95901100	0.68773600	-2.96913900
Ni	0.79574400	0.40008700	0.26430900
C	1.66381600	0.56349100	1.97007700
C	2.52731600	-0.10504800	1.26834500
C	1.45569200	1.07369700	3.35051400
H	1.25257500	2.15116100	3.34257700
H	0.58297300	0.59470400	3.81237700
H	2.32525300	0.89428200	4.00195900
C	3.82898500	-0.78492300	1.59269800
H	4.16174900	-0.46990900	2.59073300
H	3.71961200	-1.87565100	1.60740900
H	4.63204600	-0.55165500	0.88609200

C 3.81695300 2.09247100 -0.19467300

TS2c

C 2.72686800 1.23677900 -0.22282200
C 2.99298600 -0.15945000 -0.30173700
C 4.33492800 -0.65487500 -0.36375600
C 5.40825500 0.27332000 -0.33610000
C 5.15213400 1.62264100 -0.25087400
H 3.65233000 3.16597400 -0.12922100
C 4.53873100 -2.05374900 -0.44200500
H 6.42772300 -0.10203500 -0.38015600
H 5.97477400 2.33276800 -0.22689200
C 3.45085600 -2.89455800 -0.45777100
C 2.15642600 -2.33942900 -0.39524900
H 5.55254200 -2.44451300 -0.48882300
H 3.56249600 -3.97227100 -0.51749100
H 1.28168300 -2.97733000 -0.40912700
N 1.91562600 -1.03243800 -0.31627300
Si 0.86895700 1.73509200 -0.18642800
Si -1.29557900 -0.28148800 1.82601900
C 0.75373500 3.16877000 1.08037400
H 0.91082200 2.83949900 2.11377300
H 1.50331400 3.94130900 0.86054600
H -0.22794200 3.65591100 1.03293700
C 0.54687800 2.56781000 -1.88694400
H 1.21141500 3.42725100 -2.05087800
H 0.70134700 1.86089000 -2.71077200
H -0.48649600 2.93044300 -1.95817300
C -2.18226400 1.30825100 2.34619000
H -1.62886500 2.21252500 2.08283900
H -3.18191800 1.37852600 1.90802600
H -2.29669000 1.29018800 3.43875100
C -2.35810900 -1.72632300 2.47125400
H -1.89647800 -2.69156400 2.22981800
H -2.44247100 -1.66091700 3.56466600
H -3.37137800 -1.72250500 2.05671300
C 0.31492100 -0.45750100 2.85004700
H 0.02624800 -0.52508200 3.90968700
H 0.86543300 -1.36963000 2.59807500
H 0.98986500 0.39334100 2.72845900
Ni 0.04966900 -0.41324300 -0.16820800
C -1.16360500 -1.75729700 -0.73223700
C -1.83810000 -0.70404600 -0.27523000
C -1.50583300 -2.96799900 -1.52841100
H -0.69519100 -3.26362400 -2.20540000
H -1.68337000 -3.81940200 -0.85433200
H -2.42319000 -2.83292000 -2.12097900
C -3.16545300 -0.13214300 -0.58352300
C -4.30330700 -0.95949900 -0.62662600
C -3.32191400 1.23165500 -0.88633100
C -5.55228100 -0.44045400 -0.96988900
H -4.20295900 -2.01313000 -0.38202300
C -4.56991300 1.74841600 -1.23030100
H -2.44915400 1.87711900 -0.85981100
C -5.69143300 0.91533500 -1.27283000
H -6.41842800 -1.09694200 -0.99707800
H -4.66739100 2.80475000 -1.46806400
H -6.66421700 1.32003800 -1.53896000

C 2.94298800 -0.24364900 -0.54393400
C 2.28836700 -1.29463700 0.15894100
C 3.00787000 -2.44992700 0.60280900
C 4.39562700 -2.54080200 0.31962200
C 5.02856700 -1.52827000 -0.36437900
H 4.83637900 0.39702300 -1.31416800
C 2.30656700 -3.45237100 1.31593100
H 4.94337200 -3.41800300 0.65522700
H 6.09176700 -1.59793100 -0.57958700
C 0.96189200 -3.29467200 1.55662900
C 0.31126000 -2.13961100 1.07617600
H 2.84046600 -4.33390500 1.66318900
H 0.38707200 -4.03840300 2.09873500
H -0.75258500 -2.00354000 1.23001700
N 0.93056300 -1.16996300 0.40704900
Si 1.83950700 1.25121000 -1.04670200
Si -0.67277500 2.29987400 1.18151100
C 2.89653100 2.80144600 -0.65712900
H 3.00385900 2.98419200 0.41813200
H 3.90632400 2.69611700 -1.07706100
H 2.45673300 3.70005600 -1.10652800
C 1.72553100 1.20524800 -2.96133100
H 2.71670800 1.26166700 -3.43187500
H 1.23859400 0.28695500 -3.31014100
H 1.13312100 2.05177200 -3.33168600
C -0.30633000 4.07911700 0.63481700
H -1.05209100 4.46790600 -0.06562900
H -0.32832500 4.72224400 1.52519000
H 0.67831200 4.18323300 0.17328600
C -2.28213000 2.37346300 2.20953000
H -2.55377400 1.37452600 2.57133100
H -2.13119000 3.01767800 3.08679800
H -3.13810400 2.76864700 1.65127900
C 0.61659500 1.78277800 2.50057900
H 0.50778700 2.45693700 3.36307100
H 0.44724000 0.76056500 2.85538300
H 1.64462100 1.84906800 2.13570600
Ni -0.09938600 0.41444600 -0.15255900
C -1.96146400 0.02738200 -0.28985000
C -1.74320500 1.32111800 -0.49364500
C -2.43156500 2.37779300 -1.32174700
H -3.16794300 1.90008300 -1.97946500
H -2.96558100 3.11633300 -0.71035700
H -1.71524500 2.92467800 -1.94465900
C -3.06334300 -0.90283000 -0.42831500
C -2.84203800 -2.21736200 -0.89225900
C -4.38310200 -0.53513600 -0.08386200
C -3.89699100 -3.11672000 -1.02780400
H -1.83091100 -2.51135700 -1.16085100
C -5.43180500 -1.44487700 -0.19703400
H -4.56993500 0.46949400 0.28485300
C -5.19525200 -2.73743800 -0.67430500
H -3.70676800 -4.11932600 -1.40266500
H -6.43907200 -1.14357500 0.07980300
H -6.01583100 -3.44372500 -0.76824900

TS2d

C 4.30036700 -0.38826500 -0.78512200

TS2e

C -4.50101800 -1.42121000 -0.86082400

C	-3.24251500	-0.90977400	-0.58494400
C	-4.34163900	1.25608600	-0.05278200
C	-5.60109800	0.67483800	-0.35341100
C	-5.67793000	-0.64071100	-0.74962600
H	-4.59994400	-2.45824700	-1.17495800
C	-4.20242500	2.60083400	0.36821600
H	-6.49596700	1.28546800	-0.26160300
H	-6.64317200	-1.08565900	-0.97735500
C	-2.94989300	3.09540700	0.64551900
C	-1.83166000	2.24841100	0.50202600
H	-5.08769900	3.22506900	0.46519300
H	-2.79823400	4.12018300	0.96836200
H	-0.83382400	2.62108400	0.69881300
N	-1.91469400	0.97697000	0.11714600
Si	-1.56791600	-1.84728500	-0.70298800
Si	0.83247500	-1.19616700	1.92208300
C	-1.91750800	-3.59178800	0.00849900
H	-2.10276300	-3.57732100	1.08873700
H	-2.79773400	-4.03928800	-0.47319000
H	-1.07525100	-4.27012900	-0.17491900
C	-1.27156800	-2.12716100	-2.57848900
H	-2.09087000	-2.69594000	-3.03917900
H	-1.18247000	-1.17314500	-3.11159900
H	-0.34185600	-2.68355600	-2.75119600
C	1.18525100	-3.05574600	1.92897100
H	0.42665900	-3.63781800	1.40125700
H	2.16206500	-3.28994700	1.49623300
H	1.19597000	-3.38803300	2.97629800
C	2.19318600	-0.39796000	2.99235700
H	2.03540700	0.68300000	3.08823600
H	2.16710900	-0.83072900	4.00178600
H	3.19626500	-0.56070800	2.58383600
C	-0.75677600	-0.86237000	2.93748300
H	-0.56633900	-1.20762600	3.96473400
H	-0.99881900	0.20413600	2.98677500
H	-1.63036200	-1.39323500	2.55053600
Ni	-0.26889900	-0.11277400	0.05739800
C	1.27943400	0.99608100	0.00429800
C	1.63674500	-0.28648700	0.08997900
C	1.84251500	2.30182800	-0.25636700
C	1.28022700	3.13258000	-1.25132400
C	2.92040700	2.81353800	0.50105900
C	1.80209000	4.39858300	-1.50520400
H	0.44354200	2.75617800	-1.83360500
C	3.41562600	4.09418400	0.26522100
H	3.34966400	2.20232400	1.28975800
C	2.86752200	4.88957100	-0.74478300
H	1.36887600	5.01010800	-2.29273600
H	4.24088500	4.46924500	0.86533300
H	3.26392400	5.88323400	-0.93484500
C	2.78400000	-1.07162800	-0.41706800
C	2.58542800	-2.31502600	-1.04252300
C	4.09749000	-0.57450000	-0.32660300
C	3.65938300	-3.03343700	-1.56557900
H	1.57567700	-2.70504200	-1.12432700
C	5.17108300	-1.29501900	-0.84958300
H	4.27177700	0.38675500	0.14513100
C	4.95832300	-2.52815600	-1.46948100
H	3.48088200	-3.98904000	-2.05212400
H	6.17716000	-0.89073600	-0.77109600
H	5.79590500	-3.08928500	-1.87509100

R2a

C	-3.16439100	0.45002100	-0.17132500
C	0.00000000	0.00000000	0.60459600
C	0.00000000	0.00000000	-0.60459600
C	0.00000000	0.00000000	2.06619900
H	-0.51068600	0.88473000	2.46621200
H	-0.51085600	-0.88463200	2.46621200
H	1.02154200	-0.00009800	2.46621200
C	0.00000000	0.00000000	-2.06619900
H	0.51068600	0.88473000	-2.46621200
H	0.51085600	-0.88463200	-2.46621200
H	-1.02154200	-0.00009800	-2.46621200

R2b

C	-0.60788900	-0.00002300	0.00000100
C	0.60788900	0.00002500	0.00000600
C	2.03706000	0.00001100	0.00000500
C	2.75339000	0.85785000	0.85715600
C	2.75337500	-0.85783900	-0.85714400
C	4.14604200	0.85468300	0.85400100
H	2.20554300	1.52090900	1.51966700
C	4.14602800	-0.85469200	-0.85399300
H	2.20551900	-1.52088900	-1.51965600
C	4.84706600	-0.00001100	0.00000300
H	4.68605400	1.52180500	1.52058100
H	4.68602700	-1.52182300	-1.52057600
H	5.93366000	-0.00001800	0.00000300
C	-2.03706000	-0.00000900	-0.00000200
C	-2.75339100	-0.85779700	0.85719900
C	-2.75337400	0.85778700	-0.85720500
C	-4.14604200	-0.85463200	0.85404200
H	-2.20554500	-1.52080800	1.51975900
C	-4.14602700	0.85463900	-0.85405700
H	-2.20551700	1.52079000	-1.51976400
C	-4.84706600	0.00000900	-0.00001000
H	-4.68605500	-1.52170700	1.52066900
H	-4.68602500	1.52172100	-1.52068800
H	-5.93366000	0.00001500	-0.00001300

R2c

C	-1.39433800	0.00070300	-0.00034700
C	-2.60675700	0.00055200	-0.00049700
C	-4.06625200	-0.00033900	0.00029500
H	-4.46497000	0.95732700	-0.35586500
H	-4.46450900	-0.78877700	-0.65018200
H	-4.46494200	-0.17073800	1.00837100
C	0.03548500	0.00036300	-0.00018600
C	0.75269700	-1.21177200	-0.00006600
C	0.75342300	1.21206200	-0.00006300
C	2.14534900	-1.20815100	0.00009800
H	0.20472300	-2.14914800	-0.00003300
C	2.14607700	1.20760200	0.00009600
H	0.20606000	2.14979600	-0.00003000
C	2.84738200	-0.00048300	0.00017000
H	2.68496100	-2.15156600	0.00020700
H	2.68624500	2.15069800	0.00020400
H	3.93403100	-0.00081400	0.00033200

INT4a

C	-3.62362800	-1.17834700	1.06866000
C	-2.33279300	-0.76243500	0.76250700

C	-1.57569800	-1.58795100	-0.12919600
C	-2.17141000	-2.76516800	-0.69903800
C	-3.49180700	-3.13326300	-0.33493200
C	-4.20512100	-2.35452800	0.54221500
H	-4.23229600	-0.57855400	1.74013400
C	-1.42739100	-3.52640600	-1.63401400
H	-3.92281200	-4.03291000	-0.76750500
H	-5.21797900	-2.62762300	0.82541300
C	-0.15977000	-3.12230600	-1.97467700
C	0.37149200	-1.97441600	-1.35332500
H	-1.87532300	-4.41527600	-2.07165000
H	0.44348200	-3.66844200	-2.69286200
H	1.38682600	-1.65885100	-1.57489500
N	-0.28473400	-1.23487600	-0.46342700
Si	-1.76408900	0.84299200	1.64082400
Si	-0.88110000	1.90865600	-1.99989100
C	-3.26133300	2.02553300	1.70131000
H	-3.62671800	2.29338000	0.70410500
H	-4.10470300	1.61828200	2.27170300
H	-2.95855300	2.95554700	2.19870300
C	-1.45226400	0.32276400	3.44447800
H	-2.27037300	-0.32568900	3.78093600
H	-0.51880300	-0.23835600	3.56071200
H	-1.41681100	1.18467300	4.12058700
C	-1.29393500	3.70105000	-2.51283800
H	-0.40190600	4.32430100	-2.63656600
H	-1.83446600	3.70409700	-3.46822300
H	-1.93738600	4.18899200	-1.76971300
C	0.20475500	1.16795700	-3.37489900
H	0.38068800	0.09881100	-3.21424200
H	-0.29189900	1.27993800	-4.34740700
H	1.18235100	1.65808300	-3.44888500
C	-2.54839200	1.00276500	-2.07084200
H	-3.02800500	1.30442000	-3.01184600
H	-2.45575800	-0.08540500	-2.08599400
H	-3.23311100	1.26952500	-1.26066000
Ni	0.85733000	0.17969300	0.47900900
C	-0.26666800	1.80383300	0.97211400
C	0.10215600	2.04252800	-0.37046800
C	0.26036700	2.73555600	2.07223600
H	0.29883400	2.25031000	3.05139400
H	1.26019900	3.12213600	1.86694500
H	-0.40436800	3.60838100	2.17045700
C	1.21001200	3.08440100	-0.61895700
H	2.06888600	2.94311300	0.04265600
H	1.59189500	3.03924300	-1.64483700
H	0.84470100	4.11024300	-0.46430200
C	3.81549300	0.78207000	1.06092300
C	4.04906000	0.73293800	-0.46365900
C	2.57795900	-2.34358700	1.28119400
C	4.02753800	-0.57051700	-1.21992600
C	3.98120000	-2.33445000	0.63892600
C	4.01455400	-1.83670200	-0.78492000
H	3.92391800	1.84034300	1.33528900
H	5.02330200	1.21101900	-0.66225900
H	1.89743000	-2.92138200	0.63709600
H	4.35501200	-3.36638500	0.64827800
H	4.64758100	0.27813000	1.57252100
H	3.31448700	1.39117800	-0.94397100
H	2.65873900	-2.93239400	2.20817400
H	4.04626600	-0.42859200	-2.30285600
H	4.66421700	-1.76336100	1.27414000
H	4.00217100	-2.61622900	-1.54864700
C	2.47598300	0.31367000	1.64145000
C	1.94584400	-1.00657600	1.65780900

H	2.18675300	0.92982500	2.49407800
H	1.21685600	-1.16532700	2.45988300

INT4b

C	-4.80893800	0.79721500	-0.13472500
C	-3.46451400	0.46008100	-0.18857700
C	-2.54363400	1.36737100	0.42186100
C	-3.00038500	2.57286200	1.04947500
C	-4.39054400	2.85545900	1.06875300
C	-5.27836000	1.97995300	0.48737800
H	-5.54228800	0.13310400	-0.58800500
C	-2.04098800	3.43938700	1.62891100
H	-4.73500300	3.76925000	1.54678200
H	-6.34384500	2.19459600	0.50104800
C	-0.70529800	3.11593400	1.57602300
C	-0.32607900	1.91201400	0.94555700
H	-2.37624800	4.35591400	2.10928500
H	0.05824800	3.75534900	2.00622900
H	0.72450000	1.63990600	0.88403300
N	-1.19413900	1.07017100	0.39988100
Si	-2.76336500	-1.13122800	-1.03033500
Si	1.25703200	-3.24435900	1.38268300
C	-3.75314100	-2.59838600	-0.30174700
H	-3.59617700	-2.69626100	0.77915200
H	-4.83354700	-2.49784600	-0.47503300
H	-3.43177200	-3.53891400	-0.76640400
C	-3.25999100	-1.00661100	-2.87558200
H	-4.34904800	-0.94788400	-3.00892000
H	-2.81716700	-0.12404900	-3.35271200
H	-2.90581100	-1.88849000	-3.42390300
C	0.56845600	-5.00611200	1.57630000
H	1.23861100	-5.75131600	1.13063700
H	0.43673200	-5.27114200	2.63318200
H	-0.40566300	-5.10305900	1.08166300
C	2.86107100	-3.12984900	2.40187300
H	3.28537600	-2.11860700	2.36802100
H	2.68062100	-3.38036200	3.45509400
H	3.62784400	-3.81931400	2.02813900
C	0.00120700	-2.03819900	2.14841800
H	-0.27096500	-2.36051500	3.16224800
H	0.40016000	-1.01972300	2.23209000
H	-0.94007200	-2.00218000	1.57783600
Ni	-0.48270200	-0.73017800	-0.43350200
C	0.91502000	-1.90198200	-1.11628700
C	1.58723400	-2.86781100	-0.42763200
C	1.20892300	-1.71346100	-2.60276200
H	0.60139700	-0.92107000	-3.05856400
H	2.26488100	-1.45595200	-2.78095900
H	1.01337200	-2.63177200	-3.17762700
C	2.63082400	-3.74893200	-1.11769500
H	3.43943000	-3.15200100	-1.56366500
H	3.10280400	-4.46552800	-0.43494500
H	2.18629700	-4.33205100	-1.93749900
C	4.11802200	1.44657500	-1.50884500
C	4.02073200	0.71964400	-0.15007200
C	2.69421700	4.29162700	-0.69482900
C	3.64596300	1.53177300	1.06517100
C	3.85996300	3.97690700	0.26765900
C	3.57696500	2.85842000	1.24998900
H	4.44137900	0.70514800	-2.24969800
H	4.98360700	0.22276500	0.05167400
H	1.82272300	4.60228200	-0.09839800

H	4.06641800	4.89031000	0.83956000
H	4.91359500	2.19565200	-1.47765400
H	3.29134500	-0.09793100	-0.24306900
H	2.96173300	5.18207200	-1.28653400
H	3.40929900	0.91240000	1.93301000
H	4.76924500	3.78047600	-0.30563600
H	3.27179000	3.19182500	2.24314500
C	2.81022800	2.04548300	-1.98262400
C	2.23609500	3.20674800	-1.63907400
H	2.25902800	1.42646200	-2.69045300
H	1.28216400	3.43381000	-2.11862900

INT4c

C	3.96705900	1.64109900	0.88533300
C	2.64970600	1.38814400	0.51398700
C	1.63824600	1.62817100	1.50066000
C	2.00366700	2.17226800	2.78118100
C	3.36945500	2.38943600	3.09425400
C	4.33978300	2.11771000	2.16171300
H	4.76287200	1.47908600	0.16242000
C	0.98089200	2.51452500	3.70040400
H	3.62538800	2.78551300	4.07428200
H	5.38907100	2.28514400	2.39011700
C	-0.33311900	2.33500600	3.33924200
C	-0.61419200	1.75479300	2.08766600
H	1.25241800	2.93266000	4.66674000
H	-1.15144200	2.61193900	3.99687600
H	-1.64488500	1.57315100	1.79928000
N	0.31003400	1.37444000	1.20840600
Si	2.46002800	0.81305500	-1.31207300
Si	-0.43793200	3.23447300	-1.62577200
C	3.32795400	2.11121000	-2.41454200
H	2.78962400	3.06105700	-2.47891700
H	4.34933100	2.32590300	-2.07594200
H	3.40108400	1.70758800	-3.43296600
C	3.56287300	-0.72522800	-1.45651000
H	4.56143200	-0.51884500	-1.05266800
H	3.15886200	-1.58112600	-0.91098100
H	3.69138800	-1.02119900	-2.50437400
C	-0.34599000	4.10881500	-3.32287500
H	-1.11244500	3.74919600	-4.01874500
H	-0.48680300	5.19153800	-3.20674500
H	0.62994100	3.95233300	-3.79945100
C	-2.12467600	3.68756300	-0.86237500
H	-2.28758600	3.17220800	0.09073900
H	-2.15768500	4.76716800	-0.66474300
H	-2.97272500	3.44942500	-1.51343900
C	0.83085000	4.13591500	-0.52895300
H	0.76017200	5.20288100	-0.78132800
H	0.59068900	4.03786500	0.53359900
H	1.87266600	3.83962100	-0.66325300
Ni	-0.30018300	0.05219400	-0.28958000
C	0.72751700	0.44496200	-1.98363900
C	-0.35859900	1.36019700	-1.96993800
C	0.78248300	-0.67721300	-3.02670400
H	1.34521900	-1.53842800	-2.65949000
H	-0.20728200	-1.03804700	-3.31609900
H	1.27928000	-0.33455200	-3.95092400
C	-1.55286500	1.04102500	-2.88707700
H	-1.83832100	-0.01157300	-2.83239100
H	-2.44351700	1.61958200	-2.62196900
H	-1.32710700	1.26245200	-3.94183500
C	-0.99749700	-1.65728200	0.10694800

N	-0.44422600	-2.92659300	0.09510600
N	-2.34257000	-1.88024600	0.36040000
C	-1.38220500	-3.99077000	0.50519600
C	0.94401600	-3.27320600	0.09672900
C	-2.73537900	-3.29743900	0.37375400
C	-3.33901000	-0.87319000	0.54814400
H	-1.17396300	-4.30410500	1.53912000
H	-1.29075500	-4.87123700	-0.13695600
C	1.74522800	-3.00006200	1.22729800
C	1.45078800	-4.02225400	-0.98649100
H	-3.40976000	-3.51090600	1.20975600
H	-3.25137700	-3.57576800	-0.55664800
C	-3.50661200	-0.32546700	1.83948400
C	-4.20604100	-0.52173800	-0.50474200
C	3.06560600	-3.46403500	1.23750700
C	1.20117100	-2.25065000	2.41933300
C	2.77665200	-4.47083500	-0.93256200
C	0.59217200	-4.36753200	-2.18146200
C	-4.49480900	0.64521800	2.03431000
C	-2.67486700	-0.81704600	3.00104700
C	-5.18542200	0.45295500	-0.26811100
C	-4.14146900	-1.20688600	-1.84896300
C	3.58152400	-4.19652700	0.16960800
H	3.68959600	-3.25608800	2.10330000
H	0.98240200	-1.20848700	2.16598800
H	0.26380900	-2.69131200	2.77944800
H	1.92039100	-2.26608300	3.24436900
H	3.17588000	-5.04005200	-1.76873700
H	0.01764100	-5.28932400	-2.01224000
H	-0.12264900	-3.57211700	-2.40590500
H	1.21252600	-4.53675700	-3.06756600
C	-5.32308000	1.04384500	0.98438400
H	-4.62706400	1.07719100	3.02364600
H	-2.90081400	-1.86701400	3.22959200
H	-1.60389100	-0.76005200	2.78881800
H	-2.88259000	-0.23217400	3.90281800
H	-5.84759200	0.74357000	-1.08046700
H	-3.14131300	-1.59121100	-2.05887800
H	-4.84066600	-2.05401000	-1.88804600
H	-4.42122100	-0.52051100	-2.65421200
H	4.60864800	-4.55064800	0.19725700
H	-6.08461800	1.80153800	1.14901000

TS3a

C	-3.92350600	0.76660700	1.13352100
C	-2.63181100	0.38501200	0.80410400
C	-2.47027600	-0.54392900	-0.25970400
C	-3.59498200	-1.01913300	-1.00335700
C	-4.89465300	-0.60792700	-0.60820400
C	-5.05513800	0.25986200	0.44853500
H	-4.08597400	1.48640000	1.93327200
C	-3.35862000	-1.85800900	-2.12182000
H	-5.75398900	-0.97848700	-1.16187600
H	-6.05117300	0.57740600	0.74617500
C	-2.06377700	-2.17821400	-2.45741600
C	-1.00714800	-1.70842000	-1.64788900
H	-4.19958900	-2.22441100	-2.70556200
H	-1.83593900	-2.79882600	-3.31839400
H	0.01985900	-1.97344000	-1.87838500
N	-1.18255800	-0.94210000	-0.57466700
Si	-1.03021700	1.06930500	1.63472100
Si	1.02701100	2.41806000	-1.72855300

C	-1.25384900	2.96296000	1.62721200
H	-1.21801400	3.37998000	0.61599600
H	-2.22021700	3.23775200	2.07146100
H	-0.46621200	3.44979000	2.21319100
C	-1.16531700	0.57011400	3.47870600
H	-2.15407100	0.85665100	3.86194400
H	-1.05638200	-0.51109200	3.62253500
H	-0.41821100	1.07227200	4.10304000
C	1.08471700	4.31225200	-1.95697200
H	2.08490500	4.74067300	-1.83232000
H	0.73707600	4.57705500	-2.96398200
H	0.42104600	4.81364700	-1.24093700
C	2.13888500	1.63288500	-3.06103900
H	2.06410100	0.53878700	-3.03130300
H	1.84007500	1.96074500	-4.06511000
H	3.19513600	1.89607800	-2.92860600
C	-0.75868400	1.94599500	-2.15761700
H	-1.04318700	2.52773200	-3.04491100
H	-0.86818400	0.88917000	-2.40942100
H	-1.47973600	2.18199300	-1.36973000
Ni	0.33063700	-0.33548500	0.59115600
C	1.31758900	1.27530800	1.03457400
C	1.74934500	2.04999500	-0.01305100
C	2.04894800	1.44423800	2.36695100
H	1.57828600	0.89432800	3.18407000
H	3.08767300	1.09030400	2.30326700
H	2.10259200	2.49916600	2.67204000
C	3.05422400	2.84683400	0.16337400
H	3.84413800	2.25222000	0.63957400
H	3.46028600	3.20509500	-0.78820700
H	2.90305700	3.73517800	0.79501800
C	3.14651100	-1.76895600	1.44939500
C	3.62232100	-1.30596900	0.05685300
C	0.63959900	-3.68538000	0.45408900
C	3.08091400	-1.96854400	-1.18411300
C	1.94363900	-4.07935400	-0.27142100
C	2.39567500	-3.10949000	-1.33792500
H	3.68668100	-1.15022200	2.17519600
H	4.72128100	-1.39153700	0.03193400
H	-0.17795400	-3.63160600	-0.27792800
H	1.76758900	-5.05377000	-0.74426600
H	3.49243900	-2.79208600	1.63782000
H	3.41155600	-0.23379000	-0.03402200
H	0.36611500	-4.52436700	1.11397200
H	3.31387900	-1.41520600	-2.09531600
H	2.73323600	-4.24914100	0.46553200
H	2.11858700	-3.37999100	-2.35809900
C	1.66037500	-1.65721500	1.78208800
C	0.62580700	-2.44399900	1.32204200
H	1.46026600	-1.12211100	2.70585900
H	-0.30081200	-2.37229700	1.89493300

Pro

C	1.99585300	2.08360100	-0.49683200
C	1.68017200	0.83549900	0.02259200
C	2.75237500	-0.11368200	0.13051900
C	4.08377800	0.24199500	-0.26834400
C	4.33505000	1.53726000	-0.78899200
C	3.30510500	2.43857200	-0.90597500
H	1.21943200	2.83625900	-0.59689600
C	5.10432800	-0.73265000	-0.12959600
H	5.34667100	1.79854300	-1.09162400
H	3.48891600	3.43188700	-1.30707900
C	4.79470400	-1.97561800	0.36769600
C	3.44943000	-2.23912600	0.72007500
H	6.12130700	-0.48175900	-0.42357100
H	5.55001600	-2.74649800	0.48704400
H	3.17574500	-3.22090200	1.10609300
Si	-0.10846200	0.47335600	0.62518900
C	-0.02069800	-0.35952300	2.32348600
H	-0.99827400	-0.41209900	2.81048300
H	0.38529300	-1.36875800	2.22988400
H	0.65174800	0.20851000	2.97882400
C	-0.89158100	2.19705500	0.81970600
H	-1.00657800	2.70692600	-0.14365600
H	-1.88313400	2.14875300	1.27618900
H	-0.26812300	2.82986300	1.46320400
C	-1.01461000	-0.53295100	-0.73157500
C	-2.35629900	-0.59830900	-0.95609300
C	-0.04628400	-1.22251500	-1.69301100
H	0.37800500	-0.51576300	-2.42094200
H	0.79773600	-1.64963700	-1.14439800
H	-0.51376200	-2.03600700	-2.25391700
C	-2.87194900	-1.24261700	-2.25074400
H	-3.01379200	-2.32769700	-2.14513800
H	-3.84431800	-0.83251500	-2.54444700
H	-2.19469100	-1.07879700	-3.09382900
Si	-3.84046700	-0.05483400	0.11739200
C	-4.49079200	1.62905700	-0.47389500
H	-3.76809400	2.43298700	-0.29832600
H	-4.70814700	1.61074900	-1.54879100
H	-5.42062700	1.89391600	0.04525900
C	-3.60970900	-0.04024800	2.00188000
H	-3.24496100	-1.01065100	2.35771300
H	-2.94184500	0.73176500	2.38945700
H	-4.59479400	0.12281400	2.45849800
C	-5.22522900	-1.33620000	-0.14478800
H	-6.06774700	-1.09865700	0.51692700
H	-5.61227000	-1.36158900	-1.16856200
H	-4.88908900	-2.34930400	0.10793300
N	2.47121700	-1.36274900	0.61155400