3,4-Polymerization of Isoprene by Using NSN- and NPN-Ligated Rare-earth Metal Precursors: Switching of Stereo Selectivity and Mechanism

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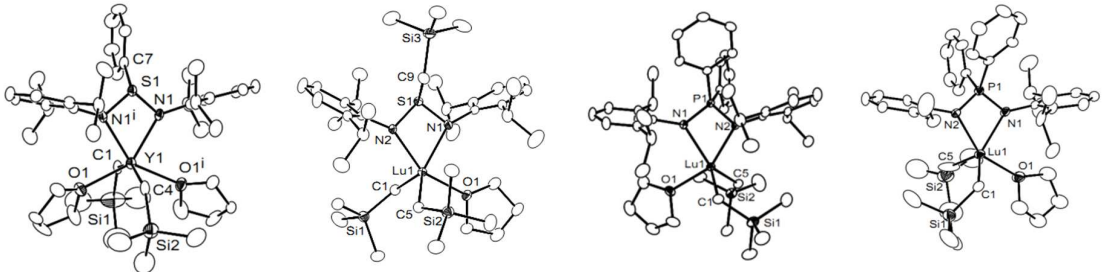
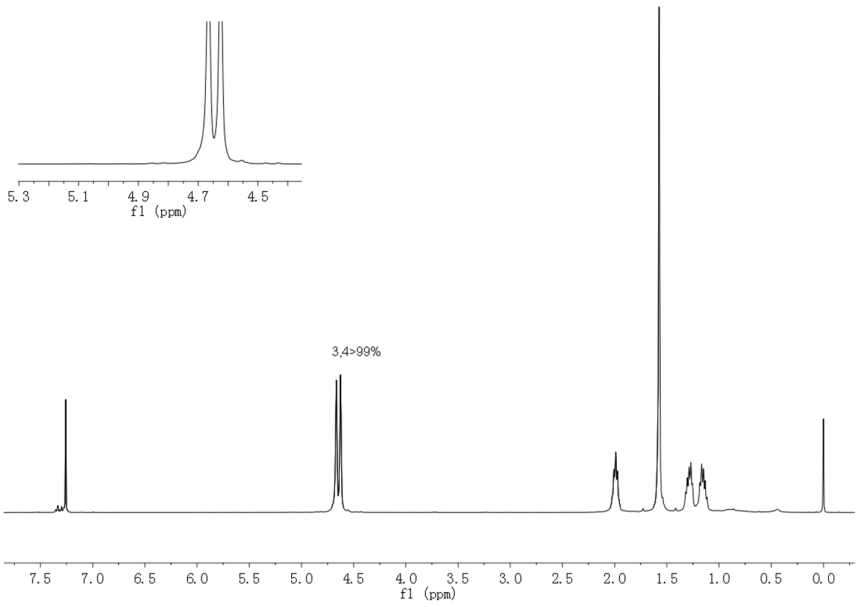
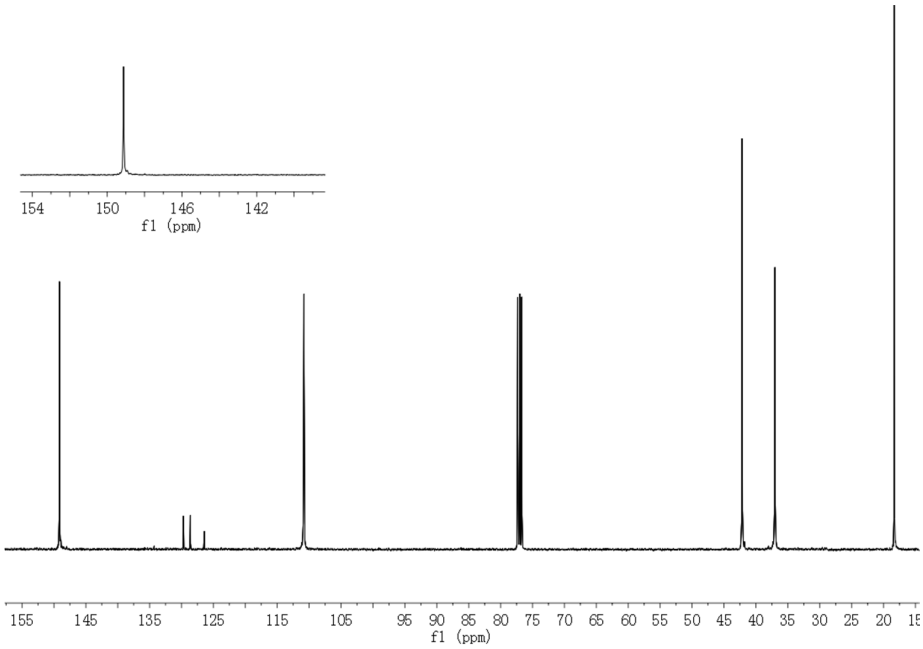


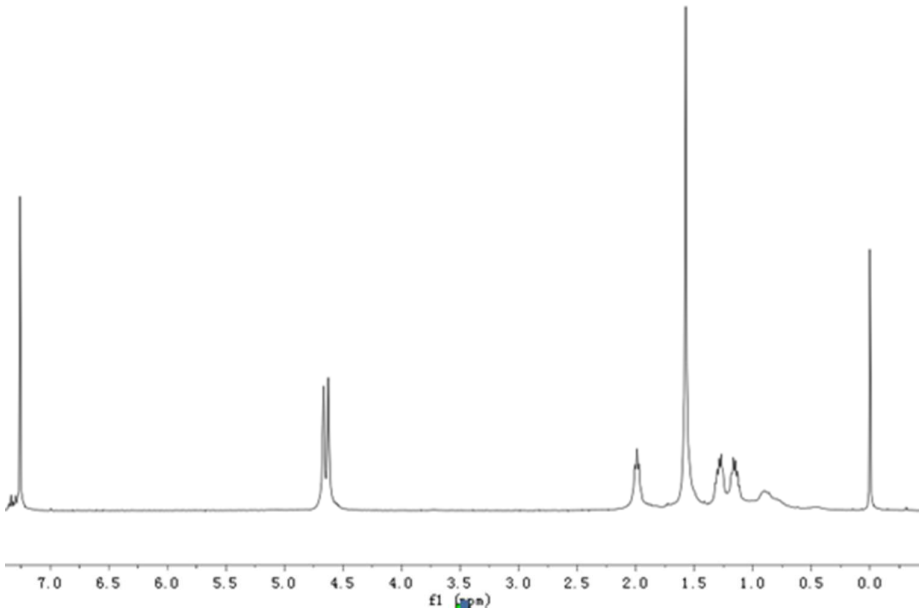
SFigure 1 X-Ray structures of complex **1b**, **1e, 2** and **3** (from left to right) with thermal ellipsoids at 30% probability. Hydrogen atoms are omitted for clarity.



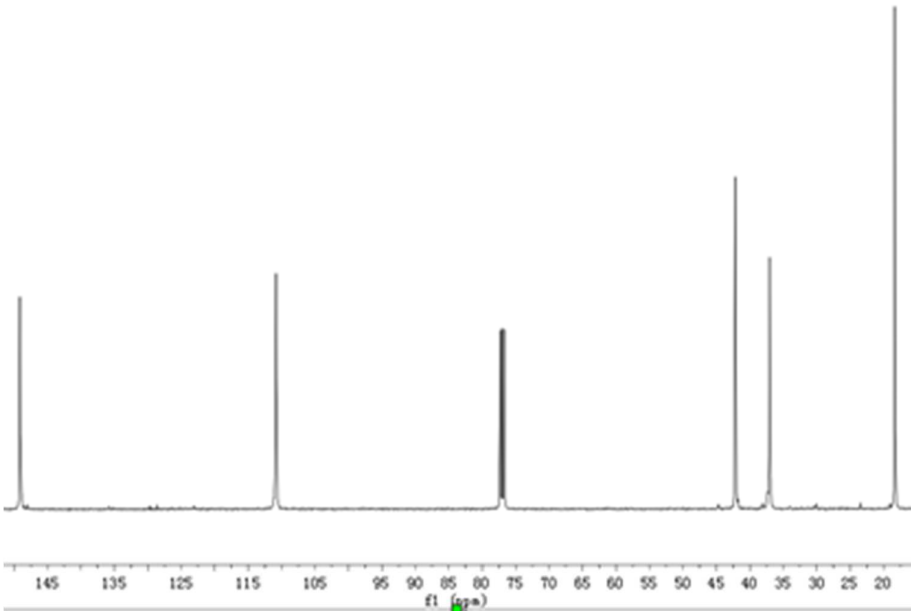
SFigure 2. ^{1}H NMR of polyisoprene samples (Run 12, Table 1)



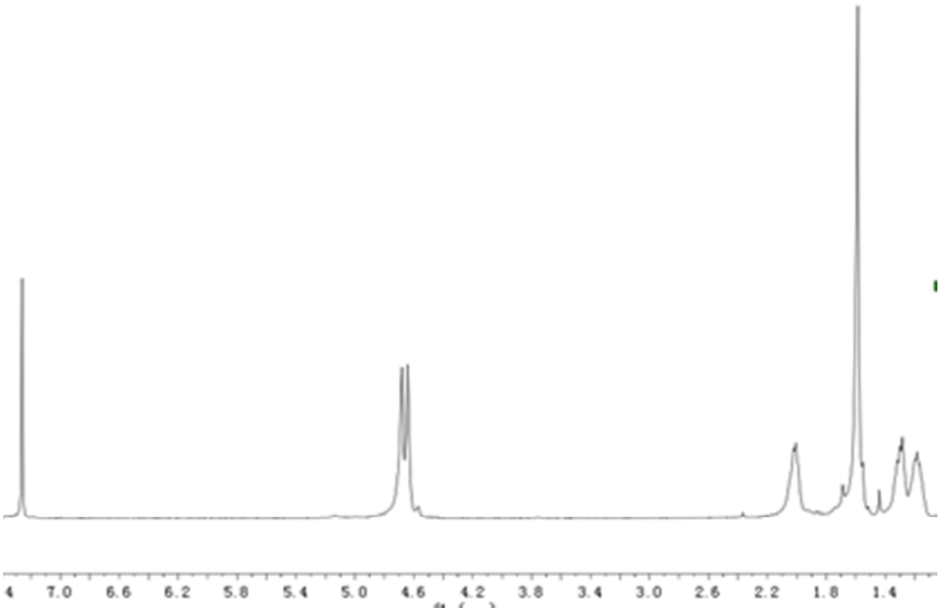
SFigure 3. ^{13}C NMR of polyisoprene samples (Run 12,Table 1)



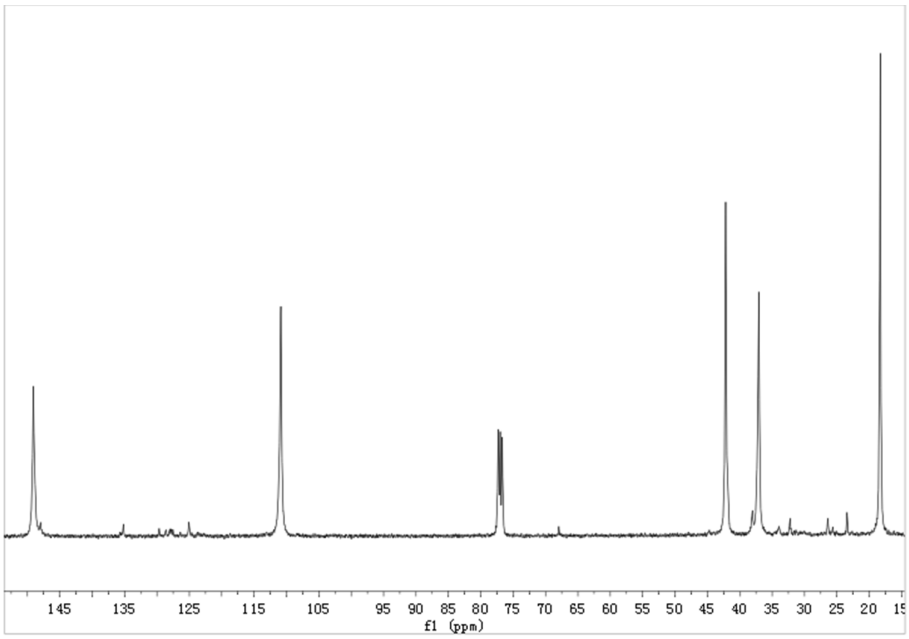
SFigure 4. ^{1}H NMR of polyisoprene samples (Run 13, Table 1)



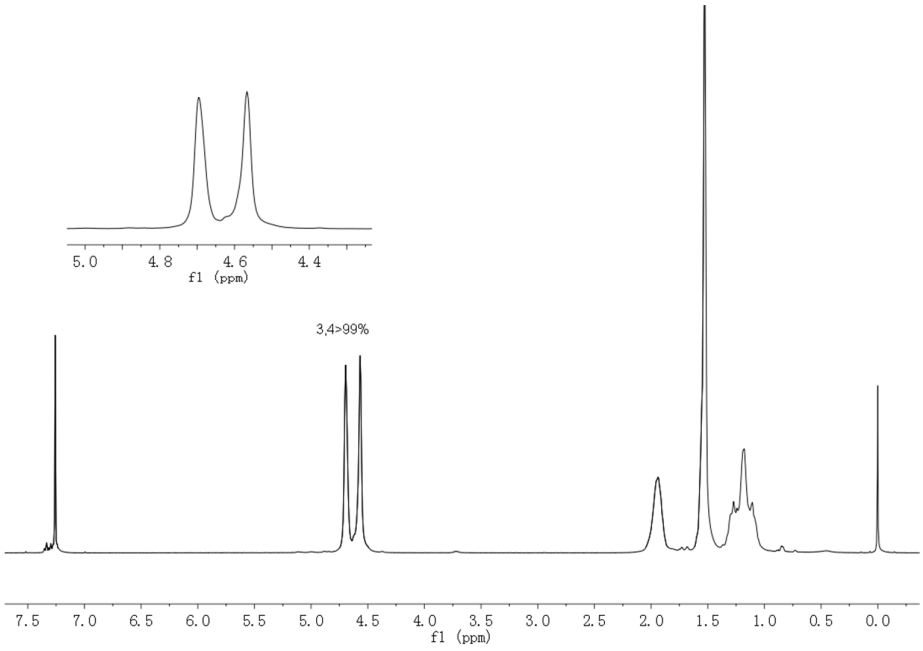
SFigure 5. ^{13}C NMR of polyisoprene samples (Run 13, Table 1)



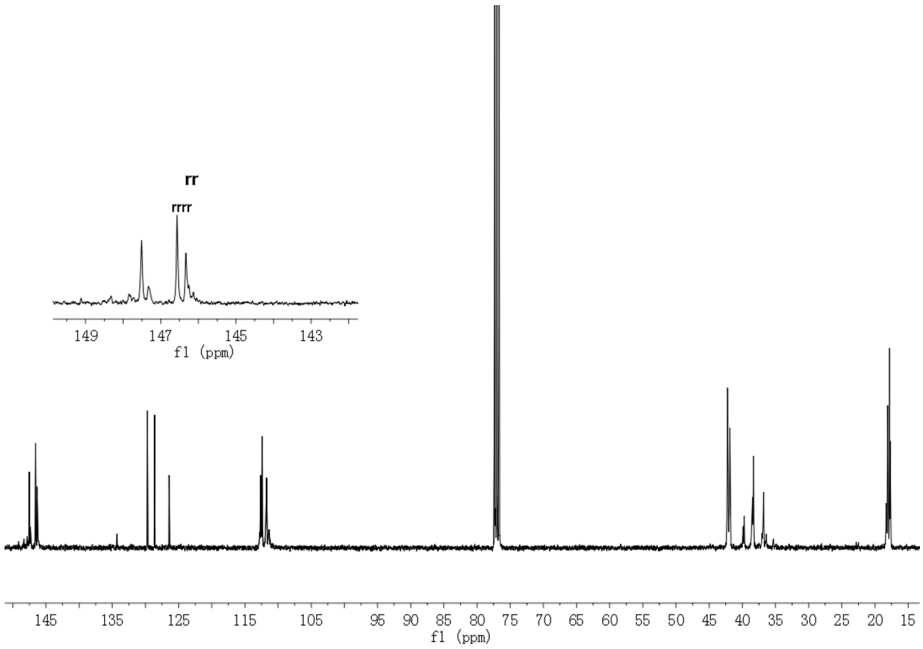
SFigure 6. ^{1}H NMR of polyisoprene samples (Run 14, Table 1)



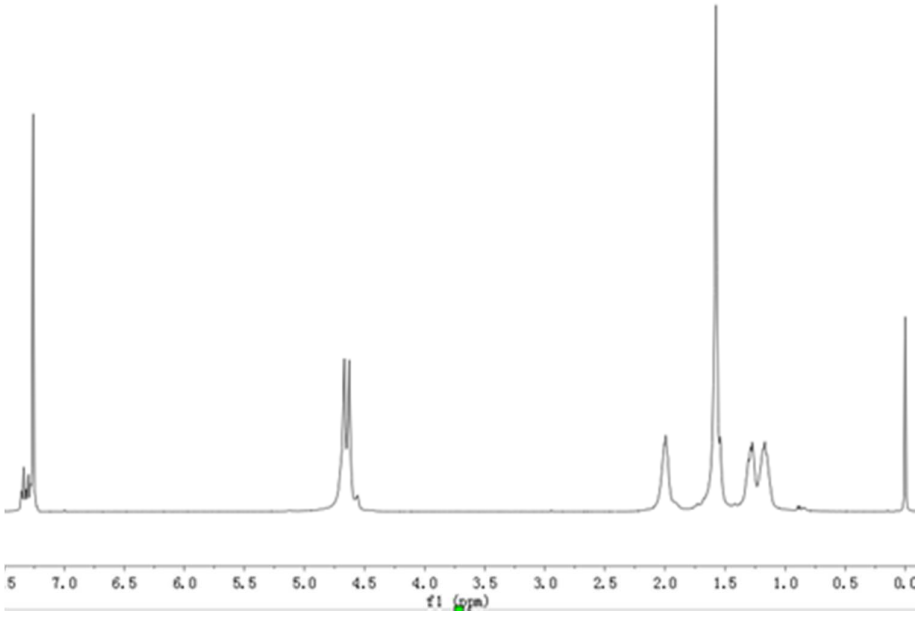
SFigure 7. ^{13}C NMR of polyisoprene samples (Run 14, Table 1)



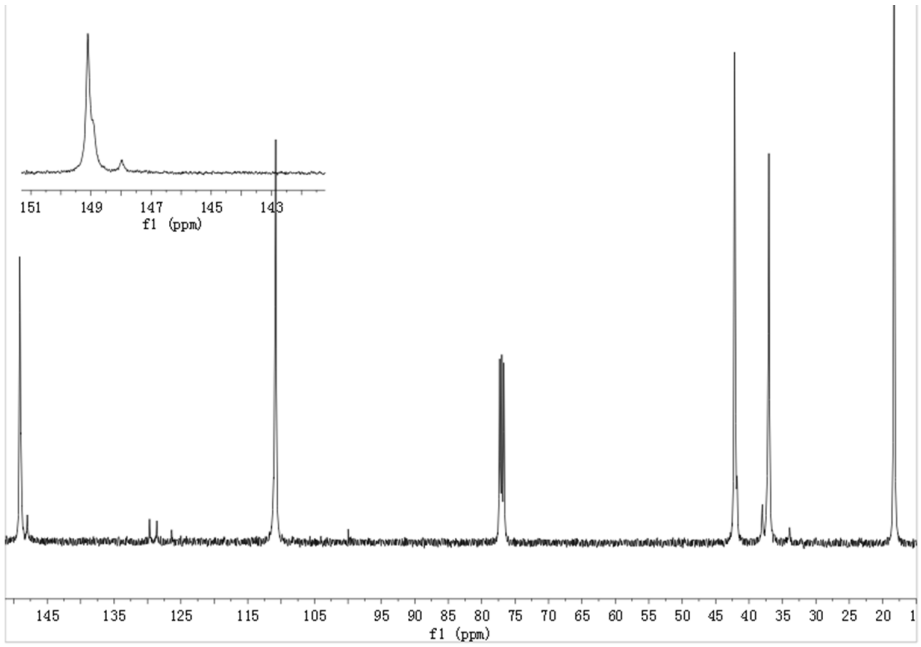
SFigure 8. ^{1}H NMR of polyisoprene samples (Run 18, Table 1)



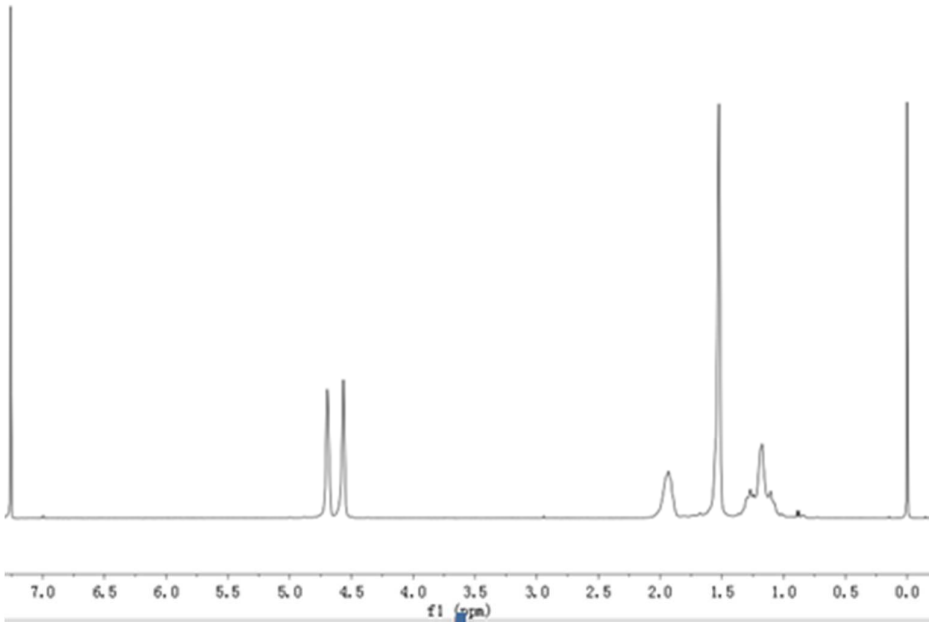
SFigure 9. ^{13}C NMR of polyisoprene samples (Run 18, Table 1)



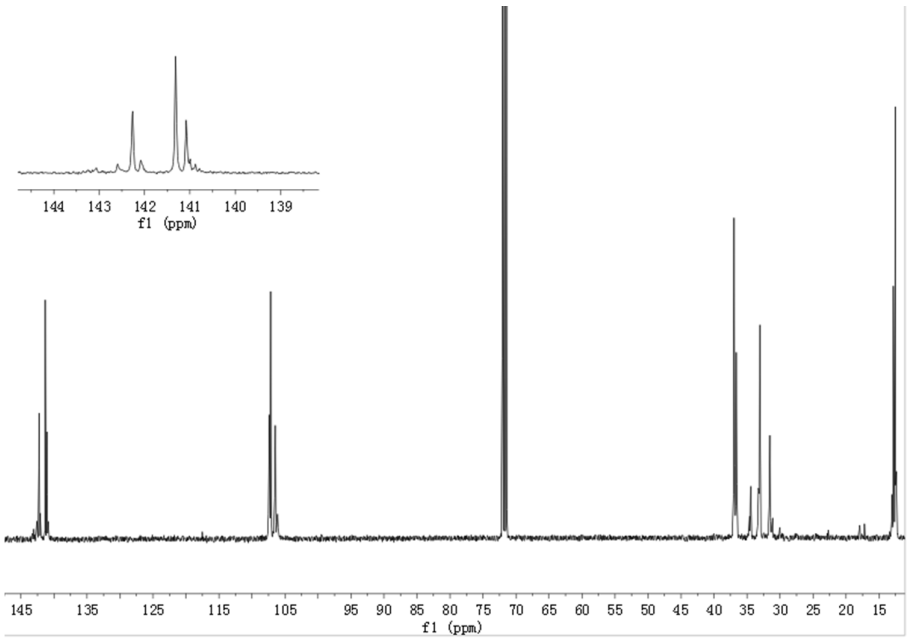
SFigure 10 ^{1}H NMR of polyisoprene samples (Run 19, Table 1)



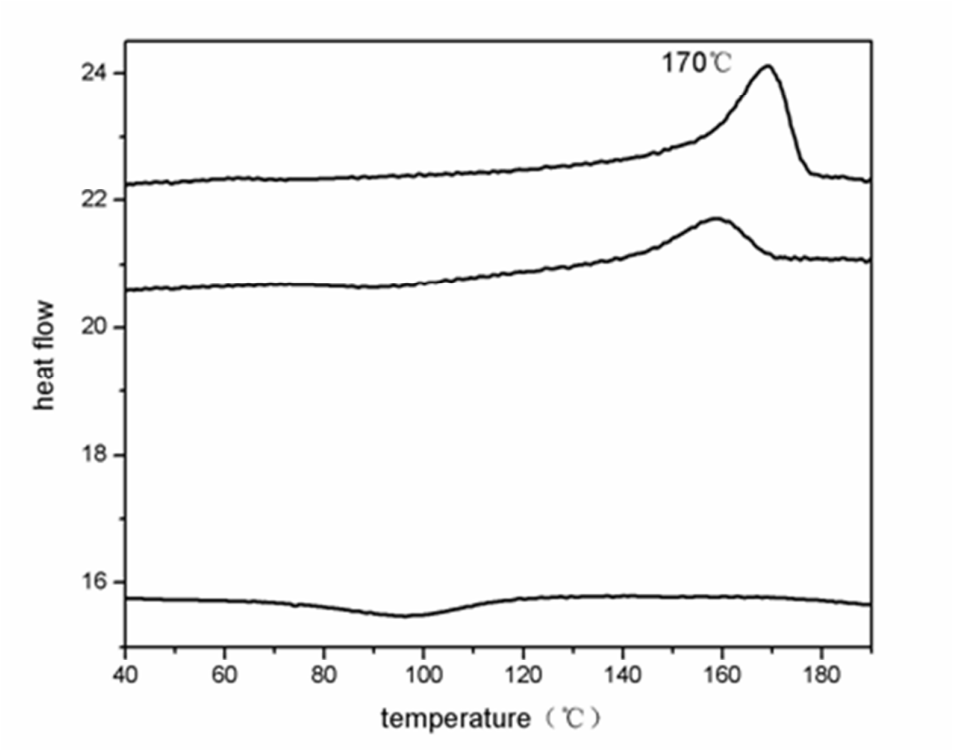
SFigure 11 ^{13}C NMR of polyisoprene samples (Run 19, Table 1)



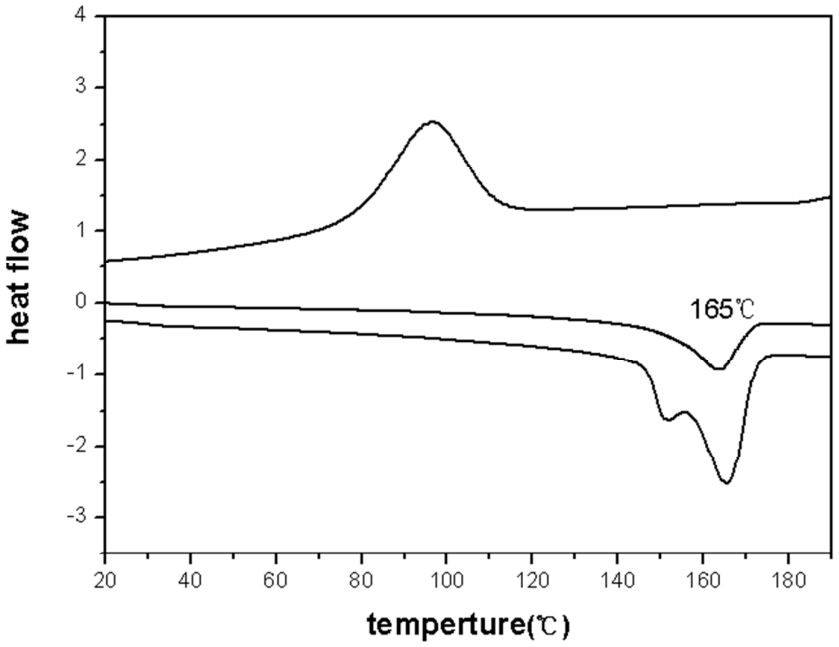
SFigure 12. ^{1}H NMR of polyisoprene samples (Run 20, Table 1)



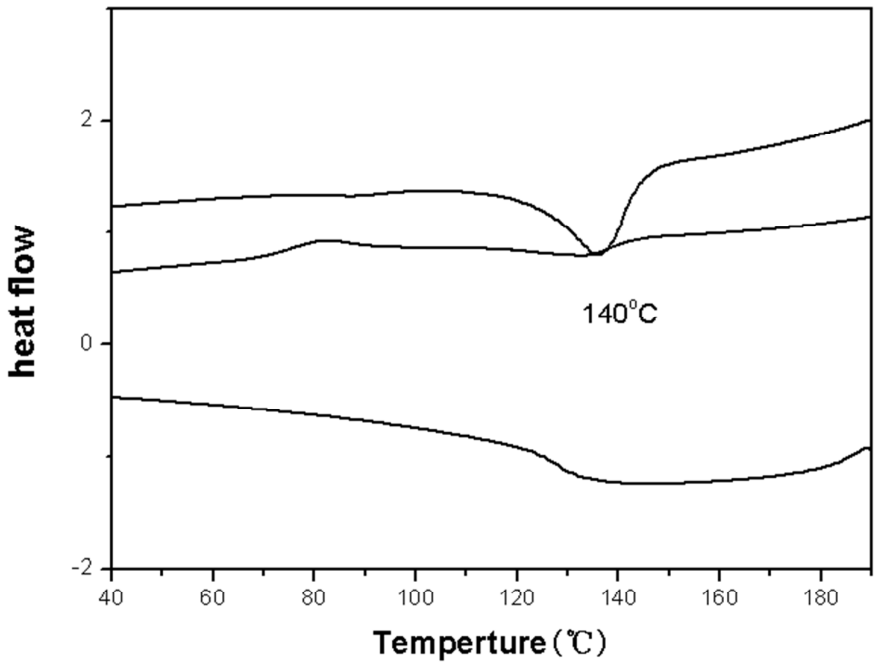
SFigure 13. ^{13}C NMR of polyisoprene samples (Run 20, Table 1)



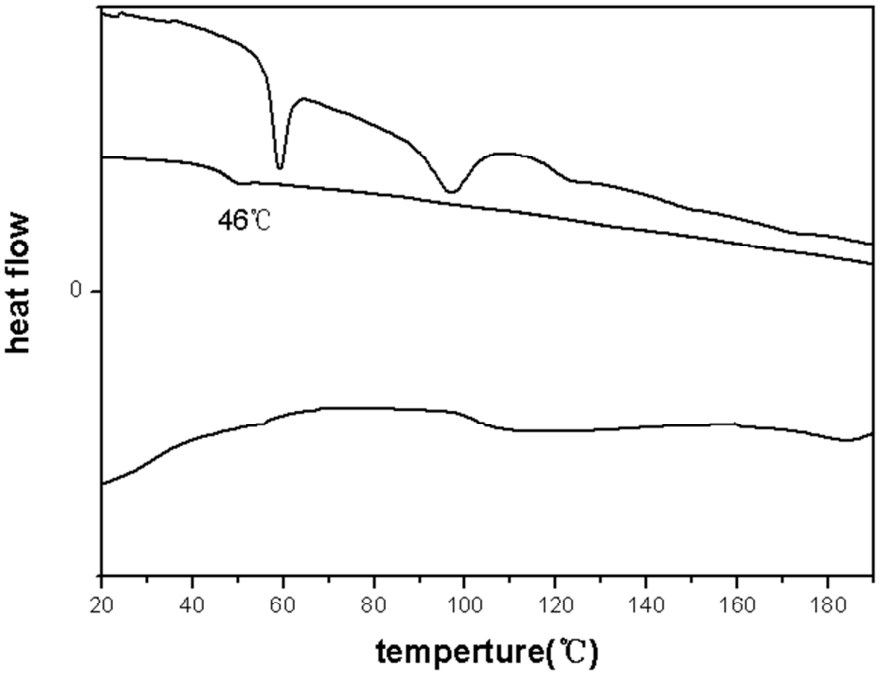
SFigure 14. DSC chart of polyisoprene samples (Run 12，Table 1).



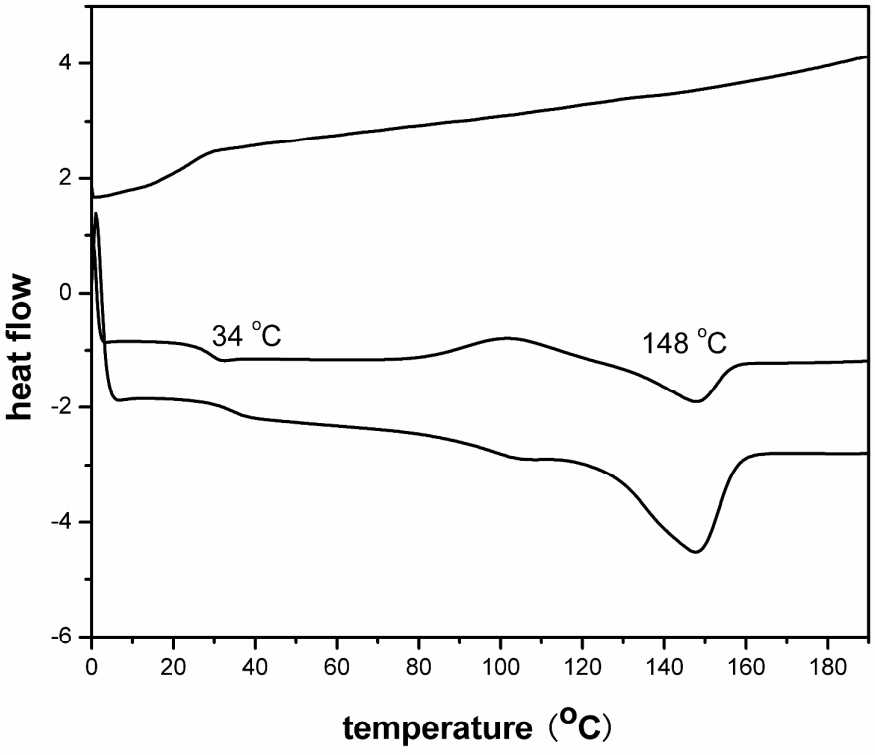
SFigure 15. DSC chart of polyisoprene samples (Run 13，Table 1).



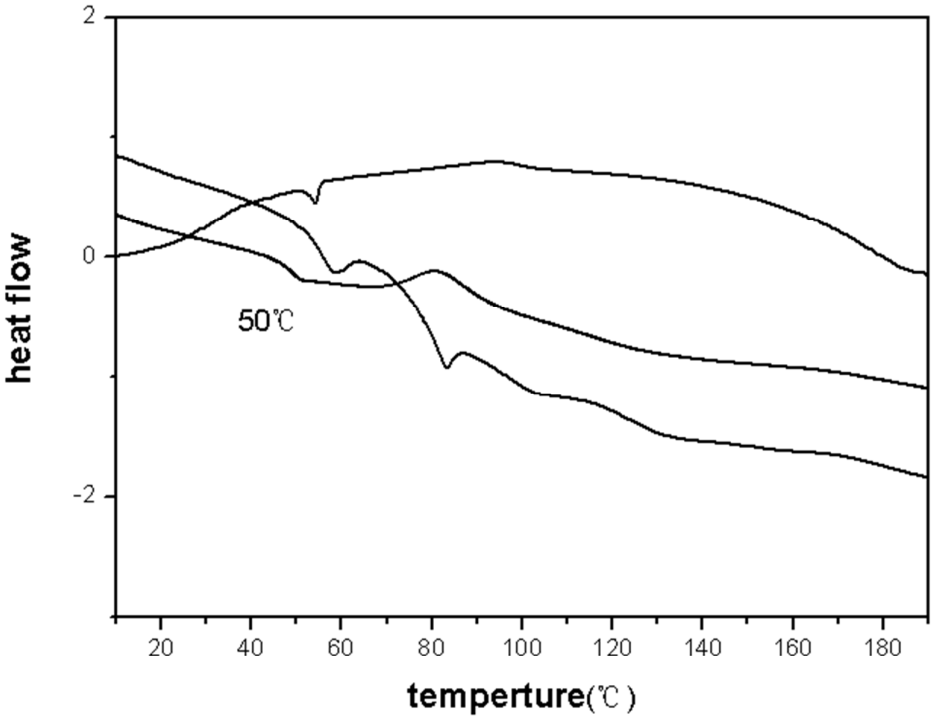
SFigure 16. DSC chart of polyisoprene samples (Run 14，Table 1).



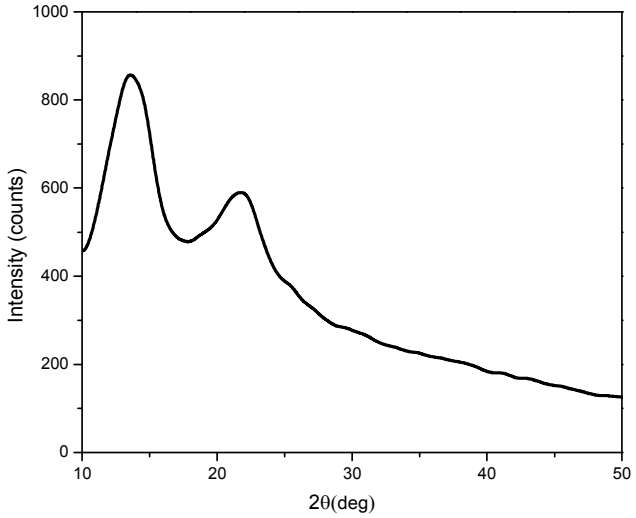
SFigure 17. DSC chart of polyisoprene samples (Run 18, Table 1).



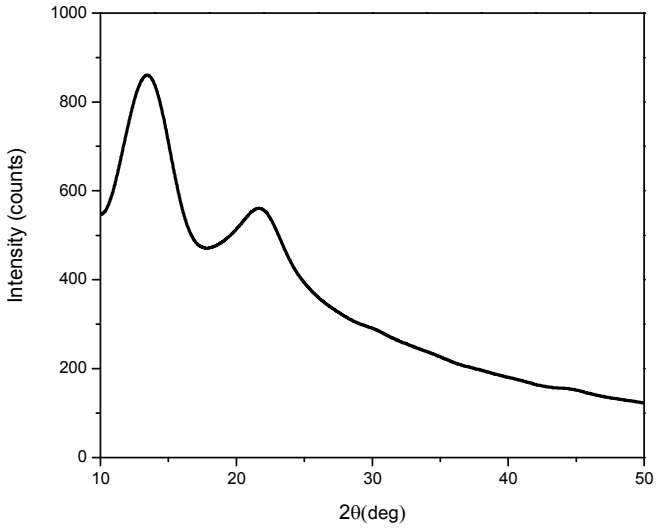
SFigure 18. DSC chart of polyisoprene samples (Run 19, Table 1).



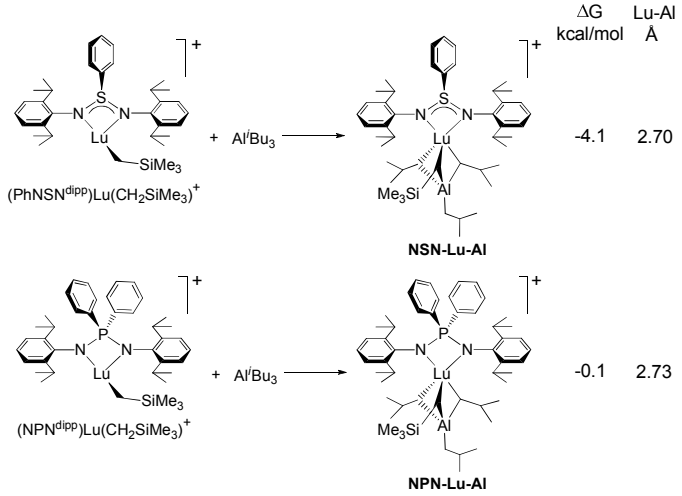
SFigure 19. DSC chart of polyisoprene samples (Run 20, Table 1).



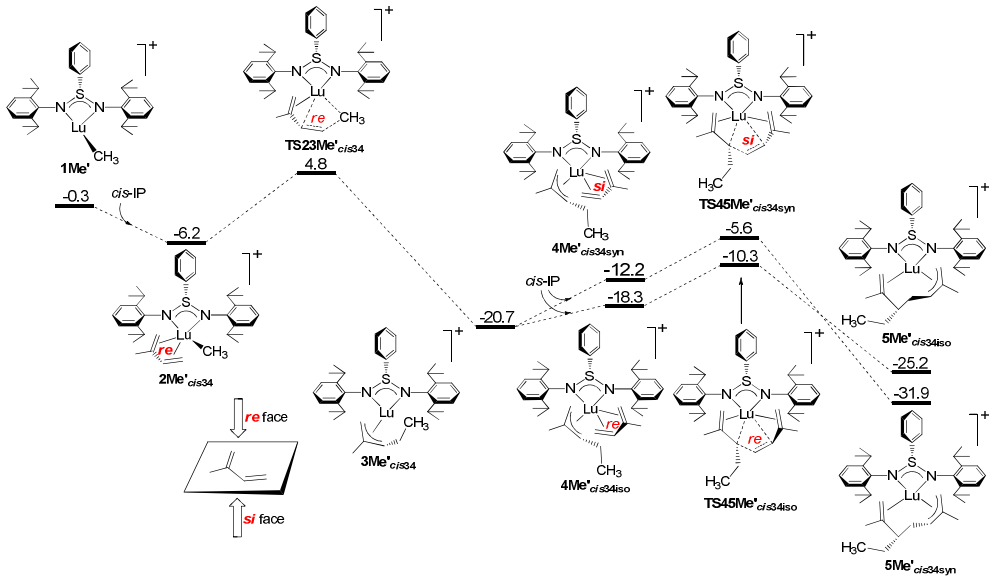
SFigure 20. Wide-angle X-ray diffraction (WAXD) trace of the 3,4-PIP (Run 12,Table 1).



SFigure 21. Wide-angle X-ray diffraction (WAXD) trace of the 3,4-PIP (Run 18,Table 1).



SFigure22. The reactions of Al^{i}Bu$_3$ with (PhNSN^{dipp})Lu(CH$_2$SiMe$_3$)$^+$ and (NPN^{dipp})Lu(CH$_2$SiMe$_3$)$^+$ forming the bimetallic complexes **NSN-Lu-Al** and **NPN-Lu-Al**, respectively.



SFigure 23 Free energy profiles calculated for the 3,4-insertion and 4,3-insertion of the first isoprene as well as 3,4-insertion insertion of the second isoprene catalyzed by **1Me′** , the isomer of **1Me**. The energy reference point is **1Me** + 2 *tans*-IP.

STable1. Crystal data and structure refinement for **1a**.

Identification code	2
Empirical formula	C_{42} H_{69} Lu N_2 O S Si_2
Formula weight	881.21
Temperature	195(2) K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.587 Å α = 90° b = 17.918 Å β =118.69° c = 21.641Å γ = 90°
Volume	4621.8Å^3
Z, Calculated density	4, 1.266 Mg/m^3
Absorption coefficient	2.263mm^{-1}
F(000)	1832
Crystal size	0.11 x 0.09 x 0.06 mm
Theta range for data collection	1.71 to 26.05°
Limiting indices	-16<=h<=16, -22<=k<=13, -25<=l<=26
Reflections collected / unique	28699 / 9092 [R(int) = 0.0500]
Completeness to theta = 25.04	99.6%
Absorption correction	None
Max. and min. transmission	0.8762 and 0.7889
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9092/ 6 / 438
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1182
R indices (all data)	R1 = 0.0736, wR2 = 0.061290
Largest diff. peak and hole	4.755 and -1.031e. Å $^{-3}$

STable 2. Crystal data and structure refinement for **1b**.

Identification code	2
Empirical formula	C46 H77 N2 O2 S Si2 Y
Formula weight	867.25
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Rhombohedral, R3m
Unit cell dimensions	a = 36.820 Å α = 90° b = 36.820 Å β =118.69° c = 11.156Å γ = 90°
Volume	13098.0Å^3
Z, Calculated density	9, 0.990 Mg/m^3
Absorption coefficient	1.109mm^{-1}
F(000)	4194
Crystal size	0.14 x 0.12 x 0.09 mm
Theta range for data collection	1.92 to 25.04°
Limiting indices	-43<=h<=43, -43<=k<=41, -13<=l<=10
Reflections collected / unique	24769 / 4754 [R(int) = 0.1087]
Completeness to theta = 25.04	99.9%
Absorption correction	None
Max. and min. transmission	0.9068 and 0.8603
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4754 / 1 / 273
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0697, wR2 = 0.1994
R indices (all data)	R1 = 0.1033, wR2 = 0.2100
Largest diff. peak and hole	1.254 and -0.496e. Å $^{-3}$

STable 3. Crystal data and structure refinement for **1e**.

Identification code	2
Empirical formula	$C_{40}\ H_{75}\ Lu\ N_2\ O\ S\ Si_3$
Formula weight	891.32
Temperature	195(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.007(2)Å $\alpha = 90°$ b = 20.514(4) Å $\beta = 90.26(3)°$ c = 19.104(4)Å $\gamma = 90°$
Volume	4705.5(16)Å^3
Z, Calculated density	4, 1.258 Mg/m^3
Absorption coefficient	2.248mm^{-1}
F(000)	1864
Crystal size	0.13 x 0.12 x 0.07 mm
Theta range for data collection	1.46 to 26.05°
Limiting indices	-14<=h<=14, -25<=k<=25, -21<=l<=23
Reflections collected / unique	29929 / 9274 [R(int) = 0.0525]
Completeness to theta = 25.04	99.7%
Absorption correction	None
Max. and min. transmission	0.8585 and 0.7588
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9274 / 0 / 450
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.0816
R indices (all data)	R1 = 0.0571, wR2 = 0.0875
Largest diff. peak and hole	0.983 and -0.432e. Å $^{-3}$

STable 4. Crystal data and structure refinement for **2**.

Identification code	3
Empirical formula	$C_{48}\ H_{74}\ Lu\ N_2\ O\ P\ Si_2$
Formula weight	957.21
Temperature	197(2) K
Wavelength	0.71073Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.884 Å α = 78.5° b = 12.506 Å β =81.9° c = 19.448Å γ = 62.2°
Volume	2503.61Å^3
Z, Calculated density	2, 1.270 Mg/m^3
Absorption coefficient	2.085mm^{-1}
F(000)	996
Crystal size	0.14 x 0.13 x 0.08 mm
Theta range for data collection	1.86 to 26.05°
Limiting indices	-14<=h<=13, -15<=k<=7, -24<=l<=22
Reflections collected / unique	13735 / 9653 [R(int) = 0.0152]
Completeness to theta = 25.04	97.5%
Absorption correction	None
Max. and min. transmission	0.8509 and 0.7590
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9653 / 0 / 510
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0274, wR2 = 0.0646
R indices (all data)	R1 = 0.0303, wR2 = 0.0662
Largest diff. peak and hole	0.852 and -0.425e. Å^{-3}

STable 5. Crystal data and structure refinement for **3**.

Identification code	1
Empirical formula	$C_{44}H_{66}LuN_2OPSi_2$
Formula weight	901.11
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 14.316Å α = 90° b = 14.631 Å β = 90° c = 22.305 Å γ = 90°
Volume	4672.0 $Å^3$
Z, Calculated density	4, 1.281Mg/m^3
Absorption coefficient	2.230 mm^{-1}
F(000)	1864
Crystal size	0.11 x 0.07 x 0.06mm
Theta range for data collection	1.66 to 25.05°
Limiting indices	-16<=h<=17, -17<=k<=17, -19<=l<=26
Reflections collected / unique	27901 / 8262 [R(int) = 0.0734]
Completeness to theta = 26.02	100.0%
Absorption correction	None
Max. and min. transmission	0.8778 and 0.7915
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8262 / 6 / 439
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.0982
R indices (all data)	R1 = 0.0711, wR2 = 0.1060
Largest diff. peak and hole	1.230 and -0.497 e. $Å^{-3}$

STable 6. Cartesian coordinates for all of the calculated structures *trans*-IP

C	-2.336862	-0.418989	0.000039
H	-1.909428	-1.417831	0.000050
H	-3.421019	-0.357360	0.000052
C	-1.578920	0.686611	0.000011
H	-2.070904	1.659509	0.000002
C	-0.111616	0.729138	-0.000009
C	0.522378	1.914970	-0.000029
H	-0.026788	2.853433	-0.000027
H	1.606526	1.985277	-0.000047
C	0.652227	-0.573456	-0.000011
H	0.404769	-1.178437	0.881643
H	0.404754	-1.178447	-0.881654
H	1.731989	-0.398636	-0.000020

Transition state between *trans*-IP and *cis*-IP

C	-2.314967	0.632856	-1.156095
H	-1.855047	0.506020	-2.133881
H	-3.401416	0.624937	-1.124008
C	-1.584809	0.802613	-0.052048
H	-2.095277	0.926791	0.905097
C	-0.090603	0.808774	-0.013255
C	0.597718	1.951505	0.081407
H	0.100969	2.917572	0.113485
H	1.684434	1.958195	0.126212
C	0.583024	-0.543450	-0.058197
H	0.245521	-1.179991	0.770870
H	0.324841	-1.076588	-0.982510
H	1.672721	-0.452999	-0.001713

cis-IP

C	-2.424781	1.655561	0.222899
H	-2.090774	2.551099	0.740899
H	-3.495851	1.543262	0.079640
C	-1.561934	0.728395	-0.209638
H	-1.958906	-0.176687	-0.673180
C	-0.089672	0.787045	-0.084005
C	0.592668	1.939033	-0.170263
H	0.095339	2.883604	-0.371061
H	1.673030	1.969003	-0.055179
C	0.605867	-0.539339	0.124756
H	0.264927	-1.025253	1.048455
H	0.380868	-1.233214	-0.696867
H	1.692122	-0.421182	0.180533

1Me

Lu	-0.141089	0.910425	1.364522
C	-0.586925	-0.546785	3.072562
H	-0.990027	-0.042841	3.967498
H	-1.321802	-1.322158	2.812362
H	0.316731	-1.077707	3.411471
S	0.305958	-0.158104	-1.321939
N	-1.072189	0.477233	-0.520289
N	1.329589	0.049989	0.016145
C	-0.007246	-1.925076	-1.475090
C	-0.244908	-2.401293	-2.769077
C	-0.046919	-2.776598	-0.364108
C	-0.529524	-3.758619	-2.951236
H	-0.206471	-1.729850	-3.619664
C	-0.322135	-4.128256	-0.560203
H	0.154559	-2.391631	0.629204
C	-0.565107	-4.617158	-1.851256
H	-0.714948	-4.139832	-3.947676
H	-0.346075	-4.801516	0.287926
H	-0.778293	-5.669298	-1.995777
C	-2.244917	0.677024	-1.327633
C	-3.371050	-0.164654	-1.136403
C	-2.291044	1.748568	-2.260411
C	-4.522856	0.080922	-1.893605
C	-3.460013	1.937068	-3.004721
C	-4.567389	1.111413	-2.827753
H	-5.394352	-0.546214	-1.751658
H	-3.508925	2.747254	-3.722790
H	-5.465728	1.277247	-3.410470
C	-3.389143	-1.275785	-0.086628
H	-2.361726	-1.444154	0.242393
C	-1.131424	2.729040	-2.455143
H	-0.310997	2.428076	-1.797007
C	-4.226468	-0.823569	1.138331
H	-4.232089	-1.603910	1.907581
H	-5.260297	-0.621309	0.839254
H	-3.816794	0.094278	1.578904
C	-3.930205	-2.611347	-0.649630
H	-3.350188	-2.929716	-1.520897
H	-4.981613	-2.521801	-0.941226
H	-3.860709	-3.389423	0.118576
C	-1.556444	4.162645	-2.044854
H	-1.916739	4.184095	-1.009403

H	-2.364805	4.522890	-2.688574
H	-0.709819	4.852131	-2.141028
C	-0.603737	2.710109	-3.910568
H	-1.386945	3.022284	-4.608602
H	-0.272855	1.705250	-4.193145
H	0.242176	3.398589	-4.016212
C	2.685572	0.479337	-0.229847
C	3.693992	-0.437408	-0.604561
C	3.017116	1.846019	0.003093
C	5.000316	0.040592	-0.786871
C	4.333514	2.272394	-0.173943
C	5.321876	1.375810	-0.580943
H	5.776475	-0.653796	-1.084918
H	4.596593	3.308202	-0.003531
H	6.338305	1.720920	-0.726074
C	3.422724	-1.926986	-0.802249
H	2.386626	-2.125974	-0.529111
C	1.957056	2.824481	0.515473
H	1.002347	2.561956	0.022011
C	4.323247	-2.784211	0.123177
H	4.074445	-3.844103	0.000723
H	4.178023	-2.509980	1.173116
H	5.381377	-2.653764	-0.125585
C	3.622185	-2.332562	-2.284690
H	4.659499	-2.165046	-2.593071
H	2.970860	-1.749934	-2.945180
H	3.389758	-3.394732	-2.416776
C	1.848681	2.704457	2.073557
H	2.726218	3.187457	2.515898
H	1.911360	1.667204	2.453579
H	0.970643	3.231623	2.489499
C	2.201131	4.305514	0.142587
H	2.323233	4.408917	-0.939072
H	3.096797	4.691997	0.637471
H	1.350875	4.919563	0.459265

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Lu	0.448854	-0.478241	1.547949
C	0.463156	1.061734	3.259458
H	0.793224	2.063340	2.946792
H	1.145090	0.780567	4.081086
H	-0.524499	1.200595	3.726643
S	-0.122140	0.524891	-1.179424
N	1.305572	0.334890	-0.272694

N	-1.104217	-0.093575	0.067679
C	-1.169953	-2.169786	3.655943
H	-0.508280	-1.875572	4.467006
H	-2.217834	-1.910359	3.770253
C	-0.747157	-2.862448	2.579683
H	-1.487765	-3.189329	1.850006
C	0.655494	-3.262023	2.296296
C	1.715654	-2.581070	2.799511
H	2.735703	-2.889993	2.591301
H	1.602024	-1.789309	3.544996
C	0.831025	-4.447241	1.381598
H	0.441636	-5.346426	1.876324
H	0.260655	-4.326969	0.453513
H	1.879999	-4.618347	1.131570
C	-0.444813	2.292285	-1.330875
C	-0.507700	3.162765	-0.236504
C	-0.607684	2.762364	-2.640532
C	-0.735720	4.519168	-0.461556
H	-0.386592	2.787158	0.771706
C	-0.834903	4.124519	-2.854613
H	-0.557461	2.076108	-3.478539
C	-0.898170	4.998572	-1.768078
H	-0.788955	5.202747	0.376908
H	-0.961996	4.497462	-3.863255
H	-1.074897	6.054164	-1.934947
C	2.556042	0.486364	-0.971485
C	3.014824	-0.522820	-1.861940
C	3.369154	1.616979	-0.695942
C	4.260983	-0.363293	-2.477327
C	4.614083	1.720992	-1.328780
C	5.056483	0.749434	-2.219674
H	4.619212	-1.125771	-3.159000
H	5.242812	2.578016	-1.119572
H	6.019904	0.852959	-2.704644
C	2.229324	-1.805801	-2.140233
H	1.263585	-1.740433	-1.631808
C	2.967157	2.698581	0.306524
H	1.935119	2.510753	0.605489
C	2.985826	-3.030826	-1.565308
H	2.411207	-3.949330	-1.733666
H	3.959788	-3.141361	-2.052229
H	3.160578	-2.910713	-0.489186
C	1.955587	-1.998707	-3.651795
H	1.414784	-1.140359	-4.062561

H	2.893179	-2.111351	-4.204992
H	1.355056	-2.900929	-3.814561
C	3.861328	2.611939	1.570338
H	3.780733	1.624690	2.040677
H	4.911412	2.779507	1.308732
H	3.561153	3.370283	2.302235
C	3.037053	4.114808	-0.313734
H	4.063802	4.371526	-0.593850
H	2.405247	4.181090	-1.204327
H	2.691036	4.856558	0.414990
C	-2.487359	-0.349935	-0.239251
C	-2.856287	-1.377140	-1.153152
C	-3.494769	0.384420	0.443695
C	-4.214445	-1.613141	-1.392347
C	-4.839040	0.092116	0.180968
C	-5.203221	-0.886776	-0.736106
H	-4.501673	-2.384317	-2.097427
H	-5.610644	0.648521	0.699693
H	-6.249317	-1.087532	-0.934281
C	-1.839822	-2.255959	-1.886961
H	-0.834190	-1.987523	-1.553815
C	-3.184902	1.465964	1.479574
H	-2.100895	1.581837	1.534803
C	-2.056960	-3.753750	-1.552453
H	-1.286903	-4.365487	-2.037104
H	-2.015328	-3.923309	-0.469817
H	-3.034211	-4.096042	-1.906416
C	-1.912002	-2.031176	-3.418412
H	-2.900961	-2.306332	-3.798708
H	-1.730569	-0.980262	-3.666031
H	-1.162444	-2.644932	-3.929580
C	-3.693180	1.044738	2.882086
H	-4.780387	0.916667	2.877315
H	-3.240463	0.096353	3.193217
H	-3.439297	1.811056	3.623091
C	-3.801338	2.828537	1.076214
H	-3.431530	3.149075	0.098665
H	-4.893245	2.762502	1.031627
H	-3.538198	3.591688	1.817889

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Lu	3.446612	14.194362	-10.179196
C	1.952345	15.801666	-9.496510
H	2.326708	16.516952	-8.751055

H	1.631478	16.421169	-10.352852
H	1.028530	15.377087	-9.070513
S	5.930919	13.897735	-8.583828
N	5.488686	14.874756	-9.904776
N	4.418535	13.125930	-8.544459
C	2.122513	11.343517	-10.467618
H	1.758941	10.901975	-9.545250
H	3.018979	10.895416	-10.889416
C	1.462028	12.358630	-11.058269
H	0.527123	12.696676	-10.611769
C	1.871168	13.076824	-12.293972
C	3.156678	13.102191	-12.724005
H	3.439362	13.630904	-13.629317
H	3.940522	12.489621	-12.272253
C	0.779220	13.842226	-12.996941
H	0.290626	14.548920	-12.314676
H	0.003543	13.146389	-13.340768
H	1.157460	14.392027	-13.861659
C	6.057385	14.953445	-7.127718
C	5.011241	15.762135	-6.668270
C	7.299255	14.938265	-6.479551
C	5.215566	16.562272	-5.545481
H	4.054132	15.760851	-7.174257
C	7.494249	15.747347	-5.356701
H	8.099807	14.304569	-6.844804
C	6.455011	16.555235	-4.891954
H	4.412882	17.190036	-5.178319
H	8.450589	15.742214	-4.848742
H	6.606376	17.179955	-4.020091
C	6.536772	15.591704	-10.582245
C	7.434634	14.911729	-11.450429
C	6.609664	17.002617	-10.442696
C	8.397322	15.655809	-12.140822
C	7.581230	17.701110	-11.169876
C	8.474582	17.039008	-12.005281
H	9.091030	15.146567	-12.799695
H	7.638983	18.778772	-11.075588
H	9.224872	17.597509	-12.552320
C	7.384055	13.400689	-11.685432
H	6.586119	12.980148	-11.066113
C	5.644225	17.792516	-9.559529
H	5.037485	17.076201	-9.003814
C	7.053189	13.085607	-13.166788
H	6.974196	12.002646	-13.318745

H	7.840744	13.465165	-13.825192
H	6.110929	13.558418	-13.467335
C	8.712478	12.720133	-11.272039
H	8.944792	12.924442	-10.222116
H	9.540428	13.089949	-11.884990
H	8.642440	11.635112	-11.411349
C	4.696930	18.654302	-10.432870
H	4.118402	18.025201	-11.119610
H	5.268926	19.373621	-11.028538
H	3.996762	19.209590	-9.798729
C	6.398852	18.676745	-8.537116
H	6.994740	19.442417	-9.044480
H	7.065266	18.071093	-7.915592
H	5.680473	19.184903	-7.884164
C	4.244232	11.978010	-7.697088
C	4.991308	10.782466	-7.900665
C	3.229493	12.017034	-6.700718
C	4.738945	9.680595	-7.076008
C	3.004487	10.876319	-5.919758
C	3.756407	9.719620	-6.091430
H	5.315679	8.773781	-7.214407
H	2.233657	10.902105	-5.158559
H	3.575789	8.852974	-5.466825
C	6.070098	10.637874	-8.977748
H	6.063074	11.531099	-9.606971
C	2.346388	13.242126	-6.454874
H	2.674625	14.037725	-7.126726
C	5.798341	9.424979	-9.903860
H	6.551417	9.385177	-10.699098
H	4.806471	9.495072	-10.364765
H	5.845540	8.484740	-9.346423
C	7.473030	10.513835	-8.330106
H	7.522812	9.616769	-7.704357
H	7.688280	11.382275	-7.698682
H	8.245922	10.441789	-9.102790
C	0.862662	12.929230	-6.777987
H	0.482810	12.135067	-6.127109
H	0.746946	12.600562	-7.818085
H	0.246229	13.822415	-6.626755
C	2.482308	13.754421	-4.999662
H	3.521655	14.009509	-4.774710
H	2.148107	12.993673	-4.286914
H	1.861917	14.647099	-4.858285

TS23Me$_{cis34}$

Lu	0.376490	-0.634013	1.501845
C	0.416793	0.923371	3.346250
H	1.048784	1.458474	2.607304
H	0.870037	1.134446	4.313284
H	-0.590225	1.356553	3.330470
S	-0.053640	0.463307	-1.218810
N	1.326240	0.312510	-0.239360
N	-1.088506	-0.198094	-0.031613
C	0.233774	-1.160871	4.131347
H	1.298590	-1.218130	4.345550
H	-0.346284	-0.700124	4.921607
C	-0.390324	-2.179693	3.383715
H	-1.461947	-2.311027	3.519444
C	0.264950	-3.074915	2.470316
C	1.530105	-2.839915	1.955149
H	1.988633	-3.536606	1.262774
H	2.238216	-2.179504	2.469737
C	-0.554921	-4.230413	1.940148
H	-0.657717	-4.983990	2.730862
H	-1.567692	-3.919827	1.660450
H	-0.081565	-4.707399	1.078799
C	-0.447318	2.217421	-1.377657
C	-0.566816	3.090784	-0.290597
C	-0.616492	2.673883	-2.691174
C	-0.857878	4.433466	-0.524562
H	-0.437386	2.730286	0.721806
C	-0.907675	4.022226	-2.915767
H	-0.522130	1.986836	-3.524696
C	-1.027303	4.897855	-1.835689
H	-0.953551	5.118453	0.309003
H	-1.039735	4.383188	-3.928100
H	-1.252943	5.942736	-2.010559
C	2.600518	0.483932	-0.891166
C	3.101634	-0.494600	-1.792130
C	3.391424	1.614847	-0.556186
C	4.366708	-0.301683	-2.358896
C	4.657198	1.750383	-1.138108
C	5.141150	0.809662	-2.040904
H	4.755491	-1.038801	-3.051497
H	5.269331	2.607094	-0.883224
H	6.119561	0.937113	-2.488629
C	2.333875	-1.765913	-2.161717
H	1.390363	-1.779422	-1.608676

C	2.938764	2.660030	0.463422
H	1.884719	2.476477	0.681472
C	3.131519	-3.031090	-1.754722
H	2.550548	-3.932540	-1.981475
H	4.075279	-3.086725	-2.305823
H	3.364111	-3.017935	-0.684361
C	2.005955	-1.799542	-3.675355
H	1.418214	-0.923492	-3.967786
H	2.927438	-1.807835	-4.266070
H	1.434407	-2.701833	-3.920260
C	3.748205	2.501120	1.777210
H	3.634109	1.491003	2.190666
H	4.814187	2.665010	1.588826
H	3.413852	3.228090	2.526523
C	3.063728	4.103274	-0.080407
H	4.109466	4.361261	-0.275078
H	2.497346	4.217899	-1.009275
H	2.673975	4.814408	0.656869
C	-2.459546	-0.441163	-0.396284
C	-2.801102	-1.418313	-1.371422
C	-3.484283	0.257614	0.298350
C	-4.153358	-1.642745	-1.653359
C	-4.821008	-0.022917	-0.007389
C	-5.159224	-0.954468	-0.982704
H	-4.421662	-2.378065	-2.402541
H	-5.607252	0.500105	0.523566
H	-6.199747	-1.149095	-1.213509
C	-1.764780	-2.255655	-2.126256
H	-0.767359	-2.000918	-1.760084
C	-3.190577	1.260718	1.414227
H	-2.117700	1.465830	1.403485
C	-1.978434	-3.769365	-1.869345
H	-1.201153	-4.349601	-2.379690
H	-1.938148	-3.993540	-0.798355
H	-2.951376	-4.095841	-2.249438
C	-1.811826	-1.955068	-3.645721
H	-2.791156	-2.219616	-4.057070
H	-1.635040	-0.891832	-3.840149
H	-1.048335	-2.537736	-4.171906
C	-3.555549	0.645002	2.790774
H	-4.623690	0.408554	2.829287
H	-3.000292	-0.285302	2.965380
H	-3.328927	1.347895	3.601445
C	-3.929334	2.604565	1.208699

H	-3.669691	3.044200	0.241478
H	-5.014312	2.468047	1.250501
H	-3.649954	3.308539	2.001261

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Lu	3.373728	13.843145	-10.002964
C	1.071299	14.147659	-10.227637
H	1.441444	15.128813	-9.828125
H	0.089037	14.353752	-10.647557
H	0.934241	13.434970	-9.393280
S	5.897562	13.730928	-8.459060
N	5.406120	14.618537	-9.833136
N	4.364767	13.027408	-8.251395
C	2.930129	12.185544	-11.649175
H	2.624777	11.195991	-11.314825
H	3.849374	12.191571	-12.234539
C	1.905505	13.098356	-12.016741
H	0.881811	12.749114	-12.108155
C	2.232231	14.354360	-12.758838
C	3.503380	14.801258	-12.862248
H	3.725036	15.743937	-13.352121
H	4.377954	14.229013	-12.560232
C	1.081509	15.113185	-13.371930
H	0.298299	15.345129	-12.642668
H	0.615932	14.503443	-14.156844
H	1.416011	16.048189	-13.827831
C	6.184887	14.913002	-7.125947
C	5.188277	15.718973	-6.565130
C	7.515935	15.009095	-6.699793
C	5.531737	16.631724	-5.569091
H	4.159810	15.621044	-6.887434
C	7.851368	15.931143	-5.704770
H	8.277784	14.373547	-7.137501
C	6.861804	16.739213	-5.142219
H	4.767370	17.255067	-5.121349
H	8.877957	16.012349	-5.369991
H	7.121531	17.449679	-4.366927
C	6.417111	15.363947	-10.529228
C	7.384090	14.707059	-11.335914
C	6.373563	16.782937	-10.472950
C	8.291307	15.486714	-12.063342
C	7.289309	17.514955	-11.236604
C	8.246396	16.876729	-12.020997
H	9.037455	14.996512	-12.677558

H	7.259396	18.597247	-11.211312
H	8.953756	17.460942	-12.597588
C	7.477466	13.183635	-11.450363
H	6.672793	12.738195	-10.858980
C	5.320279	17.524348	-9.647939
H	4.914521	16.818071	-8.920555
C	7.293405	12.717125	-12.917055
H	7.323792	11.623073	-12.971477
H	8.091079	13.112493	-13.553683
H	6.335148	13.061070	-13.323152
C	8.826495	12.670316	-10.886298
H	8.950702	12.969562	-9.840231
H	9.663481	13.078736	-11.461876
H	8.870124	11.577086	-10.943567
C	4.165470	18.001140	-10.566399
H	3.701622	17.152421	-11.086623
H	4.546981	18.689818	-11.327906
H	3.396315	18.520859	-9.982947
C	5.909413	18.715949	-8.857186
H	6.272265	19.501049	-9.528037
H	6.736918	18.387027	-8.221629
H	5.133924	19.154948	-8.219265
C	4.252483	11.929059	-7.326151
C	4.937291	10.703221	-7.549988
C	3.368391	12.058775	-6.221499
C	4.777259	9.666435	-6.624004
C	3.230385	10.981987	-5.337635
C	3.940221	9.800619	-5.520796
H	5.305545	8.733309	-6.779593
H	2.557050	11.073796	-4.493857
H	3.829966	8.983435	-4.818087
C	5.807564	10.435290	-8.781671
H	5.813950	11.326460	-9.414203
C	2.509597	13.301926	-5.981816
H	2.785257	14.049735	-6.730938
C	5.211048	9.280100	-9.626926
H	5.812118	9.125712	-10.530285
H	4.181327	9.507275	-9.923711
H	5.204098	8.345987	-9.056594
C	7.270321	10.119961	-8.383453
H	7.315436	9.212067	-7.773444
H	7.705528	10.942575	-7.806390
H	7.880168	9.960559	-9.279480
C	1.007527	12.965387	-6.169570

H	0.688014	12.217564	-5.437057
H	0.816940	12.555469	-7.169064
H	0.394229	13.863630	-6.033485
C	2.755176	13.912992	-4.580600
H	3.809705	14.172344	-4.449395
H	2.471689	13.205606	-3.794796
H	2.149151	14.817783	-4.453648

TS23Me$_{trans34}$

Lu	0.195864	-0.766679	1.441153
C	0.211655	0.861383	3.257504
H	0.940552	1.365215	2.599771
H	0.415101	1.240507	4.256390
H	-0.806191	1.183459	2.992686
S	-0.174002	0.442191	-1.216768
N	1.203236	0.192539	-0.241898
N	-1.254116	-0.189846	-0.053656
C	0.362557	-1.045537	4.169300
H	1.371014	-0.856199	4.525995
H	-0.403380	-0.755078	4.880387
C	0.114687	-2.209614	3.400466
H	-0.924829	-2.533223	3.292466
C	1.083329	-2.842724	2.547342
C	0.679547	-3.379970	1.340300
H	1.382041	-3.863721	0.670077
H	-0.376202	-3.587994	1.151004
C	2.564127	-2.667525	2.834173
H	2.882956	-1.613423	2.828181
H	2.799606	-3.052380	3.832288
H	3.174267	-3.195690	2.098365
C	-0.466531	2.218322	-1.339454
C	-0.532904	3.077276	-0.235997
C	-0.629740	2.704906	-2.642924
C	-0.767152	4.435290	-0.443888
H	-0.404738	2.694670	0.768248
C	-0.862709	4.068571	-2.840935
H	-0.576401	2.029216	-3.489199
C	-0.931639	4.929423	-1.744732
H	-0.821450	5.109336	0.402198
H	-0.989786	4.452729	-3.845330
H	-1.113191	5.986065	-1.899055
C	2.481397	0.365390	-0.887211
C	2.949167	-0.565211	-1.854165
C	3.307318	1.450114	-0.487243

C	4.213935	-0.368499	-2.420845
C	4.570969	1.589783	-1.072265
C	5.020864	0.698911	-2.040777
H	4.576252	-1.069524	-3.163417
H	5.208726	2.410647	-0.767655
H	5.997912	0.830024	-2.490365
C	2.153128	-1.797333	-2.289377
H	1.207362	-1.817065	-1.741685
C	2.898482	2.432231	0.610074
H	1.836588	2.279939	0.812205
C	2.923741	-3.095985	-1.937846
H	2.324986	-3.974953	-2.203384
H	3.867440	-3.146541	-2.489577
H	3.154715	-3.133636	-0.867425
C	1.834063	-1.752905	-3.804440
H	1.264174	-0.853142	-4.058172
H	2.758017	-1.750799	-4.391212
H	1.246820	-2.630985	-4.094239
C	3.695697	2.132127	1.906819
H	3.535710	1.097489	2.236980
H	4.768309	2.262675	1.730524
H	3.392620	2.810529	2.712908
C	3.090416	3.908158	0.187066
H	4.146054	4.132506	0.005229
H	2.524895	4.127969	-0.723131
H	2.739953	4.572045	0.985721
C	-2.617366	-0.405672	-0.466462
C	-2.950035	-1.419855	-1.404812
C	-3.643761	0.361092	0.148591
C	-4.296438	-1.613358	-1.735127
C	-4.975085	0.111878	-0.202685
C	-5.303611	-0.855784	-1.146379
H	-4.559536	-2.379151	-2.455133
H	-5.764490	0.685557	0.267152
H	-6.339660	-1.026368	-1.413587
C	-1.913680	-2.345172	-2.047047
H	-0.918793	-2.062479	-1.694115
C	-3.352243	1.390838	1.239638
H	-2.280661	1.598161	1.221305
C	-2.158832	-3.814805	-1.618257
H	-1.388479	-4.467264	-2.044740
H	-2.138974	-3.912914	-0.526729
H	-3.135441	-4.162280	-1.969614
C	-1.927130	-2.221501	-3.590700

H	-2.900062	-2.520419	-3.993359
H	-1.729210	-1.190488	-3.901905
H	-1.161971	-2.871307	-4.028433
C	-3.714395	0.795369	2.626389
H	-4.781786	0.555454	2.667538
H	-3.158779	-0.133010	2.815351
H	-3.489252	1.509694	3.427283
C	-4.093882	2.729392	1.014876
H	-3.849212	3.147225	0.034014
H	-5.178487	2.598100	1.078451
H	-3.799953	3.450554	1.786201

3Me$_{cis34}$

Lu	0.102107	-0.609146	1.422689
C	1.956270	-0.191171	3.496011
H	2.335136	-0.324057	2.466410
H	2.831641	0.172088	4.042987
H	1.232833	0.645295	3.524408
S	-0.048281	0.532981	-1.308679
N	1.204068	0.448430	-0.165907
N	-1.181735	-0.129689	-0.224343
C	1.391819	-1.482726	4.135576
H	2.122577	-2.286482	3.976795
H	1.352333	-1.312831	5.216139
C	-0.000120	-1.940770	3.694179
H	-0.783643	-1.828600	4.440854
C	-0.245527	-2.812583	2.642011
C	0.649683	-2.917688	1.519304
H	0.420958	-3.663402	0.761168
H	1.723417	-2.858973	1.735724
C	-1.610737	-3.461161	2.521203
H	-1.508660	-4.533311	2.731741
H	-2.333174	-3.048150	3.231368
H	-2.022448	-3.378782	1.507896
C	-0.521459	2.257045	-1.556638
C	-0.628875	3.193299	-0.521655
C	-0.823145	2.606648	-2.878973
C	-1.051036	4.488407	-0.815706
H	-0.365095	2.921005	0.492691
C	-1.247097	3.907657	-3.163774
H	-0.729052	1.874083	-3.673003
C	-1.362272	4.843390	-2.134822
H	-1.131838	5.223339	-0.024091
H	-1.483263	4.185781	-4.183292

H	-1.688844	5.851994	-2.356908
C	2.550259	0.577167	-0.671089
C	3.130698	-0.443392	-1.475217
C	3.322912	1.705546	-0.286664
C	4.452261	-0.287171	-1.907897
C	4.646669	1.801230	-0.732598
C	5.208299	0.823321	-1.545660
H	4.898243	-1.053067	-2.531147
H	5.241175	2.659724	-0.443546
H	6.230762	0.921702	-1.890318
C	2.386961	-1.716109	-1.889279
H	1.405893	-1.723743	-1.406176
C	2.777382	2.826120	0.599474
H	1.746560	2.573735	0.858347
C	3.140246	-2.983895	-1.412012
H	2.568560	-3.880481	-1.677018
H	4.123933	-3.054913	-1.886371
H	3.283552	-2.967745	-0.326548
C	2.173579	-1.759816	-3.423337
H	1.608662	-0.886687	-3.765522
H	3.137498	-1.769827	-3.942319
H	1.623218	-2.665158	-3.703776
C	3.591791	2.950377	1.912471
H	3.596236	2.004826	2.465438
H	4.630705	3.220791	1.698940
H	3.162713	3.730543	2.551839
C	2.772871	4.178702	-0.156454
H	3.793638	4.470234	-0.424067
H	2.179868	4.112038	-1.072731
H	2.349299	4.965498	0.478650
C	-2.523523	-0.400635	-0.648724
C	-2.819421	-1.401372	-1.607581
C	-3.571930	0.290913	0.018898
C	-4.163396	-1.662854	-1.905540
C	-4.895737	-0.024987	-0.296375
C	-5.192950	-0.987459	-1.260052
H	-4.403294	-2.417333	-2.645328
H	-5.704929	0.490517	0.203667
H	-6.225129	-1.211385	-1.501658
C	-1.739537	-2.218624	-2.319311
H	-0.763991	-1.932734	-1.919640
C	-3.251694	1.333658	1.093061
H	-2.351172	1.862924	0.773451
C	-1.920470	-3.734125	-2.050266

H	-1.113633	-4.298920	-2.530776
H	-1.901416	-3.943354	-0.975030
H	-2.873487	-4.092475	-2.451910
C	-1.740878	-1.931452	-3.841938
H	-2.694913	-2.231253	-4.287651
H	-1.592144	-0.863975	-4.038991
H	-0.938650	-2.491814	-4.334156
C	-2.967533	0.642617	2.451928
H	-3.845685	0.080965	2.787610
H	-2.149497	-0.098879	2.380582
H	-2.698508	1.374052	3.223511
C	-4.365356	2.388582	1.287585
H	-4.619528	2.861212	0.334159
H	-5.271399	1.944024	1.712365
H	-4.020256	3.164992	1.979281

3Me*cis43*

Lu	3.624631	14.204811	-10.116380
C	1.196952	11.804165	-11.162144
H	1.521783	11.849553	-10.110946
H	0.106160	11.729780	-11.167070
H	1.596911	10.874047	-11.575232
S	6.108468	13.846987	-8.550220
N	5.673146	14.852164	-9.844835
N	4.542326	13.185783	-8.441923
C	3.283430	12.976432	-12.017956
H	3.627567	11.943873	-12.129678
H	3.662197	13.519341	-12.897686
C	1.725928	12.994923	-11.989308
H	1.326875	12.871219	-13.012446
C	1.127761	14.339713	-11.533934
C	1.817985	15.505630	-11.637531
H	1.361948	16.460394	-11.389250
H	2.763508	15.562414	-12.182622
C	-0.290524	14.360627	-11.019141
H	-0.412294	13.758222	-10.112380
H	-0.960147	13.926034	-11.772182
H	-0.629538	15.378599	-10.810761
C	6.365870	14.865691	-7.081535
C	5.634154	16.023323	-6.794375
C	7.350021	14.397382	-6.201832
C	5.889594	16.713839	-5.610557
H	4.897665	16.392966	-7.496325
C	7.595254	15.093675	-5.015332

H	7.916587	13.503957	-6.440474
C	6.866522	16.247256	-4.721481
H	5.336730	17.616935	-5.382148
H	8.353784	14.737801	-4.329356
H	7.061401	16.789538	-3.804298
C	6.726008	15.477088	-10.600502
C	7.686691	14.708791	-11.313006
C	6.737707	16.895305	-10.688294
C	8.682512	15.382447	-12.029138
C	7.743941	17.516386	-11.436986
C	8.722585	16.772153	-12.087059
H	9.428370	14.807414	-12.564512
H	7.761497	18.597467	-11.508791
H	9.502089	17.271044	-12.650328
C	7.662525	13.178716	-11.381334
H	6.815562	12.808732	-10.798668
C	5.658723	17.772771	-10.050713
H	5.011053	17.123300	-9.454109
C	7.447598	12.704072	-12.841747
H	7.388281	11.610295	-12.874654
H	8.278888	13.021449	-13.479145
H	6.520245	13.117594	-13.251820
C	8.955695	12.563386	-10.792047
H	9.102236	12.877982	-9.753382
H	9.830204	12.876421	-11.371593
H	8.900146	11.469505	-10.821823
C	4.788882	18.438576	-11.148474
H	4.337435	17.684053	-11.805031
H	5.399942	19.097963	-11.772876
H	3.990452	19.037499	-10.694873
C	6.259896	18.842680	-9.107870
H	6.906092	19.529826	-9.662743
H	6.852271	18.373068	-8.316930
H	5.458670	19.432173	-8.646854
C	4.288732	12.152497	-7.483800
C	4.840776	10.855247	-7.622739
C	3.377362	12.440984	-6.431095
C	4.493203	9.878581	-6.680261
C	3.045734	11.426621	-5.529750
C	3.607421	10.155373	-5.644718
H	4.914427	8.884216	-6.769127
H	2.353555	11.628512	-4.722753
H	3.349125	9.383001	-4.930063
C	5.781838	10.473753	-8.766262

H	5.890210	11.334861	-9.430104
C	2.739706	13.828229	-6.322890
H	3.492062	14.559876	-6.629241
C	5.190996	9.314807	-9.608695
H	5.860750	9.080013	-10.443516
H	4.210446	9.588702	-10.012443
H	5.073348	8.411785	-9.001219
C	7.185260	10.097108	-8.228328
H	7.124134	9.221040	-7.574496
H	7.619157	10.923369	-7.654342
H	7.858606	9.860488	-9.059502
C	1.526773	13.931785	-7.284424
H	0.768889	13.185359	-7.024108
H	1.822106	13.719016	-8.328601
H	1.073005	14.929405	-7.250272
C	2.285401	14.197013	-4.892253
H	3.111537	14.081641	-4.184372
H	1.449000	13.572225	-4.561740
H	1.951210	15.240221	-4.868901

4Me*cis*34iso

Lu	-0.424838	-1.181078	-0.784821
C	-2.708705	-2.851716	-1.041101
H	-3.178483	-3.343411	-1.889738
S	0.566979	0.993325	1.004944
N	1.358930	-0.279049	0.216442
N	-0.921406	0.700373	0.243259
C	-1.850507	-1.578316	-3.418879
H	-2.881387	-1.243305	-3.399990
H	-1.683352	-2.626389	-3.639314
C	-0.826694	-0.685209	-3.382697
H	-1.058394	0.378284	-3.384232
C	0.600085	-1.057927	-3.486062
C	1.060993	-2.247432	-3.031077
H	2.111013	-2.510984	-3.096268
H	0.394639	-3.034810	-2.676008
C	1.496251	-0.027743	-4.123875
H	1.448843	0.930797	-3.594081
H	2.535336	-0.354458	-4.155728
H	1.157551	0.159022	-5.150746
C	-3.550393	-1.780734	-0.376342
H	-4.046724	-1.171918	-1.141625
H	-2.951294	-1.071827	0.218287
C	-4.627630	-2.376265	0.554964

H	-5.298794	-3.034383	-0.006841
H	-5.228258	-1.580897	1.008438
H	-4.172722	-2.967203	1.356299
C	-1.646619	-3.512717	-0.439652
C	-0.941667	-2.979085	0.689384
H	-1.522330	-2.459257	1.454195
H	-0.151665	-3.594784	1.111054
C	-1.106401	-4.776109	-1.084472
H	-0.011984	-4.830412	-1.042323
H	-1.428505	-4.892344	-2.124819
H	-1.479520	-5.644861	-0.527643
C	1.208637	2.559991	0.368274
C	1.185147	2.921746	-0.981849
C	1.760169	3.413318	1.331947
C	1.713719	4.152104	-1.369012
H	0.746345	2.256648	-1.714276
C	2.293833	4.642965	0.935059
H	1.770694	3.122548	2.376566
C	2.268206	5.010932	-0.411233
H	1.694131	4.445654	-2.411639
H	2.721701	5.308448	1.674533
H	2.677395	5.965898	-0.717701
C	2.649706	-0.626207	0.785049
C	2.750826	-1.310482	2.032132
C	3.837753	-0.306764	0.071134
C	4.017650	-1.642259	2.526629
C	5.078534	-0.671607	0.609483
C	5.177089	-1.329971	1.827920
H	4.094296	-2.156303	3.477041
H	5.982560	-0.423880	0.066646
H	6.147276	-1.596237	2.230255
C	-2.062627	1.455340	0.705541
C	-2.561070	1.326640	2.034376
C	-2.755024	2.283680	-0.222100
C	-3.709101	2.040482	2.398797
C	-3.908198	2.960223	0.192866
C	-4.384232	2.850573	1.493311
H	-4.083203	1.953064	3.411809
H	-4.436198	3.587471	-0.515445
H	-5.273461	3.389001	1.798514
C	1.549010	-1.695509	2.895891
H	0.635973	-1.488093	2.333793
C	3.849081	0.437334	-1.264075
H	2.812658	0.598829	-1.569233

C	-2.323459	2.457625	-1.678742
H	-1.392881	1.902801	-1.815965
C	-1.906996	0.462270	3.117314
H	-1.075530	-0.093530	2.680114
C	4.572559	-0.396206	-2.352490
H	4.095308	-1.373496	-2.484314
H	4.566371	0.139173	-3.309135
H	5.617551	-0.568290	-2.077793
C	4.541178	1.816490	-1.116266
H	4.051963	2.420044	-0.348106
H	5.592452	1.686635	-0.838494
H	4.503424	2.362620	-2.065893
C	1.561460	-3.207165	3.242285
H	1.670625	-3.818779	2.341093
H	2.392293	-3.444670	3.914107
H	0.629885	-3.483882	3.748633
C	1.532017	-0.862785	4.202736
H	2.436789	-1.059659	4.786777
H	1.489125	0.208648	3.985925
H	0.663076	-1.131630	4.814224
C	-1.350299	1.361212	4.251575
H	-0.606289	2.064630	3.862391
H	-2.159579	1.939483	4.708518
H	-0.881197	0.748908	5.028009
C	-2.900931	-0.575736	3.697780
H	-3.737399	-0.079839	4.200049
H	-3.307880	-1.215791	2.908359
H	-2.390392	-1.207734	4.433352
C	-3.393257	1.871648	-2.636465
H	-4.338030	2.413819	-2.530423
H	-3.068615	1.959231	-3.680716
H	-3.587407	0.817317	-2.408314
C	-2.056684	3.944002	-2.022550
H	-1.716880	4.035914	-3.061368
H	-2.970848	4.535813	-1.914714
H	-1.291352	4.362618	-1.363884

4Me$_{cis34syn}$

Lu	0.794321	-0.992967	-0.533227
C	3.388471	-2.781282	-0.673333
H	4.286895	-2.547771	-1.243308
S	-0.922080	1.012918	0.832547
N	0.655213	1.062935	0.205647
N	-1.247130	-0.534024	0.218932

C	2.509097	-1.323052	-3.040489
H	2.664016	-2.390140	-3.140309
H	3.396641	-0.700180	-3.006833
C	1.272155	-0.770317	-3.150077
H	1.191411	0.308800	-3.272720
C	0.020125	-1.549804	-3.254256
C	-0.121534	-2.755585	-2.652222
H	-1.047215	-3.316902	-2.723702
H	0.709071	-3.266432	-2.164912
C	-1.079174	-0.914220	-4.066273
H	-1.326470	0.087473	-3.696516
H	-0.739708	-0.795709	-5.103069
H	-1.987285	-1.516989	-4.065870
C	2.846434	-4.172287	-0.901760
H	2.690431	-4.351102	-1.976517
H	1.870887	-4.313408	-0.418870
C	3.816998	-5.250266	-0.375152
H	4.798330	-5.160490	-0.853550
H	3.430338	-6.253995	-0.582045
H	3.958233	-5.150913	0.705708
C	3.106591	-1.957630	0.397569
C	1.932630	-2.081132	1.229862
H	1.508474	-3.081578	1.343354
H	1.962899	-1.542775	2.175524
C	4.010322	-0.759405	0.645709
H	4.600612	-0.942263	1.552953
H	3.455341	0.169523	0.826719
H	4.710381	-0.591505	-0.178390
C	-1.890155	2.231221	-0.089000
C	-2.740915	3.031551	0.683223
C	-1.815740	2.390831	-1.475779
C	-3.525754	4.002978	0.054677
H	-2.785153	2.900960	1.758857
C	-2.598712	3.363644	-2.094633
H	-1.143366	1.773615	-2.057679
C	-3.453155	4.168246	-1.329404
H	-4.184753	4.627614	0.644874
H	-2.544385	3.500321	-3.167939
H	-4.058460	4.923876	-1.815131
C	-2.430063	-1.162928	0.779200
C	-2.402967	-1.743568	2.080036
C	-3.625211	-1.226353	0.011769
C	-3.561498	-2.350002	2.579003
C	-4.754261	-1.848491	0.559460

C	-4.732951	-2.402212	1.833172
H	-3.541810	-2.789074	3.569198
H	-5.666487	-1.892685	-0.023095
H	-5.619975	-2.872959	2.240177
C	1.496499	2.158449	0.627460
C	1.843896	2.359201	1.995877
C	2.046620	3.016239	-0.365888
C	2.696971	3.418185	2.327812
C	2.910791	4.046738	0.022821
C	3.231377	4.258441	1.357801
H	2.951419	3.580669	3.368150
H	3.331464	4.697528	-0.734344
H	3.893438	5.068038	1.640484
C	1.320458	1.496523	3.149398
H	0.764125	0.651848	2.738731
C	1.770334	2.850573	-1.860212
H	1.033643	2.051883	-1.972464
C	-3.754295	-0.656022	-1.400144
H	-2.785197	-0.242145	-1.687425
C	-1.165098	-1.757977	2.975862
H	-0.346050	-1.274046	2.441260
C	0.366380	2.326677	4.047113
H	0.903199	3.174405	4.485193
H	-0.474636	2.720960	3.466750
H	-0.027038	1.708055	4.860221
C	2.475781	0.912352	4.002660
H	3.034415	1.707482	4.505832
H	2.066127	0.248961	4.773051
H	3.174202	0.341380	3.383088
C	3.066438	2.435383	-2.604730
H	3.495047	1.524779	-2.169114
H	2.864961	2.263824	-3.669404
H	3.819852	3.225563	-2.527394
C	1.180460	4.138780	-2.484054
H	0.964921	3.977676	-3.547274
H	0.255237	4.424526	-1.976346
H	1.890273	4.968207	-2.407523
C	-4.808085	0.479314	-1.447220
H	-4.859754	0.904274	-2.456111
H	-5.799060	0.091279	-1.189430
H	-4.555376	1.278312	-0.745968
C	-4.142144	-1.772764	-2.403263
H	-3.408451	-2.586402	-2.390297
H	-5.118318	-2.197800	-2.150032

H	-4.209223	-1.365104	-3.418748
C	-1.416471	-0.981282	4.292198
H	-1.715710	0.050853	4.085990
H	-2.209933	-1.459185	4.875750
H	-0.505662	-0.967606	4.902389
C	-0.731224	-3.213324	3.289142
H	-0.572876	-3.782449	2.366732
H	0.199085	-3.215195	3.868253
H	-1.499621	-3.726831	3.875812

TS45Me$_{cis34iso}$

Lu	-0.436378	-1.157831	-0.781536
C	-2.849470	-2.642945	-1.073686
H	-3.447268	-3.265624	-1.735549
S	0.657746	1.004303	0.981199
N	1.385090	-0.302465	0.187366
N	-0.857960	0.739846	0.265844
C	-2.100402	-1.854345	-3.001900
H	-3.120172	-1.531015	-3.178258
H	-1.883037	-2.865598	-3.333736
C	-1.092694	-0.876329	-3.150918
H	-1.397102	0.142782	-3.371667
C	0.308352	-1.223662	-3.338375
C	0.841821	-2.386774	-2.851615
H	1.895881	-2.613546	-2.965515
H	0.217507	-3.214075	-2.511275
C	1.170830	-0.197094	-4.033233
H	1.037124	0.804741	-3.609736
H	2.229066	-0.455387	-3.992773
H	0.869675	-0.138084	-5.086654
C	-3.665253	-1.539651	-0.413020
H	-4.167472	-0.952625	-1.190055
H	-3.044444	-0.813762	0.133596
C	-4.726216	-2.092563	0.557729
H	-5.422436	-2.755218	0.032209
H	-5.303665	-1.273496	0.998298
H	-4.268797	-2.664612	1.371412
C	-1.867449	-3.392733	-0.342681
C	-1.222540	-2.899234	0.789225
H	-1.693191	-2.130763	1.402731
H	-0.488902	-3.512445	1.301845
C	-1.459137	-4.742471	-0.898586
H	-0.456440	-5.039236	-0.576244
H	-1.506790	-4.782882	-1.992188

H	-2.158923	-5.500730	-0.524215
C	1.327356	2.538572	0.299726
C	1.278639	2.873185	-1.056768
C	1.931321	3.393220	1.230534
C	1.836373	4.077098	-1.483885
H	0.799531	2.207860	-1.763008
C	2.492635	4.596496	0.793372
H	1.960179	3.124055	2.280608
C	2.443385	4.936947	-0.559566
H	1.798443	4.348605	-2.531899
H	2.960946	5.263079	1.506919
H	2.875238	5.871275	-0.897004
C	2.680544	-0.686781	0.712274
C	2.793748	-1.388736	1.947248
C	3.855862	-0.394079	-0.031778
C	4.062902	-1.754193	2.410233
C	5.100181	-0.791934	0.473809
C	5.212310	-1.459769	1.686428
H	4.150004	-2.280406	3.353360
H	5.995766	-0.565882	-0.092228
H	6.185543	-1.750781	2.063457
C	-1.965654	1.533102	0.742863
C	-2.432795	1.431740	2.085964
C	-2.660691	2.367866	-0.177461
C	-3.549212	2.181949	2.473723
C	-3.784248	3.078942	0.261429
C	-4.226494	2.999131	1.575880
H	-3.896992	2.118499	3.497799
H	-4.314283	3.712376	-0.439715
H	-5.091242	3.566668	1.898294
C	1.596645	-1.773190	2.817784
H	0.680624	-1.499938	2.287852
C	3.842530	0.340669	-1.371637
H	2.801732	0.540958	-1.635363
C	-2.257477	2.526837	-1.645217
H	-1.362594	1.924101	-1.813423
C	-1.776271	0.553209	3.156103
H	-0.983355	-0.040358	2.695552
C	4.482041	-0.532855	-2.481457
H	3.965088	-1.494225	-2.573398
H	4.443456	-0.011494	-3.445338
H	5.533465	-0.736375	-2.255726
C	4.596837	1.690492	-1.267062
H	4.163832	2.323199	-0.488329

H	5.651837	1.519175	-1.028927
H	4.544856	2.226998	-2.221292
C	1.562258	-3.302122	3.074448
H	1.599923	-3.861428	2.133105
H	2.418931	-3.611633	3.681043
H	0.649976	-3.574657	3.618006
C	1.626615	-1.011968	4.166597
H	2.527213	-1.274686	4.730780
H	1.625682	0.069860	4.003911
H	0.752463	-1.276939	4.772673
C	-1.141366	1.436309	4.261170
H	-0.384661	2.105681	3.838147
H	-1.909111	2.050702	4.742059
H	-0.669106	0.811072	5.025629
C	-2.790567	-0.438008	3.782698
H	-3.578719	0.095868	4.322526
H	-3.265628	-1.056655	3.013726
H	-2.278114	-1.094444	4.495287
C	-3.377799	2.010961	-2.585316
H	-4.290115	2.601956	-2.457462
H	-3.066614	2.093994	-3.633804
H	-3.622776	0.965292	-2.369037
C	-1.924045	4.002232	-1.979514
H	-1.611828	4.089854	-3.027251
H	-2.803203	4.638040	-1.835118
H	-1.118450	4.372664	-1.340619

TS45Me$_{cis34syn}$

Lu	0.730597	-1.023348	-0.595399
C	3.205938	-2.666864	-0.843854
H	4.197665	-2.554939	-1.278377
S	-0.918331	1.021759	0.833265
N	0.661559	1.018336	0.216386
N	-1.294007	-0.490970	0.174596
C	2.553826	-1.739089	-2.712069
H	2.553484	-2.762128	-3.076430
H	3.495245	-1.216996	-2.847511
C	1.387135	-0.961838	-2.947418
H	1.523352	0.068369	-3.265960
C	0.075591	-1.564064	-3.118575
C	-0.257789	-2.747455	-2.514709
H	-1.252757	-3.167268	-2.613727
H	0.497211	-3.413950	-2.098874
C	-0.933413	-0.785175	-3.928092

H	-0.920078	0.282670	-3.683572
H	-0.669664	-0.868507	-4.990154
H	-1.947145	-1.163666	-3.797190
C	2.743233	-4.118336	-0.865667
H	2.694641	-4.472423	-1.903156
H	1.726954	-4.231493	-0.464265
C	3.691279	-5.039189	-0.075492
H	4.708921	-4.989992	-0.478380
H	3.356240	-6.079921	-0.137297
H	3.732583	-4.758081	0.981963
C	3.057804	-1.875080	0.351064
C	2.042326	-2.073888	1.275383
H	1.501289	-3.018223	1.324367
H	2.005907	-1.468520	2.175170
C	4.011252	-0.707738	0.523960
H	4.952246	-1.088006	0.943042
H	3.626867	0.057953	1.201370
H	4.261216	-0.231214	-0.430548
C	-1.834072	2.302919	-0.054221
C	-2.652381	3.114338	0.741808
C	-1.755597	2.497181	-1.436518
C	-3.400858	4.131280	0.142148
H	-2.700538	2.957183	1.813784
C	-2.503505	3.514963	-2.026287
H	-1.109290	1.870684	-2.037202
C	-3.325220	4.330403	-1.237405
H	-4.034639	4.764251	0.750813
H	-2.446520	3.677191	-3.095861
H	-3.903004	5.120690	-1.701023
C	-2.482023	-1.114682	0.722743
C	-2.448754	-1.743040	2.000554
C	-3.683674	-1.135140	-0.035262
C	-3.608753	-2.352317	2.491345
C	-4.814927	-1.763311	0.501197
C	-4.787670	-2.362912	1.754417
H	-3.586430	-2.826478	3.465509
H	-5.733117	-1.775556	-0.073592
H	-5.676531	-2.837494	2.152873
C	1.547610	2.076127	0.634054
C	1.894417	2.276910	2.003809
C	2.154471	2.886932	-0.365924
C	2.808120	3.286517	2.328442
C	3.077544	3.867849	0.016982
C	3.402033	4.077460	1.350968

H	3.062921	3.451089	3.368343
H	3.541081	4.481919	-0.745914
H	4.110648	4.848638	1.628205
C	1.299415	1.472696	3.166237
H	0.731748	0.630813	2.764464
C	1.868755	2.733527	-1.860999
H	1.103681	1.963024	-1.978648
C	-3.810387	-0.505267	-1.421665
H	-2.831082	-0.111069	-1.701111
C	-1.197903	-1.798064	2.877184
H	-0.381920	-1.308535	2.339269
C	0.333029	2.363076	3.990334
H	0.877327	3.209462	4.421555
H	-0.467663	2.760772	3.358131
H	-0.116723	1.786781	4.805799
C	2.393923	0.886477	4.094616
H	2.951814	1.680725	4.599507
H	1.927970	0.261632	4.865316
H	3.107352	0.274719	3.532196
C	3.143688	2.278602	-2.617345
H	3.528790	1.336499	-2.208734
H	2.930930	2.140894	-3.684396
H	3.933848	3.030419	-2.524389
C	1.324270	4.048872	-2.471647
H	1.101931	3.905572	-3.535957
H	0.410118	4.362093	-1.960004
H	2.062934	4.852163	-2.386810
C	-4.827561	0.663672	-1.409262
H	-4.887594	1.120123	-2.403760
H	-5.824340	0.298929	-1.139696
H	-4.532565	1.432683	-0.691011
C	-4.240863	-1.565508	-2.467805
H	-3.544667	-2.411126	-2.482197
H	-5.237960	-1.954431	-2.237959
H	-4.280621	-1.117831	-3.468087
C	-1.414062	-1.043918	4.212651
H	-1.699248	-0.003452	4.029905
H	-2.207515	-1.520471	4.797192
H	-0.494759	-1.056945	4.810172
C	-0.778095	-3.264928	3.151282
H	-0.642243	-3.817513	2.214303
H	0.157213	-3.293787	3.722423
H	-1.546390	-3.781956	3.734575

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Lu	-0.189482	-1.161315	-0.428150
C	-3.142520	-2.965462	-1.462987
H	-3.684995	-3.885984	-1.723283
S	0.908545	1.251956	0.980938
N	1.646685	-0.066044	0.225624
N	-0.635146	0.819727	0.424297
C	-2.081236	-2.788217	-2.603640
H	-2.648153	-2.862434	-3.542268
H	-1.416044	-3.659510	-2.600912
C	-1.254687	-1.497138	-2.670108
H	-1.772278	-0.674847	-3.161831
C	0.150571	-1.540461	-2.903474
C	0.998578	-2.447615	-2.255212
H	2.068061	-2.423437	-2.438604
H	0.614911	-3.422086	-1.937048
C	0.778818	-0.394702	-3.675132
H	0.165330	0.512156	-3.637544
H	1.790616	-0.164382	-3.329335
H	0.849487	-0.688588	-4.730391
C	-4.172726	-1.820186	-1.437031
H	-4.500733	-1.653828	-2.471210
H	-3.698120	-0.880434	-1.127180
C	-5.399911	-2.103336	-0.562327
H	-5.927934	-3.000800	-0.905315
H	-6.105656	-1.267639	-0.604397
H	-5.130368	-2.255631	0.488604
C	-2.452824	-3.255624	-0.140548
C	-2.214932	-2.313688	0.808980
H	-2.666147	-1.321749	0.761716
H	-1.777720	-2.589392	1.767497
C	-2.030857	-4.686076	0.076931
H	-1.381391	-4.809186	0.947673
H	-1.531844	-5.105155	-0.804391
H	-2.930716	-5.294616	0.239047
C	1.401336	2.753110	0.106645
C	1.437825	2.851004	-1.289056
C	1.764567	3.836277	0.916007
C	1.848609	4.045931	-1.876329
H	1.154975	2.005947	-1.903661
C	2.168063	5.033868	0.317297
H	1.734850	3.745077	1.996174
C	2.211914	5.135881	-1.074127
H	1.884124	4.133099	-2.955554

H	2.448837	5.877452	0.935555
H	2.529228	6.062221	-1.537360
C	2.923555	-0.461671	0.774170
C	2.964495	-1.290781	1.930424
C	4.129358	-0.088443	0.133095
C	4.200803	-1.684416	2.447259
C	5.346793	-0.511215	0.685826
C	5.389603	-1.287087	1.837056
H	4.242218	-2.309911	3.329717
H	6.272726	-0.225074	0.201449
H	6.341792	-1.595086	2.252368
C	-1.769136	1.555936	0.919882
C	-2.200866	1.414644	2.272014
C	-2.518644	2.364160	0.021958
C	-3.351084	2.092276	2.689763
C	-3.675628	3.001475	0.488548
C	-4.090250	2.876482	1.809136
H	-3.675928	1.999394	3.719096
H	-4.251101	3.615305	-0.194204
H	-4.981731	3.387953	2.152245
C	1.678011	-1.851741	2.536248
H	0.875931	-1.119970	2.389909
C	4.157611	0.715450	-1.164005
H	3.127818	0.968928	-1.416919
C	-2.110040	2.593862	-1.433970
H	-1.192248	2.030856	-1.615743
C	-1.442535	0.578264	3.305202
H	-0.702816	-0.029536	2.777537
C	4.746343	-0.141905	-2.313960
H	4.172092	-1.065886	-2.443852
H	4.727105	0.421407	-3.254349
H	5.785537	-0.414396	-2.101625
C	4.955857	2.032543	-1.004710
H	4.532823	2.651392	-0.207656
H	6.004328	1.825393	-0.766013
H	4.925933	2.603410	-1.939390
C	1.314892	-3.159340	1.781518
H	1.255123	-3.004013	0.687867
H	2.113387	-3.896007	1.920349
H	0.376388	-3.591803	2.147229
C	1.753156	-2.126179	4.055289
H	2.442065	-2.946668	4.279431
H	2.087016	-1.232751	4.591545
H	0.763427	-2.409982	4.430988

C	-0.690083	1.496710	4.303293
H	-0.004993	2.168693	3.777252
H	-1.407387	2.106743	4.862076
H	-0.113485	0.896578	5.016490
C	-2.373386	-0.390480	4.077723
H	-3.077485	0.161067	4.708599
H	-2.951978	-1.017999	3.391660
H	-1.776149	-1.036655	4.731901
C	-3.196601	2.086363	-2.414785
H	-4.135736	2.629823	-2.268129
H	-2.872692	2.243075	-3.450503
H	-3.392018	1.019749	-2.267097
C	-1.824087	4.095332	-1.690300
H	-1.481730	4.241477	-2.721337
H	-2.733222	4.688404	-1.546976
H	-1.053503	4.468836	-1.011016

5Me$_{cis34syn}$

Lu	0.999262	-0.514137	-0.583320
C	4.316192	-1.459090	-0.995919
H	5.409573	-1.352031	-1.054248
S	-1.415281	0.517783	0.853425
N	0.042205	1.223079	0.333777
N	-1.067444	-0.959554	0.112761
C	3.782433	-1.028449	-2.424675
H	3.764682	-1.943367	-3.030630
H	4.555531	-0.393815	-2.869197
C	2.451609	-0.267862	-2.616926
H	2.597122	0.720417	-3.050870
C	1.268276	-0.923958	-3.065490
C	0.844676	-2.145342	-2.538580
H	-0.070179	-2.613101	-2.884777
H	1.575529	-2.830996	-2.100864
C	0.311877	-0.154786	-3.961086
H	0.380776	0.928464	-3.811757
H	0.586858	-0.347340	-5.006002
H	-0.727763	-0.472920	-3.832663
C	4.056055	-2.944480	-0.662781
H	4.237699	-3.521514	-1.576842
H	2.997386	-3.124566	-0.418575
C	4.944972	-3.507067	0.454937
H	6.003516	-3.421103	0.183912
H	4.732049	-4.567987	0.620922
H	4.805266	-2.985723	1.407683

C	3.869641	-0.465845	0.062281
C	3.014515	-0.779273	1.071791
H	2.737218	-1.810205	1.290004
H	2.764690	-0.043833	1.834268
C	4.439063	0.926352	-0.042196
H	5.504692	0.885861	0.222516
H	3.949259	1.629492	0.637275
H	4.382729	1.319443	-1.061807
C	-2.740104	1.341296	-0.055618
C	-3.827271	1.769435	0.716230
C	-2.711094	1.549686	-1.438569
C	-4.898563	2.415445	0.092204
H	-3.834771	1.604467	1.788025
C	-3.784932	2.192182	-2.052509
H	-1.860626	1.222986	-2.023701
C	-4.876329	2.624829	-1.287615
H	-5.742003	2.752557	0.681831
H	-3.773213	2.360598	-3.122565
H	-5.706479	3.125449	-1.770915
C	-1.835659	-2.096534	0.558958
C	-1.474374	-2.776577	1.755516
C	-2.909283	-2.582020	-0.232092
C	-2.210370	-3.900297	2.147016
C	-3.609595	-3.714754	0.200434
C	-3.274726	-4.367108	1.381789
H	-1.943892	-4.419688	3.060295
H	-4.431638	-4.087603	-0.398915
H	-3.834333	-5.238047	1.701680
C	0.367155	2.535575	0.825644
C	0.563421	2.779627	2.216153
C	0.568383	3.588316	-0.108986
C	0.896455	4.072571	2.634326
C	0.923578	4.857317	0.364694
C	1.073273	5.108830	1.723188
H	1.029227	4.268139	3.691722
H	1.077942	5.661088	-0.345247
H	1.334129	6.101596	2.069838
C	0.426832	1.697218	3.292074
H	0.296843	0.727999	2.803500
C	0.454158	3.398771	-1.622586
H	0.142666	2.367180	-1.810525
C	-3.328649	-1.930677	-1.549466
H	-2.667929	-1.080318	-1.726214
C	-0.289285	-2.355372	2.626052

H	0.157021	-1.455680	2.185214
C	-0.813681	1.962192	4.183401
H	-0.705531	2.917632	4.707076
H	-1.726111	2.006039	3.579924
H	-0.924949	1.168407	4.930204
C	1.700285	1.602234	4.171335
H	1.849857	2.520818	4.746638
H	1.603085	0.771622	4.879786
H	2.593992	1.439156	3.558255
C	1.829449	3.621304	-2.304169
H	2.585739	2.944426	-1.891867
H	1.752291	3.446665	-3.383995
H	2.172051	4.649440	-2.149487
C	-0.606676	4.344400	-2.237932
H	-0.690386	4.164161	-3.316425
H	-1.584696	4.183180	-1.777199
H	-0.321087	5.391218	-2.092941
C	-4.786144	-1.410628	-1.475193
H	-5.055748	-0.915394	-2.414599
H	-5.482130	-2.240791	-1.314649
H	-4.905653	-0.693509	-0.658154
C	-3.177112	-2.924492	-2.729257
H	-2.149191	-3.294160	-2.799699
H	-3.839866	-3.786023	-2.598311
H	-3.440939	-2.433456	-3.673236
C	-0.731155	-1.996174	4.065842
H	-1.483276	-1.201383	4.054098
H	-1.162615	-2.870188	4.563816
H	0.129974	-1.658391	4.654302
C	0.792208	-3.466008	2.651829
H	1.117463	-3.726034	1.636284
H	1.661439	-3.143598	3.237896
H	0.393281	-4.375931	3.110783

1Me′

Lu	-0.249465	-0.310091	1.362946
C	-0.332126	1.168371	3.094892
H	-0.905597	2.074058	2.848701
H	-0.777389	0.759714	4.016466
H	0.677848	1.514695	3.365313
S	0.200376	0.834587	-1.352189
N	-1.181206	0.461631	-0.457125
N	1.204171	0.427362	-0.034861
C	0.421003	-0.482217	-2.581431

C	1.521755	-0.342280	-3.439799
C	-0.447488	-1.574780	-2.690357
C	1.770648	-1.330711	-4.393732
H	2.175911	0.518942	-3.363880
C	-0.194126	-2.547038	-3.660273
H	-1.331652	-1.637272	-2.071876
C	0.915404	-2.430646	-4.502706
H	2.623446	-1.235508	-5.054420
H	-0.871222	-3.385747	-3.768228
H	1.104188	-3.187982	-5.253762
C	-2.494327	0.449365	-1.010981
C	-3.299311	-0.677548	-0.659799
C	-3.037841	1.484105	-1.808539
C	-4.594167	-0.779298	-1.169609
C	-4.334077	1.320435	-2.317881
C	-5.104622	0.203880	-2.016567
H	-5.211828	-1.629811	-0.912362
H	-4.750758	2.096517	-2.948137
H	-6.104722	0.106105	-2.420435
C	-2.773154	-1.717178	0.333658
H	-1.697016	-1.871660	0.106079
C	-2.285955	2.782615	-2.111978
H	-1.393029	2.822778	-1.482387
C	-2.950936	-1.182894	1.788241
H	-2.451661	-1.818231	2.539255
H	-4.018376	-1.192553	2.031736
H	-2.656225	-0.126840	1.918419
C	-3.425858	-3.113696	0.219409
H	-3.348538	-3.494273	-0.803154
H	-4.482628	-3.072891	0.499077
H	-2.929332	-3.818882	0.894942
C	-3.141706	4.024385	-1.753548
H	-3.468937	3.984705	-0.709970
H	-4.026312	4.092370	-2.394328
H	-2.548352	4.933426	-1.900592
C	-1.848991	2.836864	-3.598415
H	-2.728807	2.814687	-4.250161
H	-1.212650	1.983949	-3.859958
H	-1.295133	3.760750	-3.797766
C	2.616592	0.367680	-0.213007
C	3.231706	-0.904894	-0.041914
C	3.399582	1.519053	-0.460913
C	4.618151	-1.008256	-0.157241
C	4.786508	1.361462	-0.592085

C	5.391624	0.117233	-0.448001
H	5.104245	-1.966656	-0.028221
H	5.400872	2.231924	-0.789911
H	6.466378	0.022473	-0.546187
C	2.364912	-2.109515	0.332136
H	1.424355	-2.018757	-0.229951
C	2.790167	2.918989	-0.545935
H	1.718524	2.839345	-0.343048
C	2.061682	-2.077212	1.863885
H	1.226873	-2.745587	2.138926
H	1.908158	-1.053714	2.255087
H	2.937184	-2.431688	2.419233
C	2.976289	-3.478317	-0.038112
H	3.891430	-3.670824	0.531012
H	3.210068	-3.513420	-1.105990
H	2.265924	-4.281246	0.188375
C	3.397845	3.845969	0.537690
H	4.471273	3.984898	0.373786
H	3.250940	3.423442	1.536766
H	2.915979	4.829087	0.499302
C	2.981452	3.532256	-1.955814
H	2.521308	2.903833	-2.727346
H	4.046382	3.636743	-2.188547
H	2.521617	4.525433	-2.001293

2Me′*cis*34

Lu	-0.512031	0.438261	-1.605042
C	-0.883679	2.552393	-2.437077
H	-1.330515	3.185576	-1.654261
H	-1.608824	2.562740	-3.269859
H	-0.003345	3.101225	-2.799864
S	0.200536	0.191729	1.262310
N	-1.267258	0.343249	0.424551
N	1.119394	0.099268	-0.169989
C	1.057061	0.489434	-4.326232
H	1.991495	1.041891	-4.352072
H	0.210952	0.953261	-4.825631
C	0.997555	-0.724980	-3.743576
H	1.913878	-1.146562	-3.334556
C	-0.210785	-1.576045	-3.612250
C	-1.469026	-1.071253	-3.688905
H	-2.341140	-1.711026	-3.598283
H	-1.665495	-0.039038	-3.989175
C	0.039782	-3.036343	-3.328975

H	0.564791	-3.488510	-4.179969
H	0.689345	-3.169349	-2.455520
H	-0.890871	-3.586118	-3.170064
C	0.190949	-1.432596	2.052796
C	0.585292	-1.453271	3.396287
C	-0.190773	-2.607582	1.396775
C	0.597254	-2.668059	4.088347
H	0.872464	-0.534465	3.895676
C	-0.175342	-3.814230	2.094011
H	-0.507379	-2.577820	0.361602
C	0.218207	-3.843606	3.438670
H	0.897559	-2.692013	5.128501
H	-0.472315	-4.730028	1.597269
H	0.225051	-4.783830	3.976427
C	-2.468657	0.561228	1.180789
C	-3.527657	-0.377602	1.044294
C	-2.644794	1.721009	1.983097
C	-4.716718	-0.162525	1.749898
C	-3.845791	1.875063	2.684577
C	-4.872875	0.942401	2.580232
H	-5.531148	-0.869666	1.647959
H	-3.984440	2.750613	3.307601
H	-5.796248	1.085427	3.128609
C	-3.453287	-1.569284	0.088275
H	-2.413934	-1.669320	-0.241752
C	-1.599725	2.834892	2.086717
H	-0.758898	2.590312	1.434390
C	-4.334143	-1.294451	-1.158855
H	-4.279684	-2.131978	-1.865572
H	-5.379703	-1.164320	-0.862652
H	-4.020567	-0.373882	-1.669562
C	-3.863435	-2.900460	0.761355
H	-3.242152	-3.095334	1.640295
H	-4.911532	-2.875237	1.075071
H	-3.746916	-3.730765	0.054616
C	-2.181043	4.182774	1.588584
H	-2.544237	4.092021	0.559399
H	-3.013409	4.507260	2.220831
H	-1.405731	4.956861	1.620188
C	-1.068619	2.971767	3.535586
H	-1.881741	3.238467	4.218481
H	-0.627448	2.030604	3.882637
H	-0.305544	3.755695	3.587160
C	2.530901	0.375877	-0.041103

C	3.457283	-0.701111	-0.080172
C	3.001187	1.715333	0.054714
C	4.827008	-0.416684	-0.025585
C	4.381148	1.942125	0.114318
C	5.290846	0.890584	0.073637
H	5.538761	-1.233129	-0.051234
H	4.746539	2.958999	0.192974
H	6.354966	1.089150	0.121529
C	3.025305	-2.166204	-0.157673
H	1.935226	-2.191329	-0.231188
C	2.072955	2.929829	0.114419
H	1.042191	2.592282	-0.031083
C	3.626075	-2.868209	-1.401999
H	3.264881	-3.901425	-1.467323
H	3.356245	-2.341597	-2.324346
H	4.718640	-2.897280	-1.343074
C	3.437748	-2.928606	1.127285
H	4.527518	-2.936316	1.234010
H	3.005121	-2.458603	2.014477
H	3.089062	-3.966264	1.078420
C	2.391601	3.947095	-1.009934
H	3.395310	4.365034	-0.883723
H	2.338561	3.472558	-1.995401
H	1.672018	4.772331	-0.981677
C	2.161787	3.617193	1.500894
H	1.912556	2.915061	2.302794
H	3.175659	3.992239	1.675035
H	1.468395	4.464788	1.547259

TS23Me′*cis34*

Lu	-0.353459	0.253711	-1.637647
C	-0.922594	2.449329	-2.427897
H	-1.632308	2.385150	-1.578922
H	-1.430497	3.024961	-3.198838
H	-0.038354	3.013694	-2.105369
S	0.184981	0.126367	1.269619
N	-1.241100	0.279306	0.362048
N	1.186366	0.021689	-0.112467
C	-0.477665	1.084418	-4.207228
H	-0.067546	1.979869	-4.657401
H	-1.544374	0.952371	-4.370212
C	0.365928	-0.033576	-4.099672
H	1.418883	0.109890	-4.334337
C	-0.045090	-1.360470	-3.730152

C	-1.239733	-1.627625	-3.079184
H	-1.518201	-2.645140	-2.826918
H	-2.085465	-0.933038	-3.137412
C	0.946286	-2.478527	-3.954105
H	0.855877	-2.819481	-4.993517
H	1.979707	-2.150199	-3.811836
H	0.754600	-3.336151	-3.304254
C	0.141022	-1.491401	2.066653
C	0.472331	-1.506311	3.427257
C	-0.215822	-2.667490	1.398086
C	0.445126	-2.717641	4.124744
H	0.741170	-0.586679	3.935102
C	-0.240505	-3.870033	2.101850
H	-0.481330	-2.641477	0.348301
C	0.089228	-3.894231	3.463688
H	0.696667	-2.738088	5.177828
H	-0.518668	-4.786612	1.595973
H	0.065479	-4.831610	4.005922
C	-2.454846	0.582694	1.074069
C	-3.540446	-0.331444	0.992073
C	-2.611403	1.808013	1.780466
C	-4.738235	-0.019070	1.645798
C	-3.823642	2.059208	2.432400
C	-4.880020	1.156189	2.375039
H	-5.570903	-0.709351	1.583006
H	-3.945344	2.984853	2.982326
H	-5.811320	1.373495	2.884200
C	-3.485703	-1.614754	0.162269
H	-2.459057	-1.744861	-0.189692
C	-1.527979	2.888244	1.846969
H	-0.676376	2.572631	1.240544
C	-4.409671	-1.482525	-1.077445
H	-4.346981	-2.380336	-1.703739
H	-5.451127	-1.355051	-0.765179
H	-4.136732	-0.607681	-1.681686
C	-3.869216	-2.864234	0.990968
H	-3.210481	-2.970103	1.857598
H	-4.902649	-2.796376	1.344786
H	-3.785039	-3.765240	0.371771
C	-2.039517	4.226356	1.254142
H	-2.379544	4.091381	0.221772
H	-2.874709	4.619580	1.841739
H	-1.234861	4.970585	1.264518
C	-1.035192	3.092813	3.301789

H	-1.858717	3.427178	3.940770
H	-0.639802	2.159031	3.716248
H	-0.246046	3.851539	3.332447
C	2.592906	0.263300	0.112946
C	3.493459	-0.833838	0.159786
C	3.085508	1.593093	0.227021
C	4.859289	-0.578573	0.332693
C	4.459494	1.791512	0.402135
C	5.343308	0.718627	0.459956
H	5.551501	-1.411102	0.370062
H	4.842365	2.801373	0.490672
H	6.403549	0.893859	0.598479
C	3.043699	-2.287383	0.012776
H	1.959070	-2.293162	-0.113045
C	2.190303	2.829934	0.135922
H	1.150841	2.501685	0.038380
C	3.690680	-2.935935	-1.237209
H	3.316416	-3.957557	-1.370630
H	3.467309	-2.357544	-2.139803
H	4.778943	-2.984519	-1.128174
C	3.388469	-3.111724	1.278304
H	4.472023	-3.144116	1.433207
H	2.922844	-2.677481	2.167242
H	3.028615	-4.140370	1.164885
C	2.549883	3.669155	-1.117267
H	3.576933	4.040344	-1.044548
H	2.475696	3.067792	-2.031172
H	1.880161	4.532749	-1.204022
C	2.286317	3.700385	1.413292
H	2.029191	3.117280	2.302901
H	3.300838	4.091413	1.538976
H	1.600014	4.551855	1.340186

3Me′*cis*34

Lu	-0.023617	0.371623	-1.479769
C	-1.952879	1.961376	-2.740029
H	-2.290583	1.229337	-1.985425
H	-2.839659	2.581372	-2.904610
H	-1.205008	2.641534	-2.293325
S	0.245815	-0.047020	1.423151
N	-1.086974	0.340416	0.425372
N	1.331472	-0.165799	0.119915
C	-1.462335	1.326832	-4.065263
H	-1.472039	2.118171	-4.821318

H	-2.209528	0.588184	-4.383793
C	-0.063214	0.702165	-4.081249
H	0.681472	1.255024	-4.650236
C	0.213327	-0.631469	-3.806480
C	-0.618881	-1.419065	-2.936283
H	-0.367683	-2.471937	-2.824173
H	-1.700826	-1.252802	-3.000134
C	1.562276	-1.199219	-4.203346
H	1.417313	-1.894966	-5.039516
H	2.261201	-0.424340	-4.532462
H	2.026463	-1.775535	-3.394041
C	-0.026406	-1.716138	2.043629
C	-0.040202	-1.860540	3.435807
C	-0.211564	-2.816338	1.197221
C	-0.243585	-3.129093	3.987859
H	0.105036	-0.998982	4.077961
C	-0.405166	-4.076778	1.758418
H	-0.200002	-2.688186	0.120746
C	-0.422414	-4.231922	3.151401
H	-0.258552	-3.251808	5.063615
H	-0.546330	-4.937501	1.116098
H	-0.575343	-5.214728	3.580435
C	-2.315468	0.676087	1.098455
C	-3.426061	-0.204288	1.001074
C	-2.444447	1.910753	1.793416
C	-4.630738	0.161760	1.614579
C	-3.664922	2.218510	2.403082
C	-4.751947	1.353517	2.320851
H	-5.484430	-0.500874	1.539753
H	-3.767725	3.153656	2.941065
H	-5.690247	1.611499	2.797322
C	-3.381045	-1.510856	0.208250
H	-2.347081	-1.683766	-0.096407
C	-1.315463	2.938631	1.879524
H	-0.460966	2.557131	1.318292
C	-4.250063	-1.389529	-1.071202
H	-4.194279	-2.312604	-1.659592
H	-5.297874	-1.211141	-0.807912
H	-3.915230	-0.554071	-1.698052
C	-3.842482	-2.719556	1.057641
H	-3.232086	-2.816485	1.959800
H	-4.890764	-2.612704	1.354074
H	-3.750915	-3.641851	0.472532
C	-1.734144	4.278998	1.223082

H	-2.046603	4.124588	0.183968
H	-2.570541	4.732518	1.764070
H	-0.895439	4.985011	1.239763
C	-0.860988	3.163595	3.342993
H	-1.684697	3.562285	3.943841
H	-0.529006	2.224173	3.797510
H	-0.032996	3.880684	3.377881
C	2.727189	0.097263	0.374960
C	3.636966	-0.977057	0.513381
C	3.197891	1.440923	0.370006
C	5.000809	-0.686037	0.660185
C	4.565096	1.680317	0.522772
C	5.463673	0.623878	0.671475
H	5.705637	-1.502140	0.765369
H	4.937210	2.696480	0.525437
H	6.521376	0.826355	0.790520
C	3.192309	-2.437100	0.474064
H	2.104264	-2.454160	0.421050
C	2.233441	2.604911	0.133760
H	1.272475	2.355052	0.591267
C	3.750563	-3.137455	-0.790650
H	3.411266	-4.178796	-0.827432
H	3.411289	-2.627117	-1.699418
H	4.845557	-3.132608	-0.785766
C	3.615995	-3.198340	1.754298
H	4.706420	-3.242733	1.843551
H	3.213671	-2.711082	2.648087
H	3.235127	-4.224962	1.717855
C	2.019489	2.815333	-1.389911
H	2.952700	3.152859	-1.854018
H	1.775499	1.879963	-1.933113
H	1.242937	3.564049	-1.591337
C	2.685924	3.940685	0.768509
H	2.904092	3.805728	1.831993
H	3.578630	4.337314	0.274554
H	1.889174	4.686131	0.667740

4Me′*cis*34iso

Lu	0.385457	-1.330997	-0.191667
C	1.987998	-3.315294	-0.858038
H	2.029417	-4.350735	-0.524855
S	-0.243098	1.536768	0.310331
N	-1.219530	0.165604	0.073395
N	1.204146	0.658137	0.202675

C	0.707559	-3.067880	2.216833
H	1.463658	-2.564418	2.811787
H	0.980404	-4.025127	1.785221
C	-0.547236	-2.569081	2.132200
H	-0.785145	-1.667568	2.696818
C	-1.676753	-3.171704	1.380096
C	-1.463374	-4.019379	0.352396
H	-2.294006	-4.464106	-0.186367
H	-0.468775	-4.329229	0.048325
C	-3.065329	-2.793879	1.831235
H	-3.207269	-3.065579	2.885062
H	-3.238894	-1.717033	1.741674
H	-3.825582	-3.311954	1.241534
C	3.118721	-2.439301	-0.341868
H	3.307805	-2.664462	0.715352
H	2.886825	-1.355965	-0.378271
C	4.430508	-2.633515	-1.131422
H	4.762867	-3.674004	-1.057715
H	5.224797	-1.990900	-0.737228
H	4.286372	-2.400994	-2.190847
C	1.224413	-3.037681	-1.986898
C	1.029613	-1.700543	-2.476211
H	1.899344	-1.040069	-2.500989
H	0.407022	-1.595086	-3.363024
C	0.401959	-4.143660	-2.617488
H	-0.629688	-3.830428	-2.813564
H	0.387408	-5.057656	-2.016423
H	0.846317	-4.393830	-3.588858
C	-0.415652	2.559497	-1.167589
C	-0.334795	2.050781	-2.468410
C	-0.643291	3.922385	-0.937241
C	-0.482101	2.920240	-3.548109
H	-0.167887	0.993392	-2.633642
C	-0.791304	4.785517	-2.026698
H	-0.708568	4.302320	0.076386
C	-0.710238	4.284757	-3.327138
H	-0.423305	2.537746	-4.559931
H	-0.970858	5.840060	-1.858087
H	-0.826079	4.954131	-4.170886
C	-2.641546	0.347777	0.183665
C	-3.250519	0.804600	1.391251
C	-3.460790	-0.032916	-0.915765
C	-4.645918	0.895431	1.451048
C	-4.852842	0.057727	-0.789217

C	-5.447777	0.524578	0.376251
H	-5.112563	1.254991	2.360164
H	-5.478278	-0.234071	-1.624556
H	-6.526258	0.597628	0.449031
C	2.388700	1.325101	0.690736
C	3.322186	1.867900	-0.232312
C	2.659100	1.378709	2.087095
C	4.497018	2.450811	0.259494
C	3.841913	1.983969	2.525009
C	4.757743	2.517147	1.623206
H	5.212958	2.864945	-0.440103
H	4.050861	2.035642	3.587014
H	5.668959	2.980316	1.982673
C	-2.461292	1.227419	2.637747
H	-1.412628	0.949984	2.505039
C	-2.901549	-0.555817	-2.240589
H	-1.810407	-0.532021	-2.183786
C	1.709392	0.810343	3.142899
H	0.906467	0.274567	2.625775
C	3.102156	1.853842	-1.745283
H	2.145629	1.365666	-1.939202
C	-3.339578	0.336604	-3.428707
H	-2.896085	-0.035799	-4.359919
H	-4.428175	0.321107	-3.543573
H	-3.020239	1.370880	-3.275520
C	-3.335445	-2.023723	-2.487529
H	-2.899132	-2.395450	-3.422419
H	-3.011177	-2.671180	-1.665444
H	-4.424856	-2.096838	-2.568719
C	-2.959957	0.518855	3.923877
H	-2.325289	0.805631	4.770189
H	-3.987564	0.808785	4.162458
H	-2.928400	-0.570045	3.817216
C	-2.542731	2.764921	2.827263
H	-2.165863	3.291292	1.944390
H	-3.583165	3.068006	2.983034
H	-1.956005	3.074903	3.698716
C	1.070211	1.949168	3.977792
H	0.532717	2.650807	3.332830
H	0.368441	1.537596	4.712833
H	1.846039	2.503438	4.516053
C	2.432127	-0.193028	4.076956
H	2.935454	-0.977641	3.500401
H	3.191099	0.315369	4.679242

H	1.714635	-0.655478	4.765144
C	4.216437	1.054882	-2.467468
H	4.269898	0.026395	-2.097080
H	4.021424	1.029134	-3.545798
H	5.193988	1.522978	-2.310925
C	3.033403	3.295915	-2.307256
H	2.824783	3.268176	-3.382358
H	2.244328	3.871244	-1.815265
H	3.986652	3.813823	-2.157454

4Me′*cis*34syn

Lu	0.448183	1.244192	-0.298523
C	1.092343	4.340972	0.196518
H	0.705082	5.134224	-0.442096
S	-0.681786	-1.477769	0.135303
N	-1.383200	0.048024	-0.127175
N	0.901210	-0.895773	-0.016880
C	0.602491	3.212036	-2.640308
H	1.442633	3.850512	-2.395887
H	-0.349186	3.705488	-2.815324
C	0.752797	1.883088	-2.870584
H	-0.080275	1.329774	-3.301433
C	2.008416	1.126626	-2.661596
C	2.932685	1.517447	-1.751711
H	3.834575	0.936549	-1.589812
H	2.868279	2.464575	-1.219957
C	2.188875	-0.115576	-3.492992
H	2.999741	-0.739446	-3.112057
H	1.273754	-0.714766	-3.526642
H	2.424291	0.170057	-4.526692
C	2.574649	4.418928	0.462152
H	3.124313	4.492571	-0.488718
H	2.943813	3.518310	0.966698
C	2.931630	5.655190	1.314186
H	2.599872	6.577917	0.825766
H	4.014673	5.722559	1.463161
H	2.450667	5.602240	2.296080
C	0.163524	3.599030	0.887593
C	0.467098	2.459746	1.736692
H	1.452125	2.456980	2.208804
H	-0.321152	2.192715	2.441742
C	-1.308491	3.880823	0.627330
H	-1.870411	2.987628	0.313449
H	-1.451783	4.656483	-0.130175

H	-1.786746	4.214750	1.555597
C	-0.916586	-1.941768	1.867691
C	-0.510194	-1.141843	2.940805
C	-1.542327	-3.176470	2.084884
C	-0.731279	-1.587648	4.243274
H	-0.026762	-0.190190	2.760890
C	-1.756763	-3.615690	3.394292
H	-1.854445	-3.786622	1.244883
C	-1.351022	-2.823211	4.469457
H	-0.419233	-0.976721	5.081764
H	-2.236305	-4.570603	3.570339
H	-1.515925	-3.164781	5.484102
C	-2.779829	0.039332	-0.500926
C	-3.768911	0.416635	0.449243
C	-3.167665	-0.288932	-1.831688
C	-5.108324	0.473759	0.042344
C	-4.520874	-0.224515	-2.180505
C	-5.487851	0.158505	-1.256815
H	-5.865757	0.760238	0.761484
H	-4.822207	-0.478531	-3.189751
H	-6.530801	0.204159	-1.547028
C	2.001212	-1.821601	0.045525
C	3.046855	-1.556145	0.976181
C	2.123536	-2.932781	-0.844133
C	4.177053	-2.383368	0.989569
C	3.264928	-3.738707	-0.765728
C	4.291658	-3.469884	0.132956
H	4.972794	-2.177739	1.695839
H	3.354046	-4.591671	-1.426879
H	5.168882	-4.104785	0.166413
C	-2.175781	-0.744431	-2.903774
H	-1.162916	-0.620288	-2.506731
C	-3.453599	0.715958	1.916231
H	-2.367267	0.755270	2.027667
C	1.043615	-3.340693	-1.853445
H	0.358645	-2.501079	-1.998654
C	3.002287	-0.417444	1.997878
H	2.060480	0.122186	1.869446
C	-4.001979	-0.420245	2.818845
H	-3.574824	-1.386520	2.542079
H	-3.755901	-0.218718	3.867238
H	-5.091568	-0.480144	2.724949
C	-4.052814	2.068377	2.380713
H	-3.723944	2.286379	3.403281

H	-3.744414	2.890563	1.729785
H	-5.146847	2.028855	2.385139
C	-2.380470	-2.245377	-3.234718
H	-3.385838	-2.409007	-3.635893
H	-1.651705	-2.575443	-3.984641
H	-2.264699	-2.860763	-2.337460
C	-2.296844	0.104287	-4.195065
H	-3.262329	-0.065735	-4.681605
H	-2.220504	1.175964	-3.977225
H	-1.512404	-0.175155	-4.908608
C	0.241529	-4.551907	-1.305109
H	0.908388	-5.413274	-1.193885
H	-0.189710	-4.334135	-0.323702
H	-0.566268	-4.821719	-1.994645
C	1.621068	-3.713100	-3.243677
H	2.275411	-2.928188	-3.631608
H	2.192713	-4.644765	-3.197110
H	0.797516	-3.866378	-3.950655
C	3.033718	-0.971779	3.445027
H	3.972892	-1.501545	3.633749
H	2.956932	-0.148304	4.165189
H	2.205148	-1.665480	3.610570
C	4.163999	0.586771	1.789025
H	4.090129	1.407335	2.512736
H	5.131424	0.095434	1.933257
H	4.148252	1.007351	0.777632

TS45Me′*cis*34iso

Lu	0.206162	-1.404922	-0.070391
C	2.099871	-3.344633	-0.827393
H	2.400843	-4.388581	-0.773294
S	-0.344368	1.518507	0.319827
N	-1.339073	0.175039	0.073407
N	1.080661	0.603794	0.224511
C	1.197328	-3.805370	1.104420
H	2.203711	-3.991852	1.463097
H	0.703430	-4.680032	0.690012
C	0.413155	-2.903312	1.862671
H	0.872975	-2.405705	2.712146
C	-1.038185	-2.861207	1.744634
C	-1.682423	-3.270347	0.609846
H	-2.759138	-3.181590	0.520990
H	-1.191071	-3.864081	-0.160302
C	-1.810546	-2.253560	2.888855

H	-1.909615	-2.999421	3.687962
H	-1.293206	-1.389360	3.317046
H	-2.811296	-1.945842	2.579400
C	3.264315	-2.400457	-0.550045
H	3.659900	-2.600117	0.452559
H	2.962635	-1.340850	-0.533667
C	4.401127	-2.574317	-1.574915
H	4.765252	-3.607518	-1.568252
H	5.244219	-1.919767	-1.332996
H	4.066780	-2.342118	-2.591020
C	1.172295	-3.103575	-1.903776
C	0.907589	-1.837565	-2.420936
H	1.639839	-1.034672	-2.334524
H	0.199604	-1.732400	-3.238190
C	0.392447	-4.293929	-2.426137
H	-0.558751	-4.001419	-2.880259
H	0.199426	-5.044424	-1.652286
H	0.989080	-4.788185	-3.203767
C	-0.459138	2.555604	-1.159797
C	-0.381232	2.048245	-2.460798
C	-0.628420	3.927023	-0.930917
C	-0.471308	2.925028	-3.540997
H	-0.263217	0.984444	-2.624500
C	-0.723210	4.798286	-2.020020
H	-0.689077	4.308260	0.082200
C	-0.643394	4.297715	-3.320390
H	-0.414289	2.542701	-4.553085
H	-0.859078	5.859314	-1.851003
H	-0.717151	4.972863	-4.164249
C	-2.766613	0.342388	0.108538
C	-3.451307	0.868329	1.246031
C	-3.521880	-0.119980	-1.007761
C	-4.848934	0.935061	1.222771
C	-4.919808	-0.050716	-0.963055
C	-5.585596	0.476184	0.135920
H	-5.370134	1.347361	2.077748
H	-5.492497	-0.404264	-1.812367
H	-6.667535	0.531175	0.146728
C	2.263368	1.219475	0.780751
C	3.242684	1.770131	-0.089929
C	2.488860	1.215231	2.186735
C	4.425550	2.281700	0.458813
C	3.682243	1.751659	2.682692
C	4.649329	2.276062	1.830746

H	5.174863	2.702601	-0.201097
H	3.856904	1.759416	3.751933
H	5.567949	2.684032	2.235524
C	-2.737332	1.414640	2.488384
H	-1.702852	1.061382	2.482502
C	-2.887607	-0.671971	-2.287190
H	-1.801690	-0.667877	-2.154007
C	1.469962	0.677910	3.193697
H	0.680206	0.161566	2.638295
C	3.049752	1.870146	-1.604361
H	2.093683	1.405393	-1.852992
C	-3.225390	0.230480	-3.501236
H	-2.724844	-0.143482	-4.403010
H	-4.304129	0.229452	-3.688401
H	-2.906819	1.260121	-3.320175
C	-3.331677	-2.129066	-2.573070
H	-2.838921	-2.503304	-3.479078
H	-3.083069	-2.789112	-1.736669
H	-4.413137	-2.180472	-2.735451
C	-3.380319	0.936909	3.815643
H	-2.758622	1.260977	4.658274
H	-4.375029	1.371704	3.952378
H	-3.472635	-0.151715	3.846711
C	-2.737966	2.966962	2.461168
H	-2.293488	3.351216	1.538286
H	-3.767573	3.335861	2.516442
H	-2.177791	3.365183	3.314685
C	0.823225	1.842954	3.986493
H	0.340697	2.554550	3.309541
H	0.072782	1.458960	4.687766
H	1.588405	2.377903	4.558551
C	2.106363	-0.342019	4.171283
H	2.611708	-1.148713	3.628380
H	2.845983	0.143441	4.815374
H	1.334943	-0.775172	4.818979
C	4.174993	1.137872	-2.377243
H	4.227109	0.081831	-2.098491
H	3.994487	1.206693	-3.456174
H	5.148505	1.592989	-2.167995
C	2.992553	3.354807	-2.046648
H	2.815840	3.417120	-3.126070
H	2.187692	3.886244	-1.532447
H	3.940141	3.856167	-1.823422

TS45Me′*cis*34syn

Lu	-0.136695	1.344681	0.207599
C	0.337372	4.257826	-0.438568
H	0.988109	5.064925	-0.107603
S	0.206323	-1.630892	0.069262
N	1.303070	-0.335415	0.119414
N	-1.142388	-0.613611	0.087701
C	0.152878	3.846488	1.669138
H	-0.648299	4.580255	1.634323
H	1.125760	4.264451	1.907498
C	-0.139014	2.597648	2.295573
H	0.601103	2.191206	2.981103
C	-1.490802	2.065460	2.344000
C	-2.406915	2.360745	1.369956
H	-3.395588	1.915870	1.381569
H	-2.266071	3.192121	0.681631
C	-1.829329	1.090563	3.444684
H	-2.710547	0.496617	3.195916
H	-0.999254	0.414002	3.671788
H	-2.043143	1.653714	4.362215
C	-0.990028	4.786205	-0.962232
H	-1.514408	5.317131	-0.157466
H	-1.660447	3.973896	-1.271284
C	-0.799413	5.751920	-2.146894
H	-0.172271	6.603235	-1.860458
H	-1.765269	6.144683	-2.481449
H	-0.322492	5.252984	-2.996885
C	1.066021	3.253184	-1.168168
C	0.467657	2.341909	-2.030332
H	-0.513575	2.539587	-2.459293
H	1.087732	1.633918	-2.573414
C	2.543841	3.116919	-0.843941
H	2.844593	2.081145	-0.650746
H	2.828781	3.724899	0.018896
H	3.134513	3.458939	-1.702380
C	0.271282	-2.396420	-1.570045
C	0.104110	-1.680957	-2.759746
C	0.500003	-3.778290	-1.588174
C	0.168262	-2.356757	-3.977715
H	-0.082794	-0.615070	-2.733746
C	0.557688	-4.448735	-2.813346
H	0.627601	-4.322907	-0.659416
C	0.393161	-3.739036	-4.003876
H	0.038548	-1.811589	-4.904927

H	0.729671	-5.517750	-2.834718
H	0.437481	-4.259154	-4.953012
C	2.647864	-0.661168	0.538772
C	3.689284	-0.749834	-0.427753
C	2.951551	-0.825301	1.920717
C	5.000109	-0.978367	0.010845
C	4.276691	-1.064017	2.301192
C	5.298023	-1.134106	1.359520
H	5.796528	-1.048822	-0.720014
H	4.511596	-1.197941	3.350247
H	6.318316	-1.317085	1.675158
C	-2.461054	-1.182436	0.090548
C	-3.374679	-0.752806	-0.914695
C	-2.906504	-2.084202	1.102652
C	-4.690517	-1.230842	-0.890964
C	-4.225151	-2.550381	1.058612
C	-5.117549	-2.129436	0.078352
H	-5.386620	-0.900424	-1.653002
H	-4.562350	-3.248405	1.814685
H	-6.136376	-2.497786	0.072715
C	1.885794	-0.792677	3.017564
H	0.948984	-0.443176	2.571814
C	3.442100	-0.676016	-1.936885
H	2.402599	-0.377248	-2.093987
C	-2.005701	-2.603795	2.229207
H	-1.117020	-1.969806	2.287742
C	-2.995696	0.206550	-2.046720
H	-1.939165	0.470247	-1.925328
C	3.652450	-2.074569	-2.575046
H	2.995247	-2.819610	-2.121677
H	3.441416	-2.033260	-3.649290
H	4.690556	-2.395735	-2.438577
C	4.370539	0.344429	-2.644061
H	4.106503	0.410371	-3.705840
H	4.291731	1.340720	-2.201629
H	5.416218	0.026894	-2.581628
C	1.647561	-2.215759	3.586511
H	2.567670	-2.597593	4.041114
H	0.865518	-2.194142	4.354872
H	1.342981	-2.906519	2.794332
C	2.262051	0.181308	4.162152
H	3.140386	-0.177736	4.707126
H	2.492402	1.179486	3.773417
H	1.435579	0.259536	4.878101

C	-1.564877	-4.062218	1.933558
H	-2.442455	-4.716954	1.917065
H	-1.069890	-4.140756	0.961011
H	-0.877406	-4.419472	2.708665
C	-2.695694	-2.558167	3.617032
H	-3.087810	-1.561314	3.835521
H	-3.522593	-3.272725	3.670946
H	-1.971547	-2.828266	4.394178
C	-3.159300	-0.474103	-3.429280
H	-4.209051	-0.730370	-3.604546
H	-2.838630	0.205929	-4.227894
H	-2.566243	-1.390587	-3.483241
C	-3.830419	1.511865	-1.997841
H	-3.519680	2.192320	-2.800402
H	-4.893552	1.292599	-2.137797
H	-3.716040	2.019859	-1.035338

5Me′*cis*34iso

Lu	0.069744	-1.249338	-0.016394
C	2.181792	-3.847349	-0.721746
H	2.545108	-4.822618	-1.077863
S	-0.470917	1.676934	0.345799
N	-1.457314	0.335962	0.057214
N	0.950484	0.750584	0.252434
C	1.344476	-4.189539	0.570763
H	2.015502	-4.812078	1.175564
H	0.513956	-4.844675	0.284357
C	0.821874	-3.066647	1.481503
H	1.465770	-2.867284	2.337187
C	-0.578877	-2.955464	1.753384
C	-1.540354	-3.061728	0.749077
H	-2.594300	-2.937310	0.974619
H	-1.329301	-3.642368	-0.154708
C	-1.012504	-2.477081	3.124373
H	-1.107850	-3.353651	3.778235
H	-0.274519	-1.814665	3.586841
H	-1.981848	-1.972289	3.101715
C	3.416909	-2.990367	-0.384782
H	3.860894	-3.404381	0.528606
H	3.124914	-1.964148	-0.111552
C	4.484796	-2.961257	-1.485531
H	4.857292	-3.971860	-1.688964
H	5.339670	-2.350145	-1.179297
H	4.104309	-2.553073	-2.427922

C	1.289320	-3.323587	-1.835056
C	1.242455	-2.021532	-2.227383
H	1.995618	-1.297841	-1.912457
H	0.617522	-1.719652	-3.066925
C	0.426005	-4.346898	-2.528370
H	-0.356327	-3.890101	-3.140755
H	-0.034420	-5.050169	-1.827295
H	1.066609	-4.944478	-3.191311
C	-0.555010	2.744831	-1.110508
C	-0.513187	2.261768	-2.421929
C	-0.665955	4.116504	-0.850589
C	-0.580336	3.162819	-3.483417
H	-0.441464	1.197598	-2.608324
C	-0.733010	5.013358	-1.920913
H	-0.704352	4.477463	0.171292
C	-0.690228	4.536767	-3.232153
H	-0.552165	2.799740	-4.503722
H	-0.821941	6.075454	-1.729122
H	-0.745178	5.232041	-4.060944
C	-2.880888	0.510427	0.046105
C	-3.592153	1.016804	1.169466
C	-3.596265	0.086839	-1.108903
C	-4.982565	1.150240	1.082485
C	-4.989463	0.217718	-1.131251
C	-5.682076	0.760206	-0.054769
H	-5.527859	1.552810	1.927735
H	-5.538110	-0.105600	-2.008072
H	-6.759388	0.866922	-0.096188
C	2.147089	1.358283	0.779572
C	3.141595	1.825359	-0.121002
C	2.367231	1.433403	2.183267
C	4.330852	2.350992	0.398328
C	3.567455	1.981425	2.649063
C	4.545469	2.435757	1.769433
H	5.093321	2.708604	-0.283361
H	3.740640	2.050377	3.716396
H	5.468740	2.854521	2.151956
C	-2.914543	1.420238	2.483534
H	-1.866960	1.110015	2.449316
C	-2.919781	-0.544890	-2.328185
H	-1.834736	-0.506815	-2.166523
C	1.342321	0.957263	3.215038
H	0.529090	0.449645	2.684750
C	2.966333	1.790900	-1.639505

H	1.987105	1.355824	-1.852714
C	-3.233566	0.235547	-3.628546
H	-2.695987	-0.206619	-4.476177
H	-4.304329	0.192172	-3.851066
H	-2.944675	1.285560	-3.531263
C	-3.334345	-2.031383	-2.481185
H	-2.815875	-2.487778	-3.334027
H	-3.103754	-2.599634	-1.574504
H	-4.411448	-2.107672	-2.661019
C	-3.560518	0.708285	3.699317
H	-3.008554	0.959127	4.612363
H	-4.599460	1.023568	3.835175
H	-3.546370	-0.378394	3.568166
C	-2.967698	2.957155	2.679005
H	-2.497005	3.477964	1.838193
H	-4.008068	3.292336	2.743951
H	-2.452077	3.243317	3.602399
C	0.738920	2.160042	3.984305
H	0.264275	2.865872	3.295476
H	-0.011432	1.813716	4.704695
H	1.524331	2.690244	4.532771
C	1.963583	-0.058270	4.206741
H	2.387891	-0.916260	3.674318
H	2.760499	0.408481	4.793347
H	1.199755	-0.417194	4.906252
C	4.056366	0.917006	-2.310044
H	4.057615	-0.100436	-1.903730
H	3.887693	0.864436	-3.392001
H	5.050809	1.343871	-2.143209
C	2.992942	3.222070	-2.232278
H	2.826243	3.183346	-3.314552
H	2.214159	3.844029	-1.782664
H	3.964012	3.695247	-2.052112

5Me′*cis*34syn

Lu	-0.591281	-0.961833	-0.519688
C	-3.917052	-2.503797	-0.220898
H	-4.226930	-3.544887	-0.381078
S	1.235896	1.260664	0.177870
N	1.410539	-0.428299	0.118515
N	-0.422461	1.210625	-0.187441
C	-3.153074	-2.060632	-1.486102
H	-2.942770	-0.969948	-1.395650
H	-3.813594	-2.103077	-2.365659

C	-1.896470	-2.890008	-1.689155
H	-1.975270	-3.930920	-1.383707
C	-0.848633	-2.542455	-2.536081
C	-0.619309	-1.192595	-2.934466
H	0.243446	-0.986666	-3.562728
H	-1.481033	-0.567295	-3.176120
C	0.226530	-3.570374	-2.832992
H	1.233718	-3.146359	-2.744443
H	0.156130	-4.449969	-2.185943
H	0.117354	-3.906828	-3.871427
C	-5.194402	-1.666487	0.016407
H	-5.785910	-1.694766	-0.907418
H	-4.917558	-0.614827	0.171373
C	-6.054704	-2.152198	1.187160
H	-6.364131	-3.194930	1.048290
H	-6.962954	-1.547781	1.274411
H	-5.520024	-2.080645	2.141600
C	-2.958330	-2.491983	0.972411
C	-2.391519	-1.342902	1.424482
H	-2.731901	-0.367005	1.077367
H	-1.797924	-1.337442	2.336755
C	-2.729153	-3.803870	1.668658
H	-2.010509	-3.727284	2.488525
H	-2.395034	-4.578810	0.969603
H	-3.685648	-4.152609	2.081757
C	1.440151	1.757424	1.904447
C	0.824756	1.109881	2.981076
C	2.280004	2.858513	2.112449
C	1.059470	1.565012	4.276822
H	0.173882	0.262598	2.808247
C	2.505249	3.312761	3.415355
H	2.753260	3.351037	1.270224
C	1.898730	2.665852	4.492958
H	0.590846	1.068635	5.117960
H	3.153627	4.163447	3.584436
H	2.077279	3.015760	5.502406
C	2.734310	-0.978791	0.219064
C	2.987174	-1.903421	1.269730
C	3.745195	-0.697511	-0.736859
C	4.251885	-2.490466	1.368620
C	5.002163	-1.295806	-0.579055
C	5.262508	-2.177155	0.463670
H	4.453355	-3.196465	2.163862
H	5.783520	-1.077331	-1.297294

H	6.241880	-2.629621	0.563329
C	-1.025360	2.472626	-0.550552
C	-1.929940	3.091136	0.354045
C	-0.777694	3.066274	-1.820383
C	-2.567710	4.277411	-0.028058
C	-1.430541	4.261040	-2.144780
C	-2.320629	4.865383	-1.263105
H	-3.260660	4.749712	0.658097
H	-1.241282	4.721842	-3.106824
H	-2.817354	5.788440	-1.537532
C	3.525266	0.188291	-1.966752
H	2.499154	0.560744	-1.960112
C	1.873640	-2.338084	2.221835
H	1.169125	-1.507988	2.307749
C	0.181980	2.472909	-2.852984
H	0.513702	1.494068	-2.496674
C	-2.244449	2.521197	1.737364
H	-1.657934	1.608603	1.863521
C	2.368668	-2.685533	3.644042
H	2.950686	-1.859033	4.062888
H	1.510281	-2.875972	4.298423
H	2.989490	-3.587069	3.644237
C	1.126799	-3.551637	1.607757
H	0.321693	-3.895304	2.266915
H	0.689381	-3.302313	0.627022
H	1.824518	-4.379478	1.444012
C	4.481767	1.406219	-1.962132
H	5.525243	1.077188	-1.995591
H	4.292986	2.038291	-2.836026
H	4.342505	2.008915	-1.057966
C	3.700989	-0.638306	-3.266913
H	4.720930	-1.026878	-3.347083
H	3.009379	-1.487941	-3.283046
H	3.503386	-0.008605	-4.142049
C	1.425312	3.382465	-3.026778
H	1.125130	4.370208	-3.391675
H	1.952917	3.513209	-2.076671
H	2.118262	2.943284	-3.753551
C	-0.515036	2.259795	-4.220617
H	-1.411089	1.640399	-4.112978
H	-0.811571	3.217065	-4.660899
H	0.171735	1.765866	-4.917265
C	-1.832325	3.513824	2.853415
H	-2.403827	4.443885	2.769826

H	-2.031246	3.077336	3.838903
H	-0.767415	3.753048	2.786910
C	-3.749743	2.172008	1.864022
H	-3.953658	1.706798	2.835400
H	-4.361484	3.076360	1.785225
H	-4.068884	1.486474	1.069808

$Al^{i}Bu_3$

C	1.229837	14.530125	11.719913
H	1.547066	15.343593	11.045772
H	2.171311	14.010931	11.976252
Al	0.138627	13.227791	10.686139
C	0.627998	15.143376	13.004021
H	0.322415	14.322737	13.671304
C	-0.625819	15.974445	12.689808
H	-0.384304	16.801947	12.009097
H	-1.405278	15.365741	12.211943
H	-1.060792	16.409295	13.597894
C	1.657809	15.995267	13.765284
H	2.543115	15.404447	14.029368
H	1.994651	16.839560	13.149016
H	1.238371	16.405676	14.693101
C	0.637131	12.859642	8.793756
H	1.344758	13.631807	8.450700
H	1.215799	11.919639	8.776768
C	-1.372448	12.249768	11.538951
H	-1.356765	12.437117	12.624846
H	-2.312827	12.709387	11.188836
C	-1.448683	10.723100	11.296974
H	-1.505986	10.545519	10.212062
C	-0.516184	12.748220	7.768084
H	-1.195948	11.947210	8.096418
C	-0.000078	12.368675	6.369856
H	0.550831	11.421007	6.395411
H	-0.821963	12.261261	5.650009
H	0.682228	13.138623	5.985775
C	-1.332712	14.048790	7.700122
H	-1.790945	14.293919	8.669237
H	-0.695726	14.895286	7.411144
H	-2.145154	13.979158	6.966670
C	-0.189981	10.010343	11.816822
H	-0.061704	10.180326	12.894149
H	-0.241490	8.926692	11.655592
H	0.719261	10.369682	11.313407

C	-2.709332	10.110434	11.930125
H	-2.779359	9.032700	11.733327
H	-2.704460	10.252099	13.019063
H	-3.617883	10.583416	11.538850

$(PhNSN^{dipp})Lu(CH_2SiMe_3)^+$

Lu	3.756641	13.413561	10.019015
S	5.595594	14.211354	7.806130
Si	2.044254	11.268398	11.370040
N	5.335882	14.831585	9.355702
N	4.392534	13.031362	7.995349
C	3.904906	11.453422	11.208955
H	4.327247	10.640643	10.602435
H	4.392094	11.418813	12.190956
C	1.306409	9.706994	10.613158
H	1.639818	9.558670	9.579569
H	0.210454	9.729196	10.615078
H	1.623524	8.828468	11.187194
C	1.256914	12.735124	10.288398
H	1.382500	13.777883	10.651815
H	0.171573	12.595480	10.349488
H	1.458230	12.702577	9.199820
C	1.416741	11.583930	13.123204
H	1.728041	10.767059	13.784954
H	0.322894	11.643022	13.162545
H	1.815035	12.513569	13.549214
C	7.195192	13.373910	7.860152
C	7.658322	12.707535	8.999209
H	7.070166	12.702131	9.909266
C	8.894380	12.065227	8.953480
H	9.267200	11.550077	9.830314
C	9.657789	12.092027	7.779537
H	10.619448	11.594301	7.752274
C	9.189904	12.761655	6.647067
H	9.784300	12.783956	5.742084
C	7.951991	13.409945	6.681600
H	7.582921	13.936466	5.808339
C	6.196324	15.792182	9.961616
C	6.809578	16.885709	9.298233
C	7.674925	17.710460	10.031453
H	8.165511	18.532166	9.523616
C	7.896378	17.525855	11.390018
H	8.569739	18.180648	11.929105
C	7.213638	16.513772	12.061641

H	7.350312	16.398763	13.128816
C	6.363501	15.649086	11.372855
C	5.546208	14.603056	12.121092
H	5.590941	13.656225	11.547322
C	6.066595	14.240920	13.529923
H	7.115163	13.933292	13.484160
H	5.478900	13.412769	13.940840
H	5.976796	15.091520	14.212779
C	4.067387	15.093720	12.244184
H	4.032169	15.921437	12.959718
H	3.399337	14.307666	12.632189
H	3.676125	15.534504	11.305820
C	6.511938	17.288449	7.848552
H	5.773192	16.604269	7.427124
C	7.780708	17.242209	6.961393
H	8.528789	17.953021	7.327196
H	7.529688	17.514432	5.929996
H	8.230411	16.244168	6.965616
C	5.872187	18.701968	7.808909
H	6.574573	19.456335	8.176474
H	4.970731	18.738294	8.429246
H	5.601288	18.958897	6.778654
C	3.789206	12.514001	6.796374
C	2.817584	13.279650	6.093047
C	2.216772	12.718733	4.961016
H	1.483160	13.292313	4.407023
C	2.541787	11.433179	4.534401
H	2.063290	11.017166	3.655705
C	3.478370	10.683891	5.239654
H	3.721777	9.682512	4.905051
C	4.119866	11.202265	6.371212
C	5.140779	10.335439	7.109670
H	5.542281	10.920920	7.940090
C	6.316817	9.940740	6.181433
H	5.961055	9.343628	5.335477
H	7.047049	9.343662	6.739002
H	6.821928	10.829820	5.793159
C	4.464758	9.066191	7.687825
H	4.057621	8.443417	6.884290
H	3.644056	9.331786	8.363249
H	5.195774	8.470352	8.245986
C	2.420880	14.698994	6.510648
H	2.868926	14.906517	7.491152
C	2.976933	15.743559	5.508518

H	4.067677	15.677912	5.441387
H	2.703093	16.757002	5.822758
H	2.560668	15.565360	4.511584
C	0.886057	14.854812	6.652671
H	0.389910	14.717612	5.687094
H	0.643549	15.859895	7.015657
H	0.474667	14.117847	7.351637

$(NPN^{dipp})Lu(CH_2SiMe_3)^+$

Lu	14.761057	9.664417	5.723333
N	12.949874	8.639102	5.061546
N	13.777435	10.841431	4.194812
P	12.619653	9.695115	3.809096
Si	17.311166	9.564616	7.372775
C	15.636159	10.308104	7.758587
H	15.721134	11.395121	7.893371
H	15.222337	9.898893	8.687882
C	17.178508	8.849196	5.510234
H	16.530159	7.965657	5.330704
H	18.178436	8.452575	5.301458
H	17.031667	9.580747	4.688237
C	18.729498	10.802794	7.253205
H	18.483589	11.643849	6.593447
H	19.650861	10.340673	6.879880
H	18.943646	11.220500	8.243907
C	17.742237	8.044858	8.402775
H	17.926283	8.341173	9.442176
H	18.643925	7.540552	8.036442
H	16.928317	7.309477	8.416084
C	12.179083	7.494746	5.486488
C	11.234134	7.655991	6.541354
C	10.496773	6.543960	6.961555
H	9.771765	6.657493	7.757432
C	10.687157	5.289935	6.385828
H	10.101651	4.442351	6.721587
C	11.652626	5.127189	5.399691
H	11.825665	4.143007	4.981533
C	12.416660	6.208730	4.940305
C	13.549639	5.935758	3.951993
H	13.896284	6.890227	3.559179
C	13.106110	5.078125	2.744012
H	12.797735	4.076115	3.059106
H	13.939706	4.969538	2.041749
H	12.272409	5.553759	2.219073

C	14.726983	5.255812	4.699841
H	15.073658	5.877738	5.536889
H	15.567472	5.080250	4.018101
H	14.409747	4.293624	5.114862
C	11.089271	8.979720	7.298379
H	11.411875	9.790683	6.641109
C	9.644031	9.292056	7.752308
H	8.947996	9.271824	6.908950
H	9.612477	10.292478	8.198120
H	9.300490	8.580706	8.510045
C	12.024144	8.949292	8.537137
H	11.722204	8.140118	9.210271
H	11.977365	9.899665	9.081006
H	13.066974	8.773177	8.246552
C	13.721882	12.256084	3.906332
C	13.083213	13.139867	4.822679
C	13.076351	14.511631	4.540835
H	12.588355	15.188751	5.231792
C	13.684079	15.023042	3.398972
H	13.664338	16.088062	3.200889
C	14.328174	14.157940	2.520860
H	14.817317	14.557059	1.640118
C	14.365508	12.777686	2.753914
C	15.128438	11.894873	1.768294
H	15.005281	10.859764	2.081889
C	14.561502	12.016067	0.332420
H	13.501209	11.743551	0.310648
H	15.103119	11.343836	-0.342145
H	14.665777	13.038294	-0.045400
C	16.640803	12.233305	1.791436
H	16.810440	13.266916	1.472710
H	17.188707	11.571129	1.111127
H	17.053153	12.120612	2.801579
C	12.424129	12.678694	6.126463
H	12.481253	11.585669	6.176147
C	10.926515	13.071663	6.193743
H	10.820243	14.161304	6.215701
H	10.477689	12.669914	7.109504
H	10.377830	12.685620	5.332406
C	13.172912	13.261800	7.352783
H	14.234199	12.996649	7.335337
H	12.733818	12.878976	8.280978
H	13.094228	14.353618	7.359683
C	10.927809	10.330929	3.665739

C	9.830459	9.593410	4.147352
H	9.987172	8.671449	4.690951
C	8.531027	10.051483	3.918463
H	7.689666	9.478436	4.289302
C	8.315401	11.235056	3.209522
H	7.305241	11.585022	3.034107
C	9.401975	11.964691	2.718572
H	9.236874	12.880541	2.164107
C	10.705243	11.517487	2.936027
H	11.538013	12.089657	2.547299
C	12.936242	8.940646	2.177346
C	11.891651	8.701135	1.268163
H	10.879931	8.993151	1.516124
C	12.153386	8.090799	0.037498
H	11.339787	7.913572	-0.655270
C	13.453896	7.717090	-0.299033
H	13.654840	7.249495	-1.255284
C	14.502175	7.948266	0.599554
H	15.513813	7.660941	0.338798
C	14.244663	8.550170	1.828264
H	15.070248	8.727286	2.510295

NSN-Lu-Al

Lu	3.066630	14.204842	9.942491
S	5.365223	15.630424	8.669793
Si	3.515845	10.626152	12.364548
N	4.686554	15.659545	10.225311
N	4.322179	14.386589	8.159959
C	3.181548	12.178636	11.265842
C	2.961052	10.955833	14.140606
H	3.471955	11.831658	14.559040
H	3.215386	10.098571	14.776025
H	1.882807	11.121551	14.233025
C	5.393320	10.360593	12.356309
H	5.775124	10.188006	11.342079
H	5.664080	9.484283	12.958001
H	5.929779	11.220558	12.777243
C	2.683839	9.107913	11.613904
H	1.592646	9.185480	11.595072
H	2.940211	8.212845	12.193861
H	3.025331	8.936409	10.585482
C	7.027704	14.939177	8.774123
C	7.367109	13.849072	9.582979
H	6.625362	13.391089	10.224404

C	8.676111	13.370421	9.565987
H	8.951735	12.530923	10.192523
C	9.635074	13.974213	8.742032
H	10.650423	13.596994	8.733263
C	9.290018	15.060685	7.936426
H	10.033284	15.527871	7.302463
C	7.981664	15.551803	7.951367
H	7.706969	16.399259	7.333140
C	5.041755	16.755097	11.090821
C	4.648622	18.088020	10.788492
C	4.996559	19.111639	11.676737
H	4.710636	20.131469	11.447323
C	5.685886	18.845072	12.855469
H	5.944313	19.652528	13.530073
C	6.024819	17.533987	13.170623
H	6.539847	17.327042	14.101192
C	5.717314	16.474117	12.308938
C	6.079982	15.056357	12.753040
H	5.811320	14.372973	11.943931
C	7.596458	14.906255	13.025972
H	8.178064	15.157980	12.134702
H	7.825660	13.873593	13.315411
H	7.910603	15.562707	13.843711
C	5.263209	14.659215	14.010710
H	5.516021	15.309441	14.854352
H	5.485473	13.624394	14.298809
H	4.185865	14.750421	13.826996
C	3.822005	18.461185	9.555134
H	3.612059	17.553652	8.983097
C	4.594254	19.437350	8.633596
H	4.814829	20.370009	9.162503
H	3.995454	19.678716	7.748780
H	5.541446	18.996876	8.305452
C	2.458262	19.069135	9.972731
H	2.603858	20.004745	10.521234
H	1.905894	18.379374	10.620668
H	1.851828	19.282538	9.085045
C	4.311851	14.051810	6.760897
C	3.708706	14.917853	5.808286
C	3.648017	14.509231	4.471305
H	3.194140	15.163991	3.736586
C	4.148677	13.274509	4.068737
H	4.086748	12.975648	3.029063
C	4.724160	12.424662	5.007420

H	5.105862	11.461764	4.689764
C	4.825121	12.791341	6.354763
C	5.448517	11.800819	7.339075
H	5.544508	12.305200	8.303220
C	6.863738	11.358953	6.893578
H	6.824204	10.813926	5.945033
H	7.301382	10.694133	7.647175
H	7.519963	12.225450	6.771383
C	4.527243	10.566479	7.518902
H	4.411324	10.033232	6.569440
H	3.528533	10.867261	7.857967
H	4.954709	9.871686	8.252331
C	3.108682	16.276754	6.176808
H	3.226042	16.430583	7.253019
C	3.849063	17.426766	5.448938
H	4.917941	17.414735	5.685993
H	3.435020	18.395189	5.750286
H	3.736621	17.328570	4.364400
C	1.592443	16.324077	5.859925
H	1.419048	16.204895	4.785925
H	1.170609	17.286899	6.170494
H	1.058430	15.520889	6.379940
C	1.390845	14.791416	11.660209
H	1.317950	15.539987	10.825872
H	2.388659	14.975320	12.121469
Al	1.102590	12.731404	11.091792
H	3.867810	12.882480	11.788092
H	3.708083	11.854201	10.341652
C	0.368251	15.298670	12.715399
H	0.339921	14.558686	13.528068
C	-1.045017	15.415078	12.127272
H	-1.067214	16.142105	11.304871
H	-1.413264	14.458404	11.741832
H	-1.753388	15.757629	12.889161
C	0.809300	16.639417	13.326674
H	1.800235	16.565498	13.789554
H	0.857409	17.422928	12.559350
H	0.102623	16.970684	14.096082
C	1.086399	12.983673	8.971235
H	1.235181	14.027610	8.581510
H	1.908461	12.399467	8.508729
C	-0.273365	11.747488	12.139253
H	0.233230	10.979661	12.741376
H	-0.622890	12.484454	12.879117

C	-1.516009	11.091927	11.480029
H	-1.929432	11.776009	10.725617
C	-0.220942	12.548709	8.245314
H	-0.554015	11.601838	8.686231
C	0.026247	12.299052	6.748176
H	0.777889	11.516864	6.590947
H	-0.895941	11.983496	6.246735
H	0.385254	13.207850	6.248820
C	-1.336644	13.584965	8.442749
H	-1.540776	13.779792	9.501282
H	-1.066560	14.540638	7.973027
H	-2.270226	13.244883	7.982038
C	-1.161783	9.772371	10.778051
H	-0.829178	9.024666	11.509832
H	-2.030389	9.354782	10.256147
H	-0.357726	9.891623	10.040822
C	-2.620158	10.846714	12.523504
H	-3.502826	10.380686	12.069353
H	-2.262385	10.180192	13.318763
H	-2.940596	11.784016	12.993179

NPN-Lu-Al

Lu	13.723700	7.165398	4.996498
N	12.239651	5.577606	5.393116
N	11.666028	7.832349	4.564813
P	10.922380	6.357110	4.742767
Si	15.830320	6.650842	1.202431
C	15.026070	6.751987	2.956609
C	14.519697	5.968825	0.013622
H	14.179721	4.969391	0.311986
H	14.935108	5.882157	-0.998118
H	13.642969	6.625186	-0.051018
C	16.299074	8.383864	0.608715
H	15.420498	9.040995	0.591020
H	16.685663	8.335659	-0.416805
H	17.065886	8.866347	1.223139
C	17.284423	5.449029	1.216317
H	18.097571	5.761949	1.876723
H	17.698385	5.350479	0.205262
H	16.962201	4.449511	1.533841
C	12.296654	4.324371	6.102542
C	12.127654	4.314415	7.520397
C	12.270196	3.104048	8.208261
H	12.145330	3.090004	9.284326

C	12.576766	1.920382	7.542556
H	12.680279	0.994638	8.095983
C	12.758296	1.938152	6.164995
H	13.007883	1.018999	5.648035
C	12.630141	3.121908	5.426511
C	12.887117	3.065182	3.921349
H	12.717342	4.061368	3.513154
C	11.907853	2.098439	3.211512
H	12.046818	1.072581	3.568230
H	12.084278	2.113673	2.130370
H	10.870699	2.394896	3.395128
C	14.355849	2.661713	3.630964
H	15.056733	3.349933	4.119135
H	14.546444	2.671145	2.550811
H	14.561690	1.653186	4.003622
C	11.851800	5.583553	8.336273
H	11.574241	6.380917	7.644108
C	10.693428	5.417220	9.350847
H	9.769938	5.121403	8.849647
H	10.516614	6.370455	9.862186
H	10.940196	4.669517	10.111172
C	13.129735	6.021943	9.098321
H	13.421605	5.250261	9.818783
H	12.950416	6.956613	9.643096
H	13.971727	6.168329	8.414612
C	11.092886	9.152112	4.504709
C	10.909722	9.895934	5.709127
C	10.435138	11.210296	5.624825
H	10.291849	11.778521	6.536650
C	10.146006	11.802835	4.399030
H	9.778104	12.821137	4.358751
C	10.339745	11.079372	3.227304
H	10.123751	11.542482	2.271516
C	10.815065	9.762083	3.253706
C	11.030496	9.038251	1.926460
H	11.401448	8.038095	2.147506
C	9.702210	8.882407	1.145706
H	8.963961	8.338209	1.743384
H	9.874999	8.322799	0.219829
H	9.286003	9.861363	0.885632
C	12.090255	9.768786	1.063260
H	11.754621	10.778258	0.804357
H	12.264331	9.218295	0.130888
H	13.041610	9.856555	1.602626

C	11.214759	9.334981	7.103299
H	11.529470	8.292906	6.991695
C	9.966641	9.347657	8.023281
H	9.631417	10.375156	8.199372
H	10.215031	8.900685	8.993027
H	9.146102	8.781013	7.579631
C	12.360005	10.122604	7.791859
H	13.262226	10.144738	7.172748
H	12.605379	9.666861	8.758406
H	12.055717	11.159123	7.970042
C	9.369639	6.328966	5.684877
C	8.973831	5.151670	6.349560
H	9.653809	4.312490	6.429076
C	7.695906	5.061305	6.904859
H	7.396527	4.153011	7.414206
C	6.803598	6.131178	6.795620
H	5.811338	6.053964	7.223585
C	7.185701	7.295304	6.124210
H	6.491470	8.121634	6.029336
C	8.459960	7.397399	5.562301
H	8.741871	8.297704	5.031265
C	10.407191	5.631704	3.141777
C	9.105337	5.136492	2.943018
H	8.380379	5.178254	3.743482
C	8.735361	4.586900	1.711949
H	7.728881	4.209845	1.576766
C	9.652780	4.527750	0.664214
H	9.363162	4.104676	-0.290105
C	10.950341	5.017279	0.848110
H	11.667931	4.975987	0.037839
C	11.324704	5.562012	2.074347
H	12.335502	5.932954	2.192933
C	15.050016	9.287481	4.820874
H	14.555014	9.269284	5.823871
H	14.212661	9.359710	4.090720
Al	16.345527	7.645055	4.399799
C	15.749538	10.676799	4.759785
H	16.364534	10.697102	3.848522
C	16.677551	10.894957	5.963687
H	16.107710	10.887338	6.902095
H	17.453491	10.125028	6.035989
H	17.181667	11.864824	5.892560
C	14.728787	11.822757	4.651210
H	14.080059	11.702709	3.775866

H	14.083254	11.862434	5.536908
H	15.236850	12.790179	4.564109
H	14.723212	5.697100	3.107315
H	14.110811	7.306940	2.650856
C	15.872809	6.362648	6.040096
H	15.468898	5.391546	5.683769
H	15.104414	6.734957	6.770067
C	18.210566	8.137792	3.893276
H	18.337511	7.959594	2.815917
H	18.221267	9.234934	3.986073
C	17.078447	6.028657	6.967649
H	17.948979	5.838638	6.329998
C	19.467170	7.582604	4.613619
H	19.305417	7.618593	5.699866
C	20.697137	8.457220	4.312224
H	20.904884	8.479196	3.234522
H	20.542328	9.490929	4.642780
H	21.592601	8.074431	4.816636
C	19.758665	6.125288	4.225337
H	20.600388	5.721974	4.800071
H	18.896704	5.466683	4.391776
H	20.025823	6.055169	3.163048
C	16.832629	4.754015	7.792417
H	16.647683	3.888710	7.145348
H	17.701857	4.523617	8.419284
H	15.964893	4.866119	8.453111
C	17.412641	7.214815	7.883918
H	18.303169	7.003967	8.485634
H	17.604243	8.133690	7.318239
H	16.585873	7.416729	8.578344