

Supporting Information for

Dearomatization Reactions of N-Heterocycles

Mediated by Group III Complexes

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Preparation of deuterated isoquinoline, adapted from Calf, G. E.; Garnett, J. L. *J. Phys. Chem.* 1964, 68, 3887-3889

1. Pt oxide must be activated first: 100 mg of Pt oxide was measured into a round bottom flask. 50 mL of water was added. While stirring, 400 mg of NaBH₄ was slowly added. The solution bubbled. The solution was then heated at 70 °C while open to the atmosphere for 30 min. The water was decanted off. The remaining black solid was washed with 5 mL of water and then 5 mL of D₂O.
2. 1 mL of isoquinoline, 6 mL of D₂O, a stir bar, and the activated Pt oxide were combined into a high-pressure glass vessel, which was then flame-sealed under vacuum. The solution was stirred overnight at 130 °C behind a blast shield.
3. Diethyl ether was used to extract isoquinoline from D₂O; this extraction was repeated 5 times. NaOH was added to help polarize the water and to help the extraction. The ether portion was dried over NaSO₄ and then filtered through a Buchner funnel. The volatiles were then removed by using a rotovap, until a yellow oil remained.

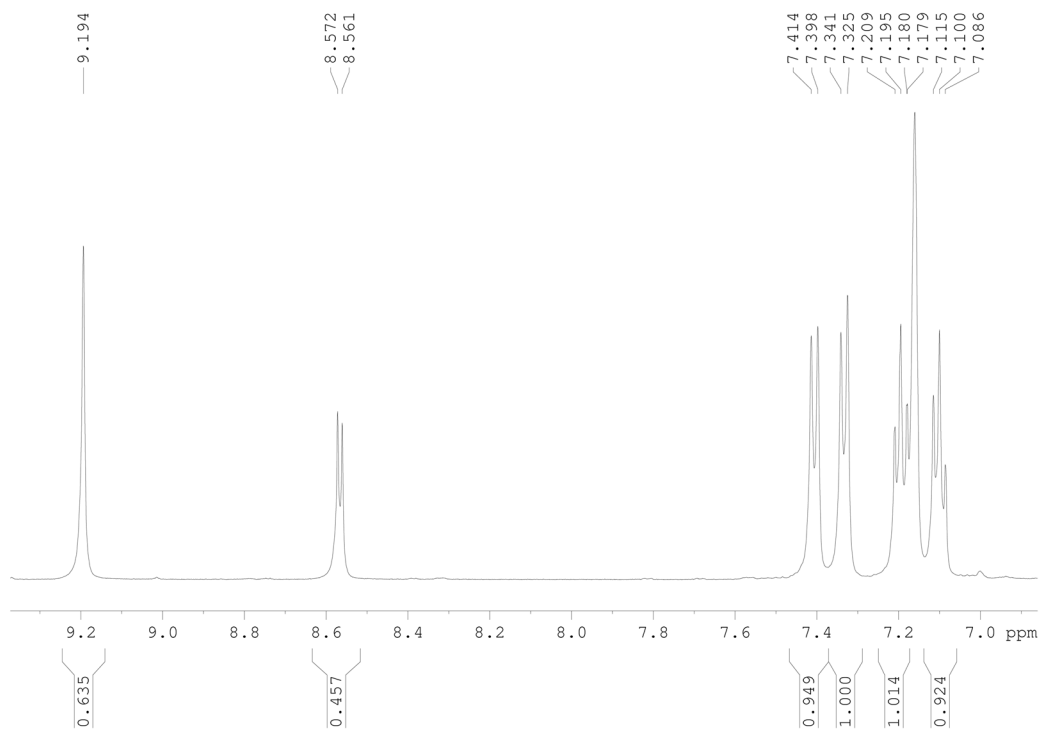
The deuterated isoquinoline was distilled over sodium, under vacuum. A clear oil resulted from the distillation. ¹H NMR spectroscopy showed deuterium incorporation at the 1-position (36%) and the 3-position (54%).

NMR spectra

Deuterated isoquinoline

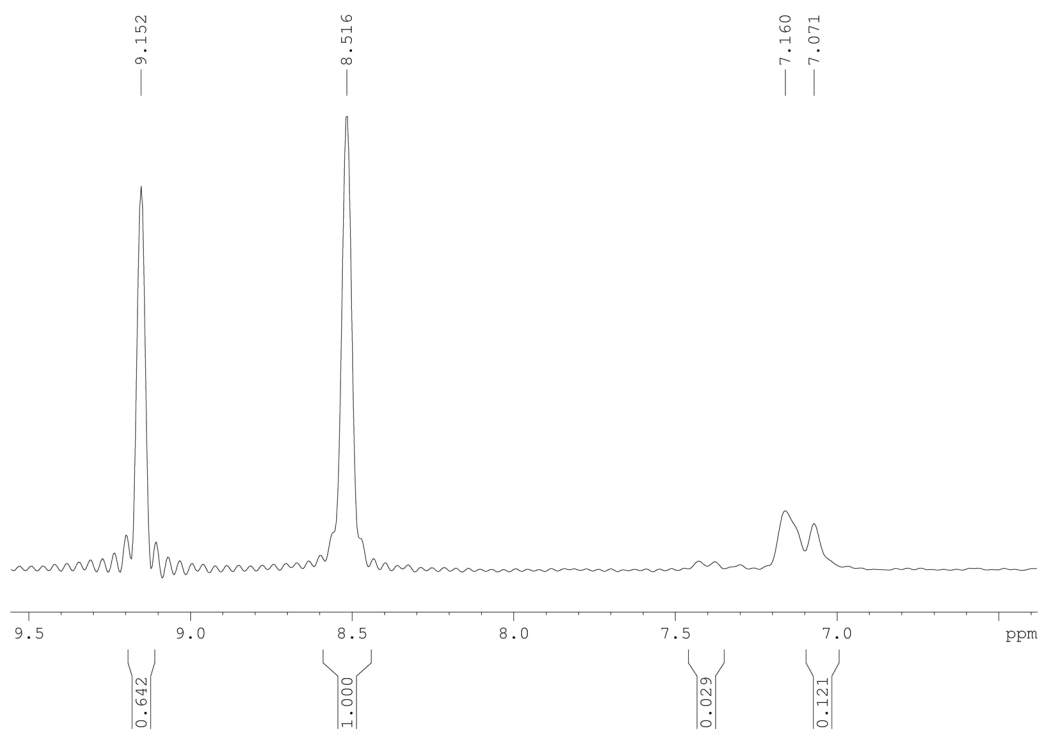
^1H NMR (500 MHz, C_6D_6)

deuterated isoquinoline in C_6D_6

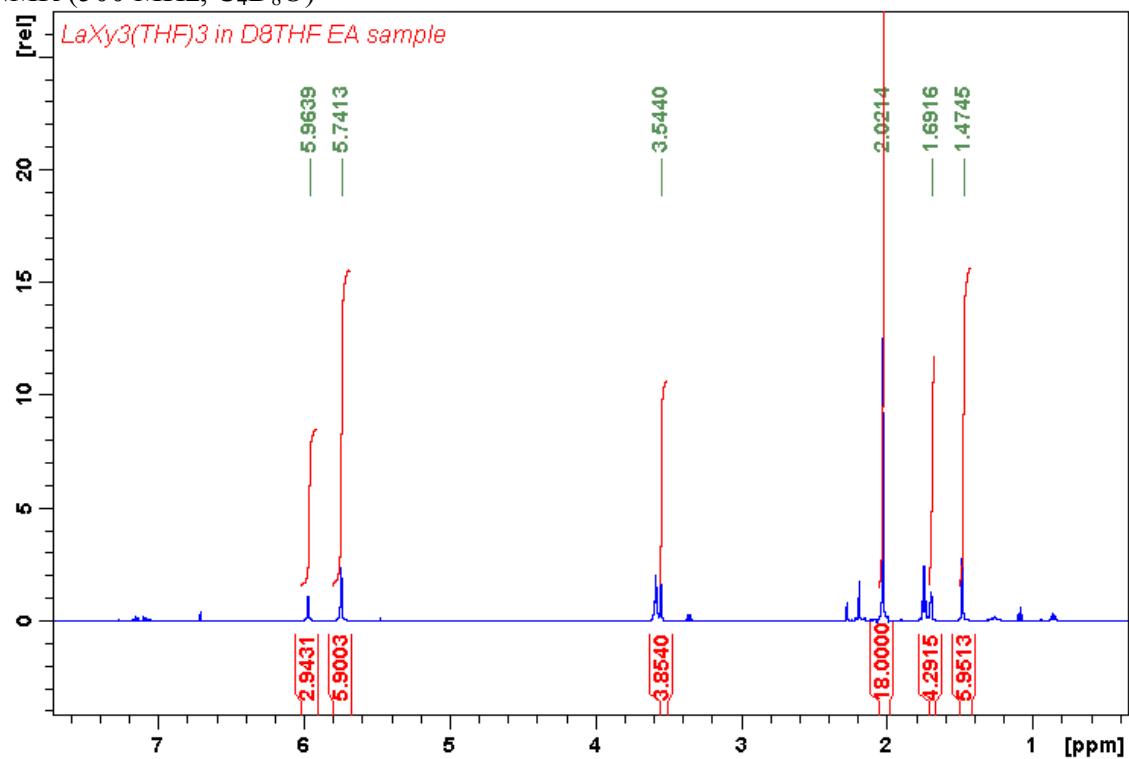


^2H NMR (500 MHz, C_6H_6)

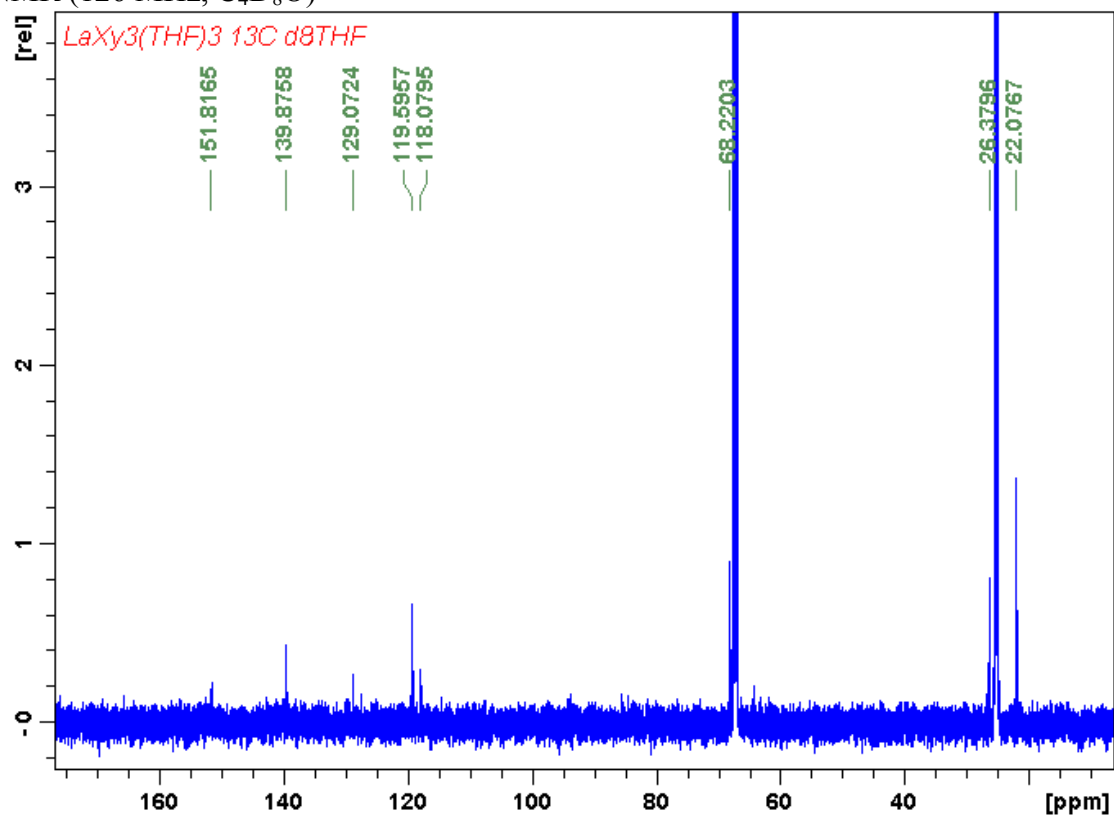
deuterated isoquinoline in C_6H_6



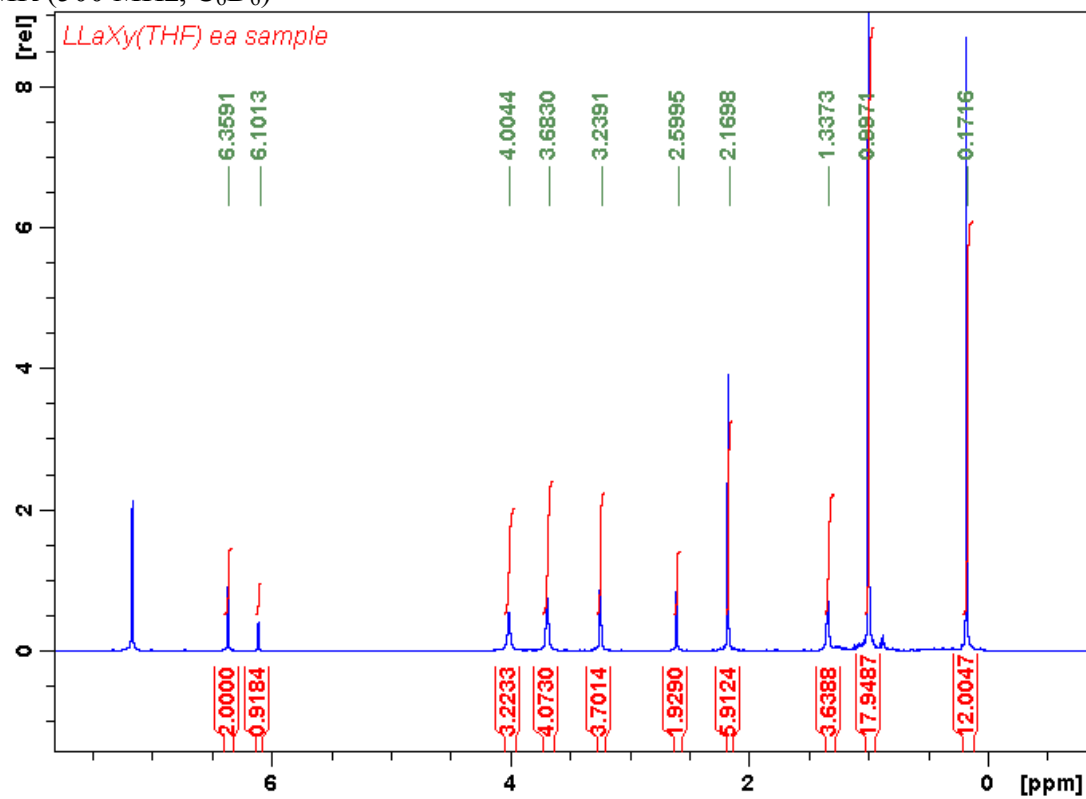
La(CH₂Ar)₃(THF)₃
¹H NMR (500 MHz, C₄D₈O)



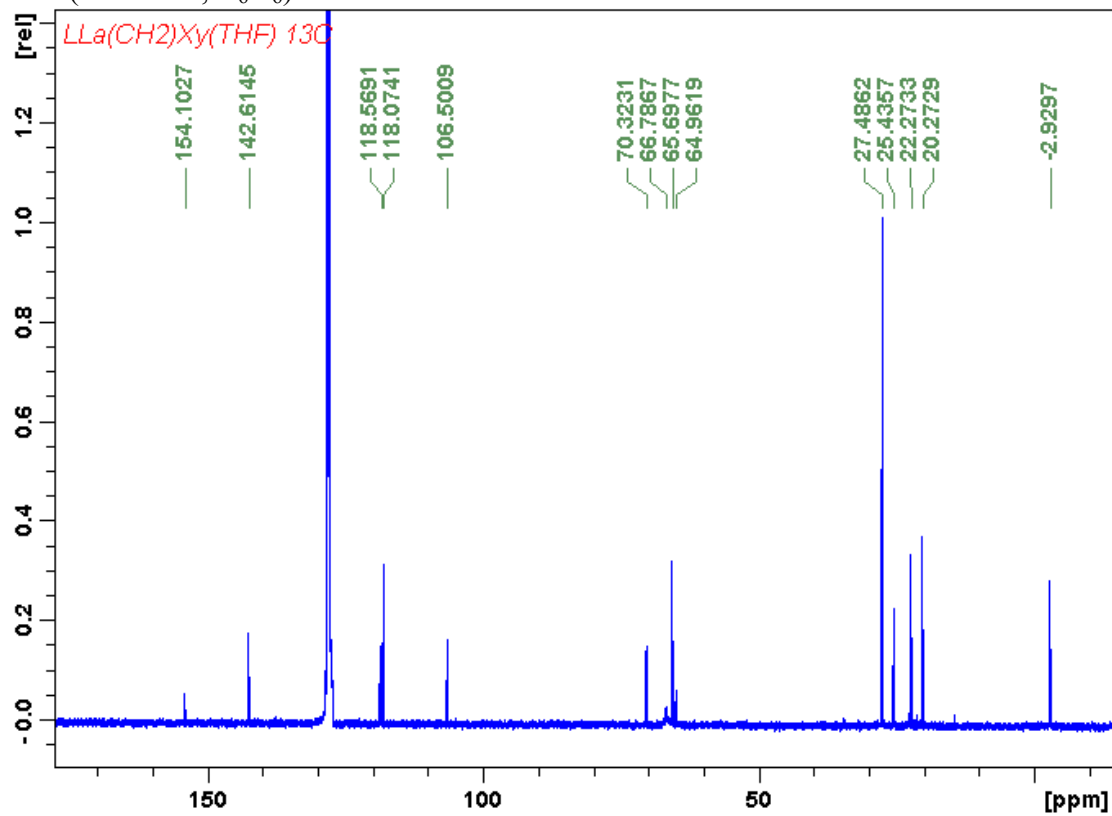
¹³C NMR (126 MHz, C₄D₈O)



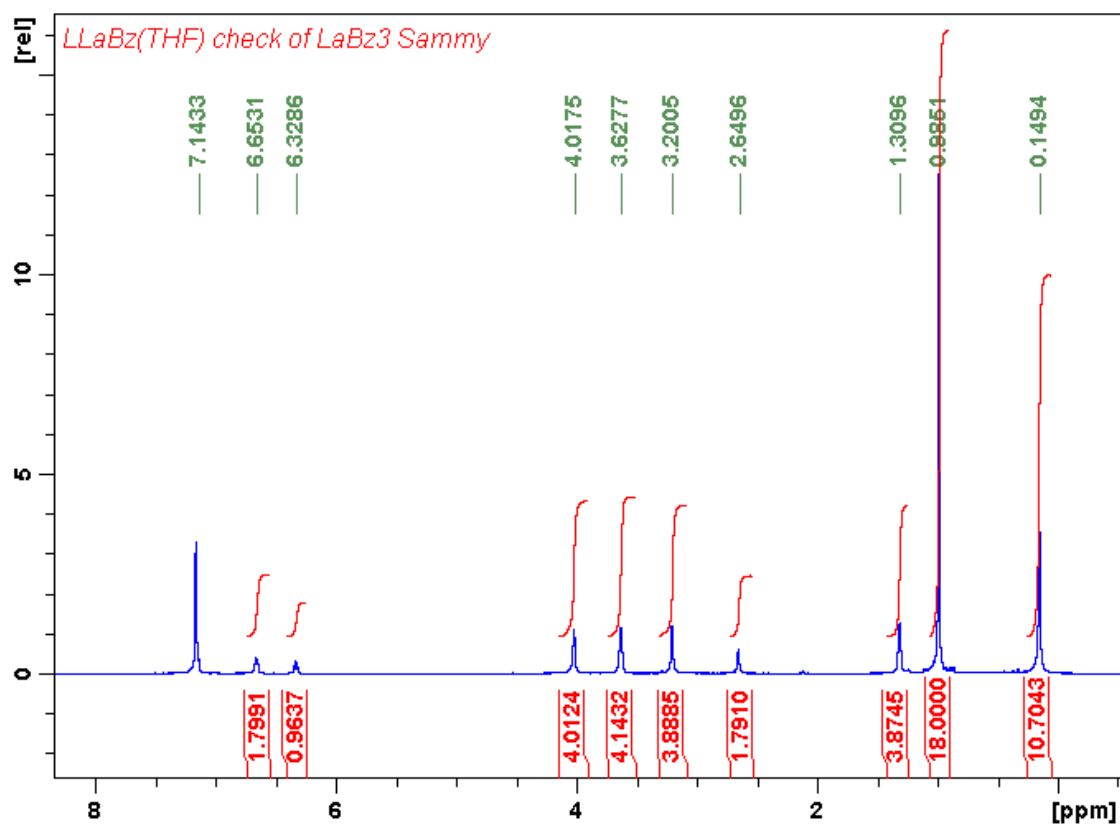
$1^{\text{La}}\text{-CH}_2\text{Ar}$ (Ar = 3,5-Me₂C₆H₃)
 ^1H NMR (500 MHz, C₆D₆)



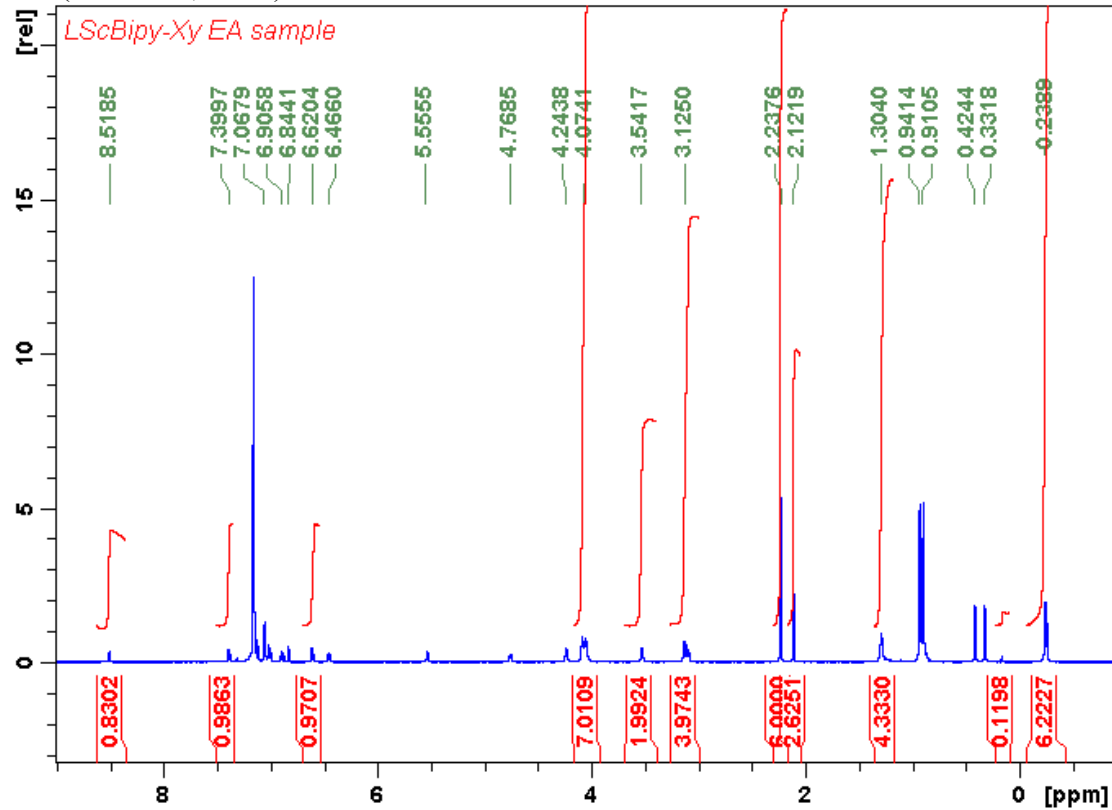
^{13}C NMR (126 MHz, C₆D₆)



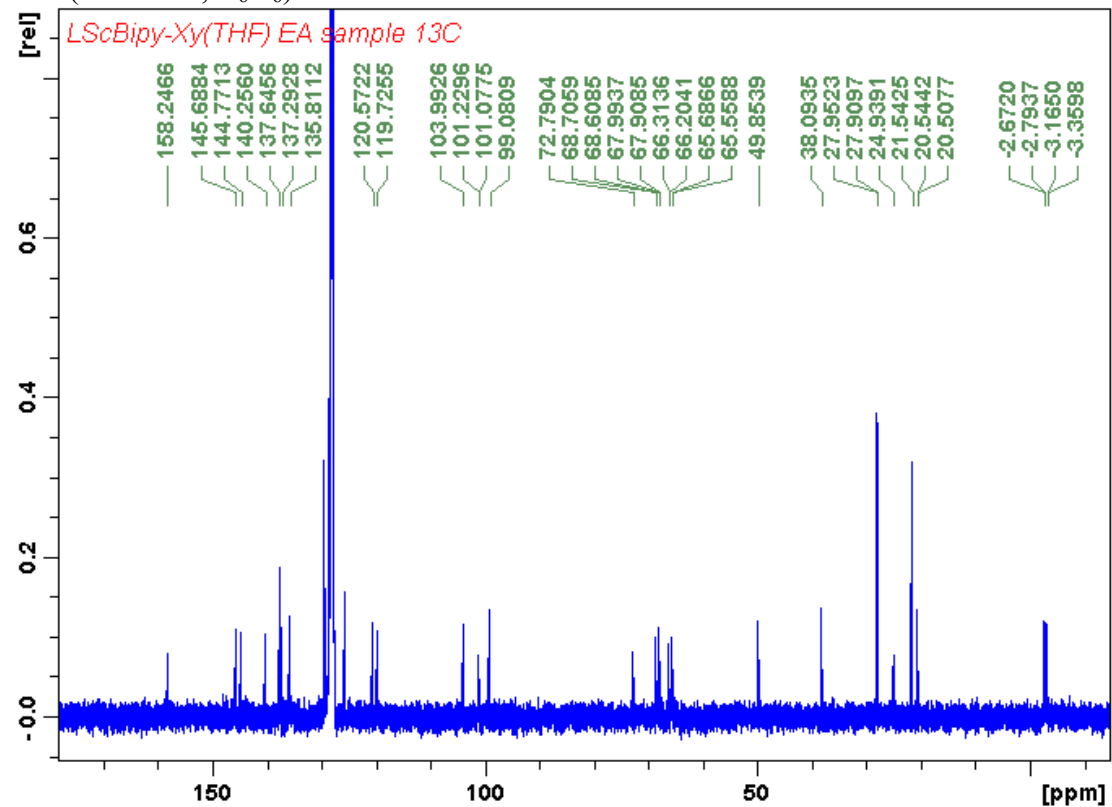
1^{La}-CH₂Ar (Ar = Ph)
¹H NMR (500 MHz, C₆D₆)



²Sc
¹H NMR (500 MHz, C₆D₆)

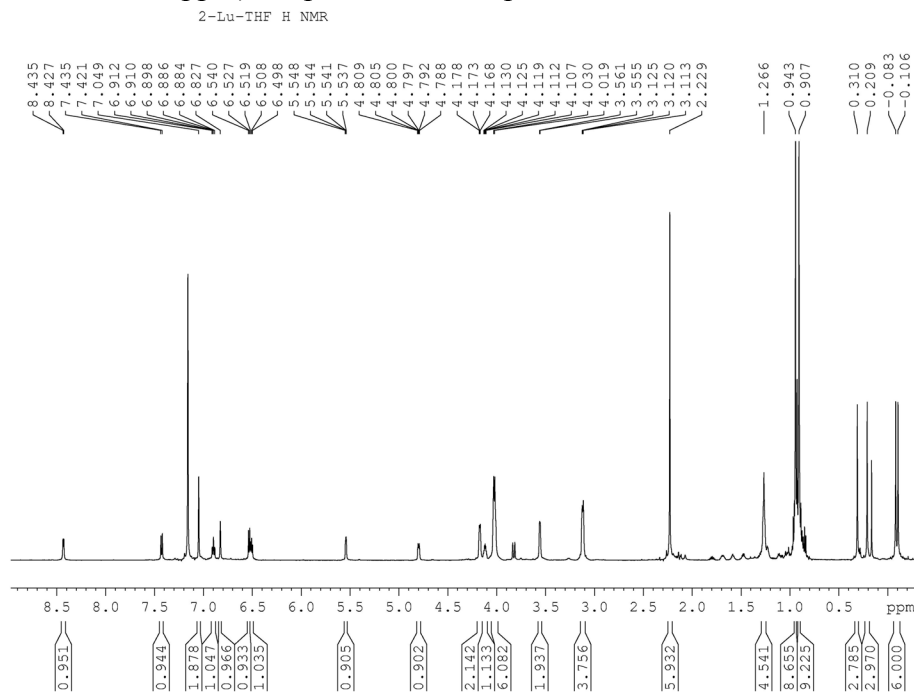


¹³C NMR (126 MHz, C₆D₆)

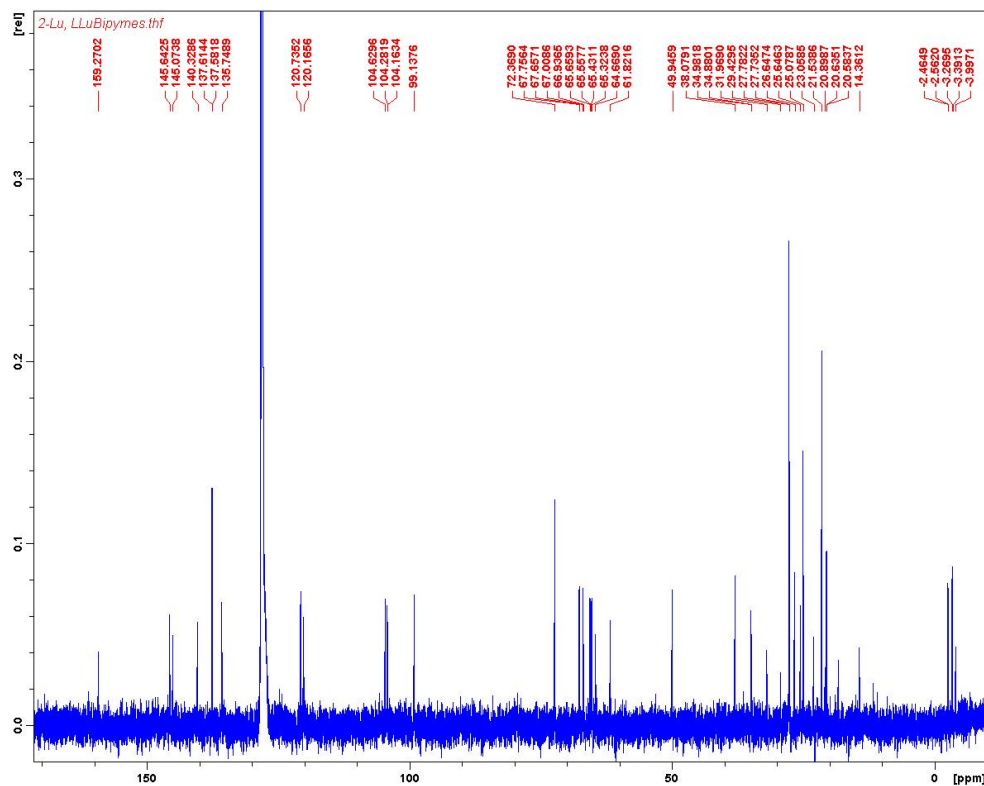


2^{Lu}

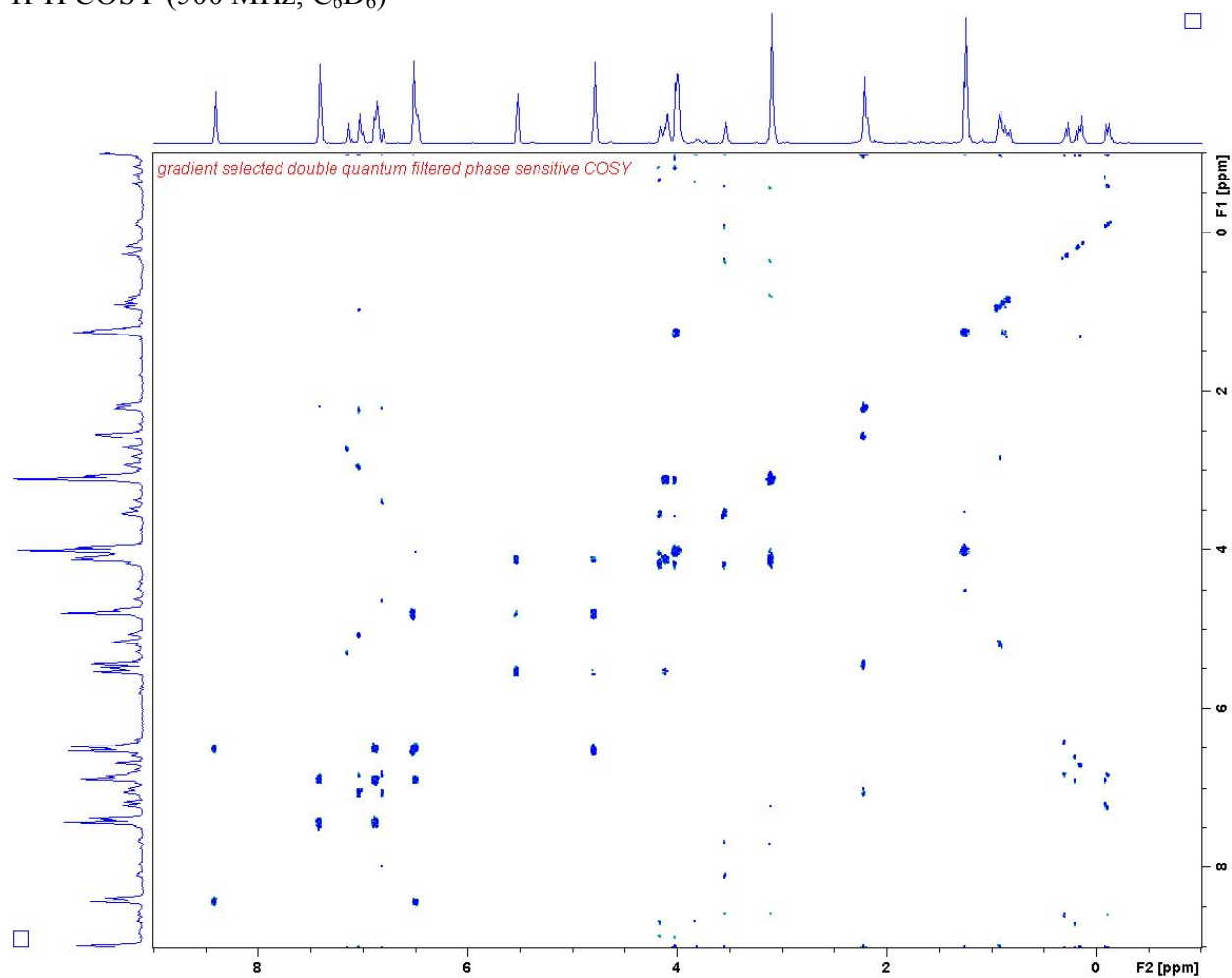
¹H NMR (600 MHz, C₆D₆) Peaks for hexanes (1.78, 1.69, 1.59, 1.47, 1.23, and 0.88) and free ligand (3.83, 0.92, and 0.16 ppm) are present in this spectrum.



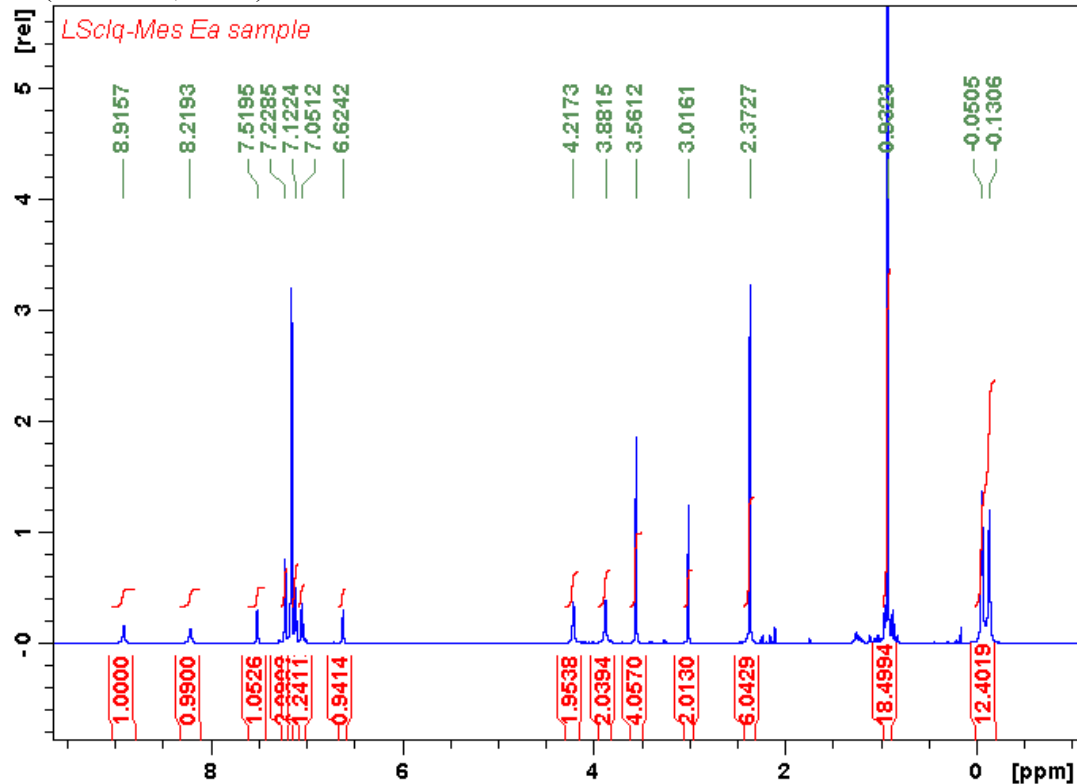
¹³C NMR (151 MHz, C₆D₆): Peaks for hexanes (14.4, 23.1, and 32.0 ppm) and free ligand (26.7, 61.8, and 64.7 ppm) are present in this spectrum.



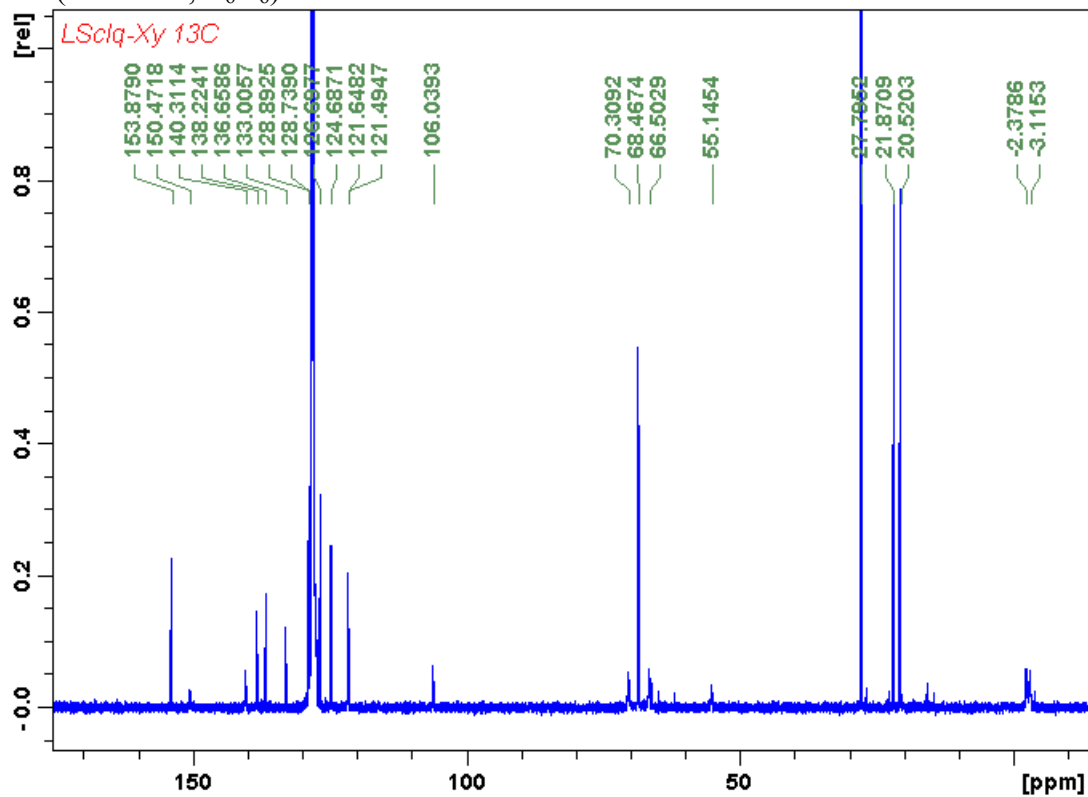
H-H COSY (500 MHz, C₆D₆)



1^{Sc}-iqn
 ^1H NMR (500 MHz, C_6D_6)

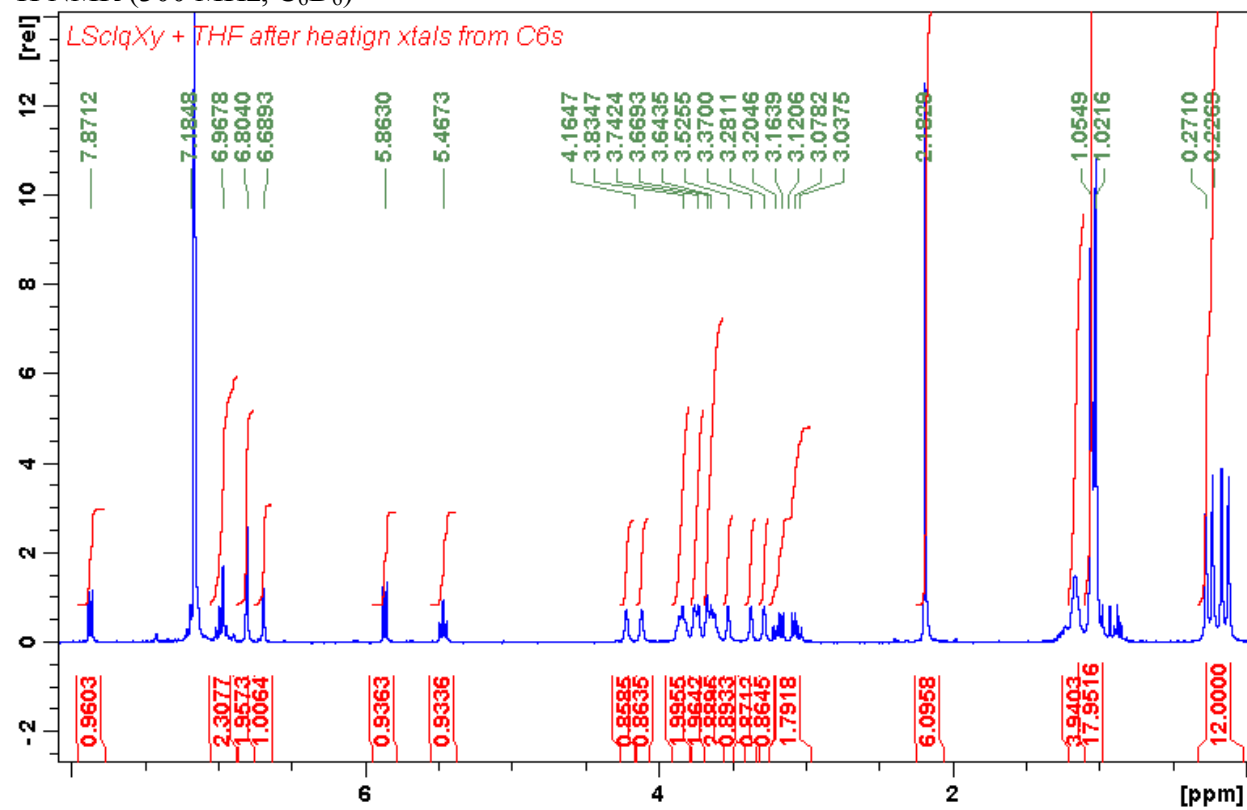


^{13}C NMR (126 MHz, C_6D_6)



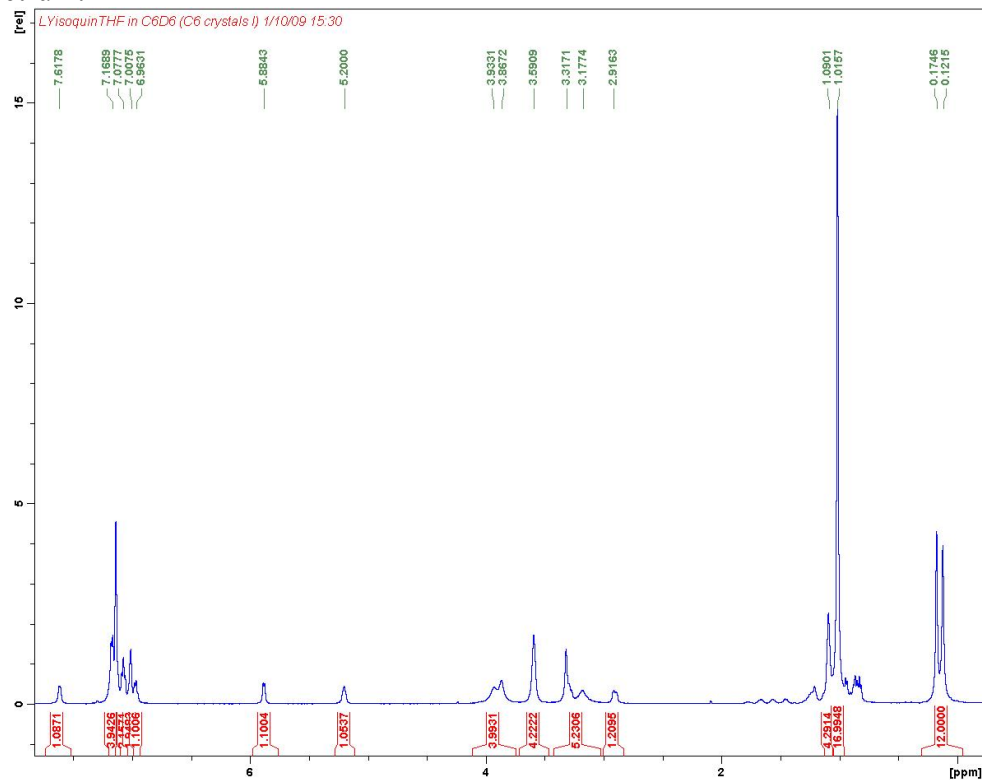
3^{Sc}-THF

^1H NMR (300 MHz, C_6D_6)

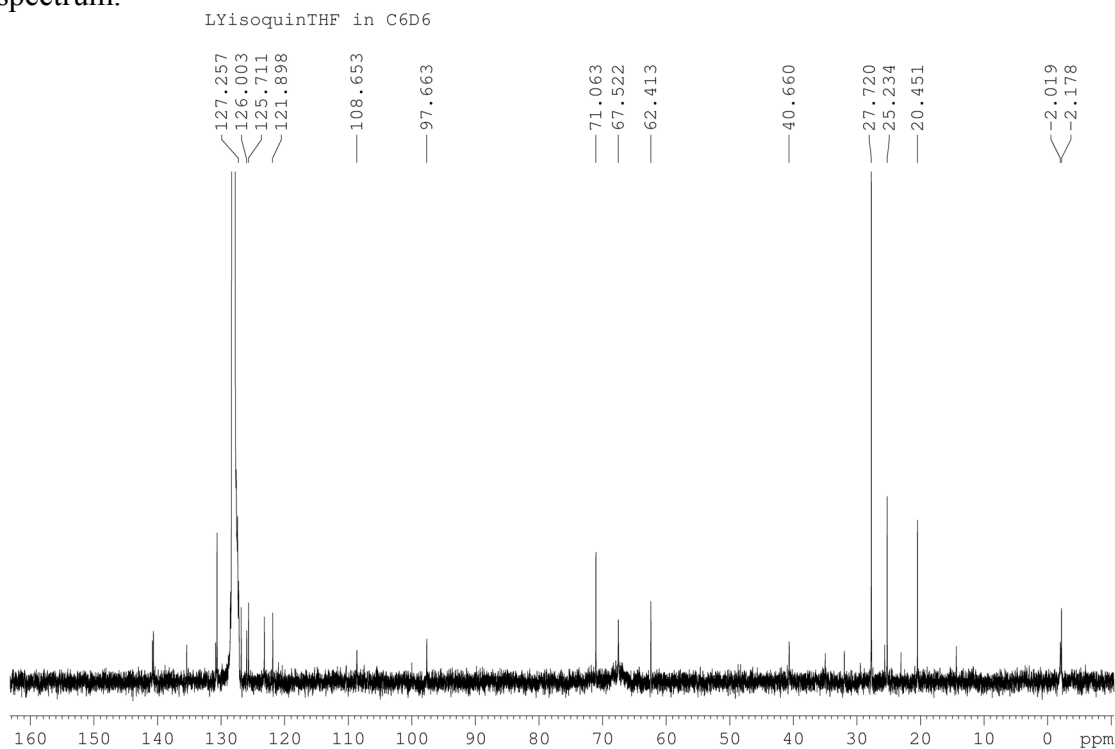


3^Y-THF

¹H NMR (500 MHz, C₆D₆): Peaks for hexanes (1.78, 1.69, 1.59, 1.47, 1.23, and 0.88) are present in this spectrum.

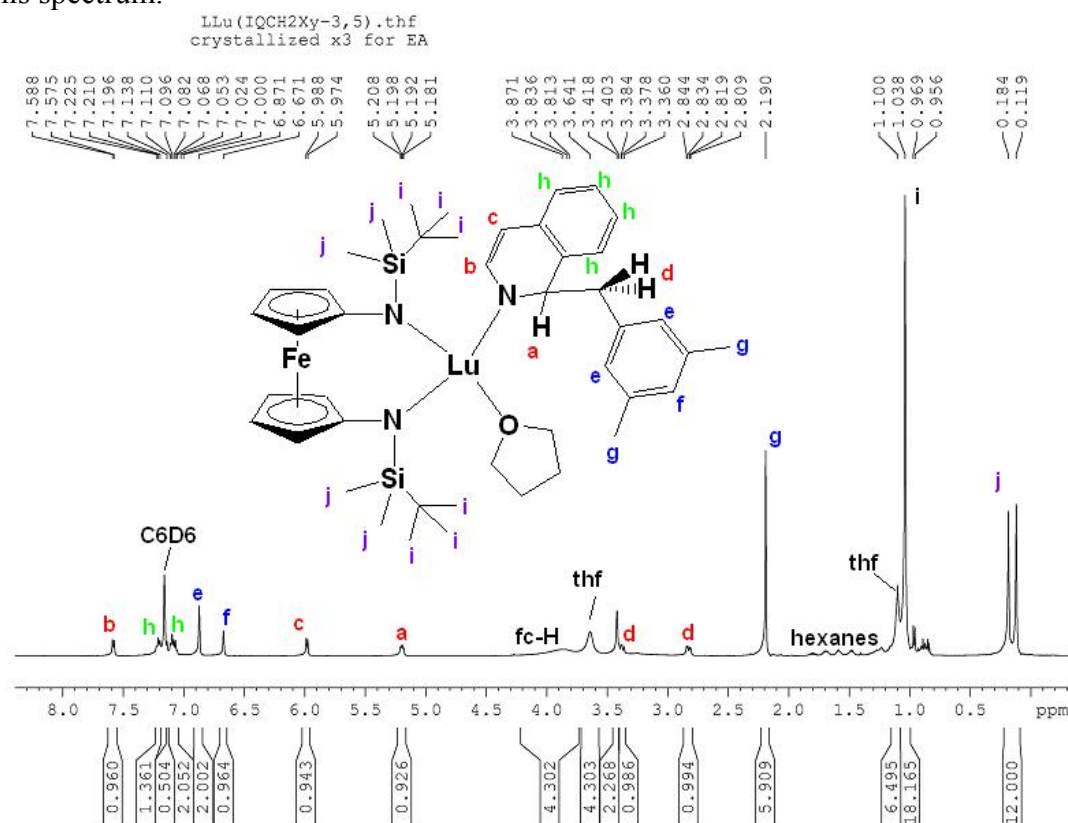


¹³C NMR (126 MHz, C₆D₆): Peaks for hexanes (35.0, 32.0, 25.6, 23.1, and 14.4 ppm) are present in this spectrum.

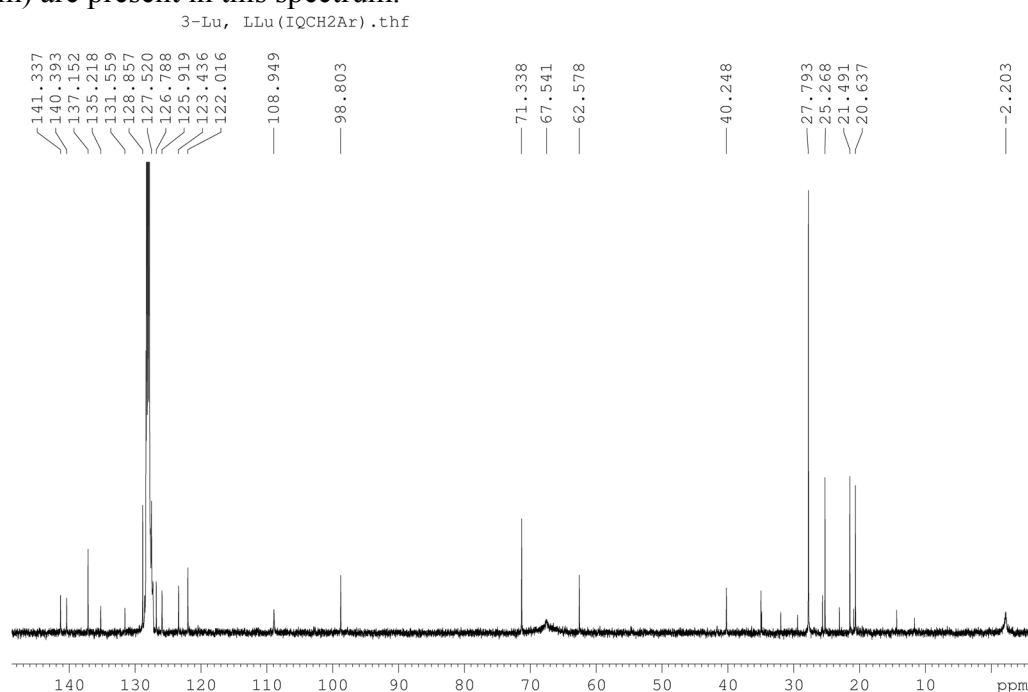


3^{Lu}-THF

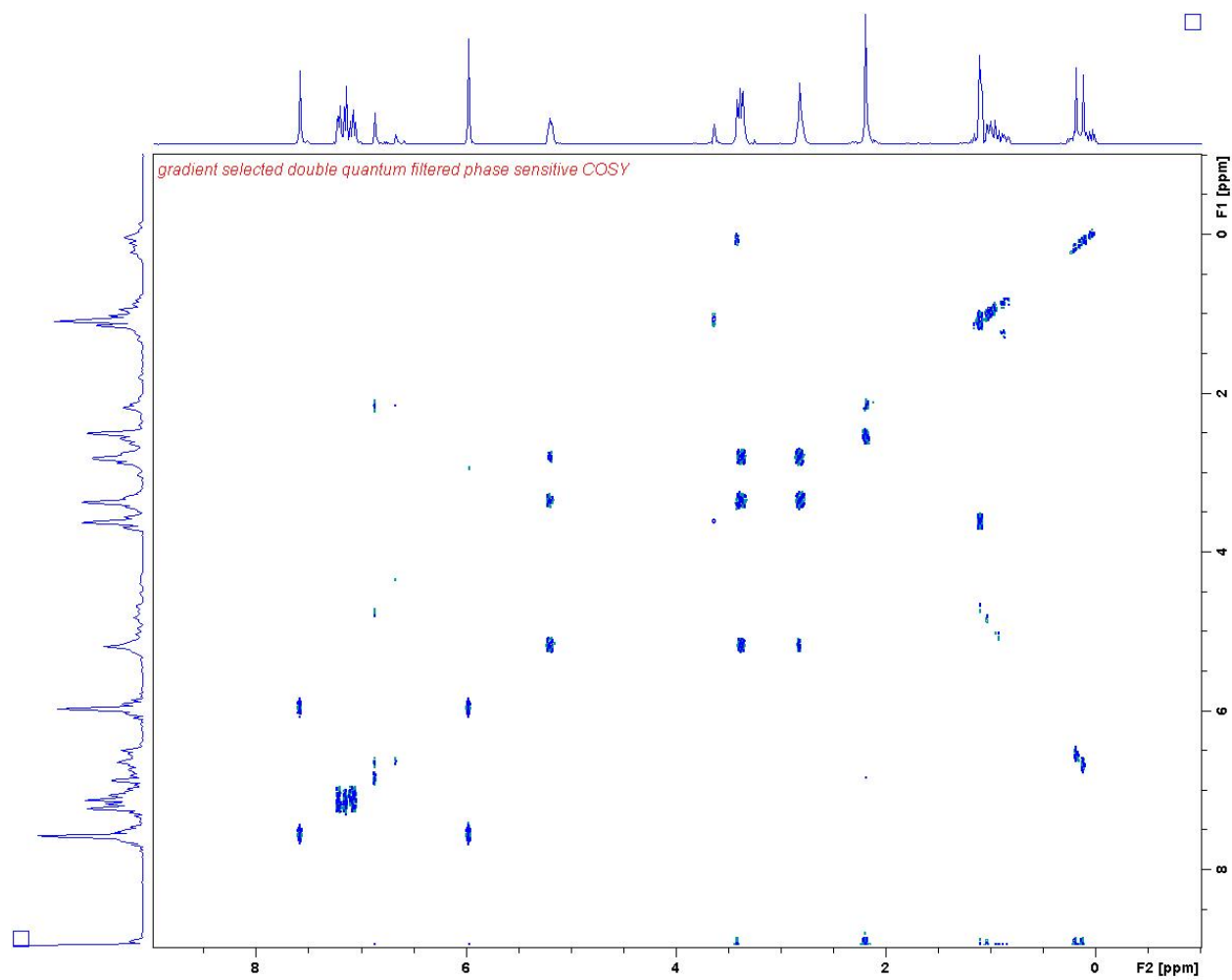
^1H NMR (500 MHz, C_6D_6): Peaks for hexanes (1.78, 1.69, 1.59, 1.47, 1.23, and 0.88) are present in this spectrum.



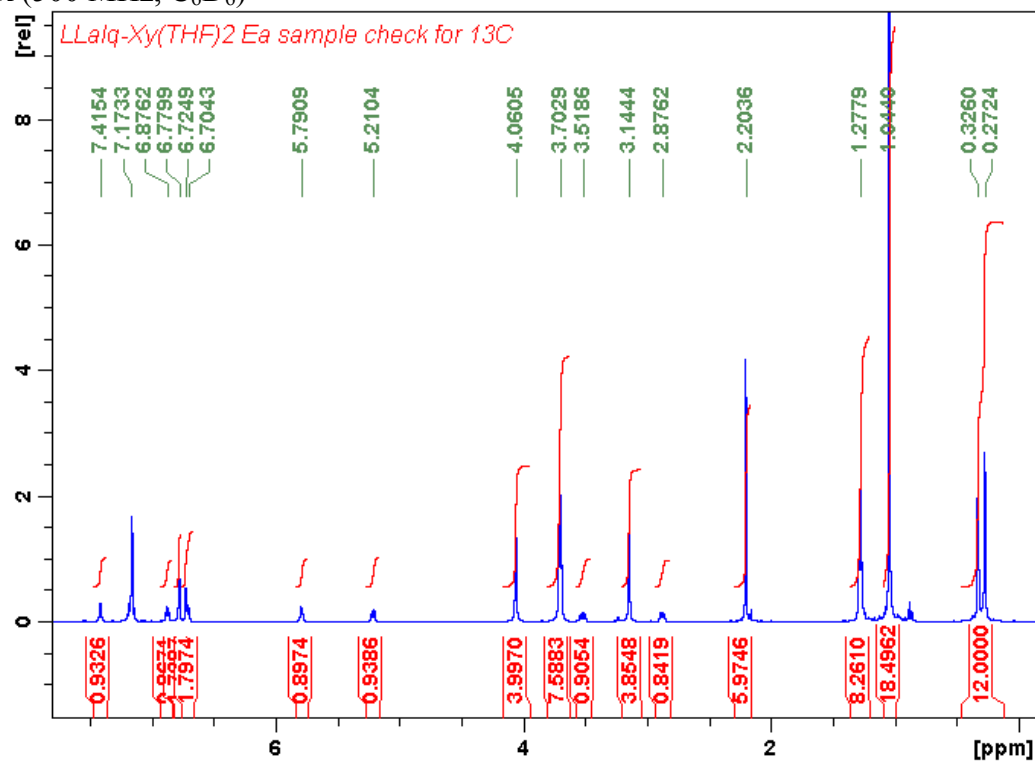
^{13}C NMR (126 MHz, C_6D_6): Peaks for hexanes (35.0, 34.9, 32.0, 29.4, 25.7, 23.1, 20.9, 14.4, and 11.7 ppm) are present in this spectrum.



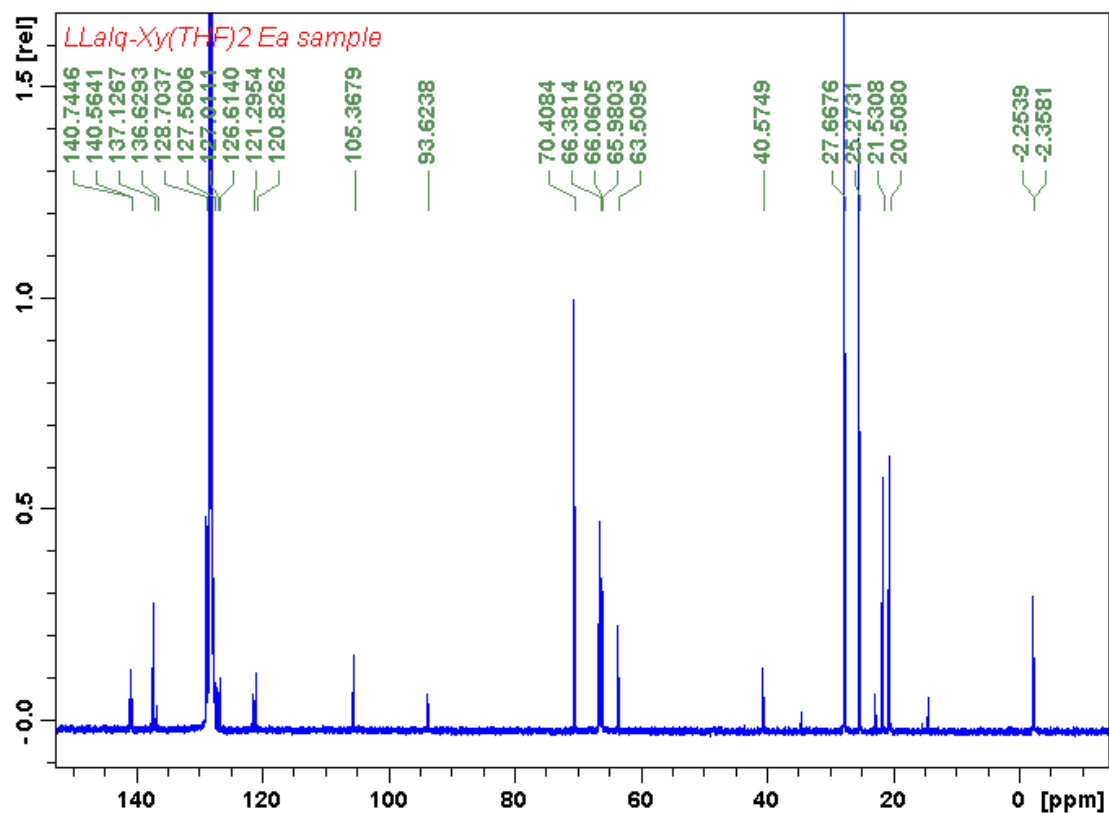
H-H COSY (500 MHz, C₆D₆)



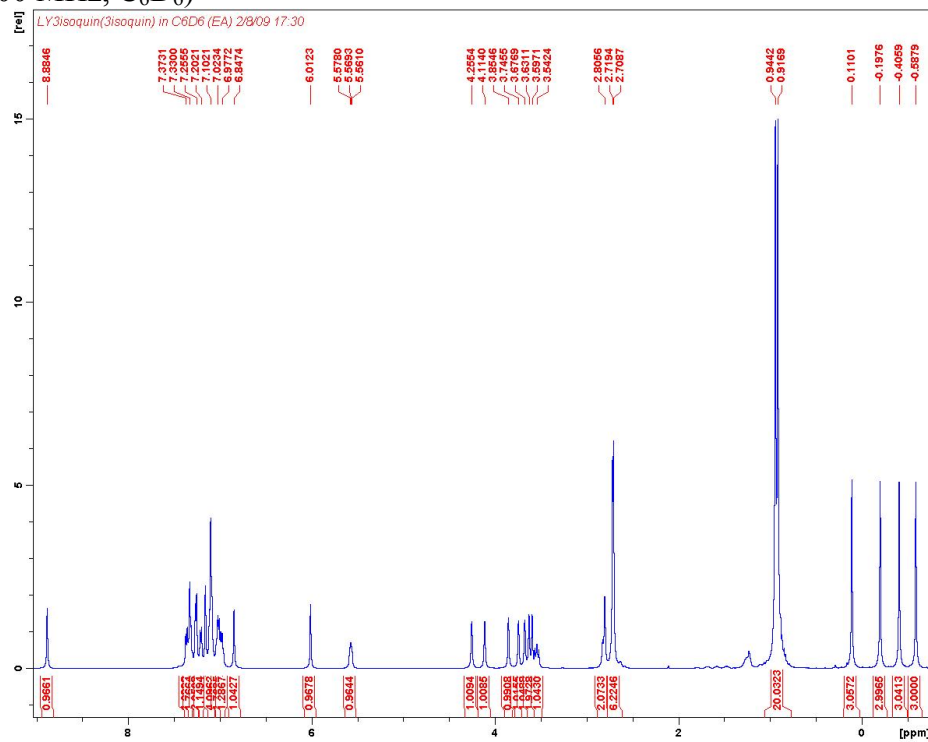
3^{La}-THF
¹H NMR (500 MHz, C₆D₆)



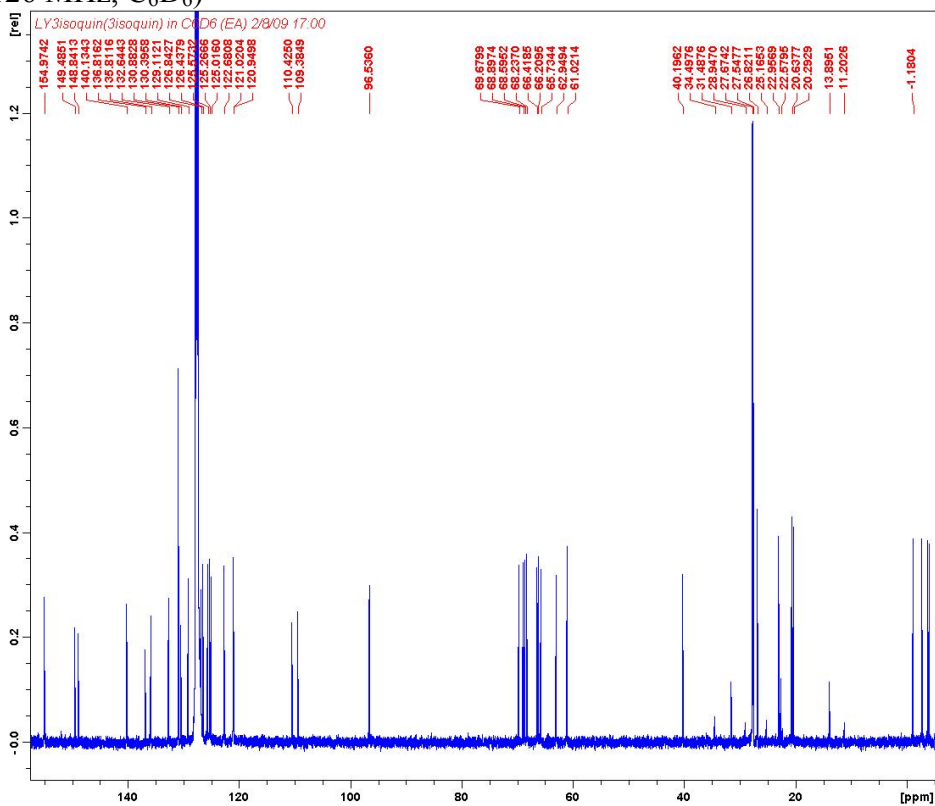
¹³C NMR (126 MHz, C₆D₆)



3^Y-iqn^{Me}
¹H NMR (500 MHz, C₆D₆)

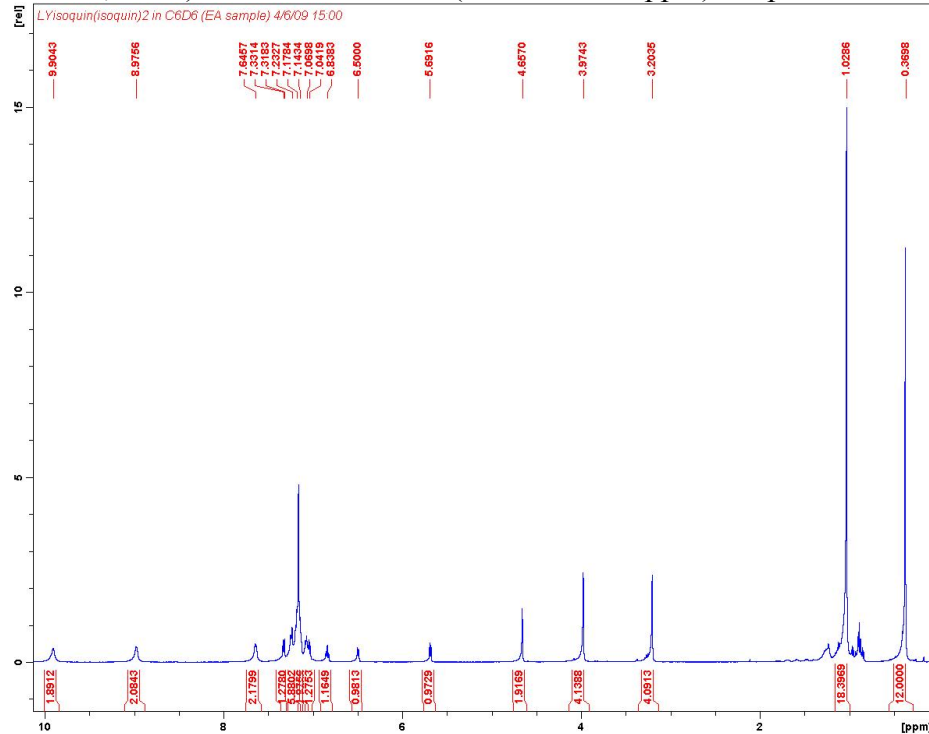


¹³C NMR (126 MHz, C₆D₆)

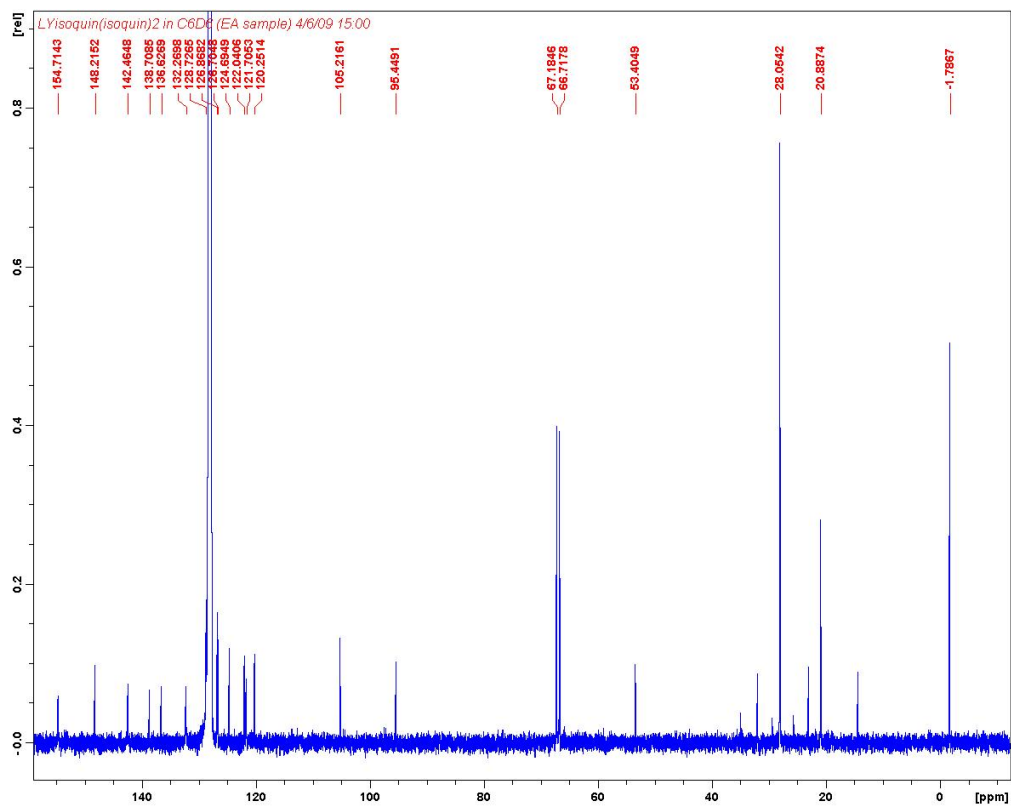


4^Y-(iqn)₂

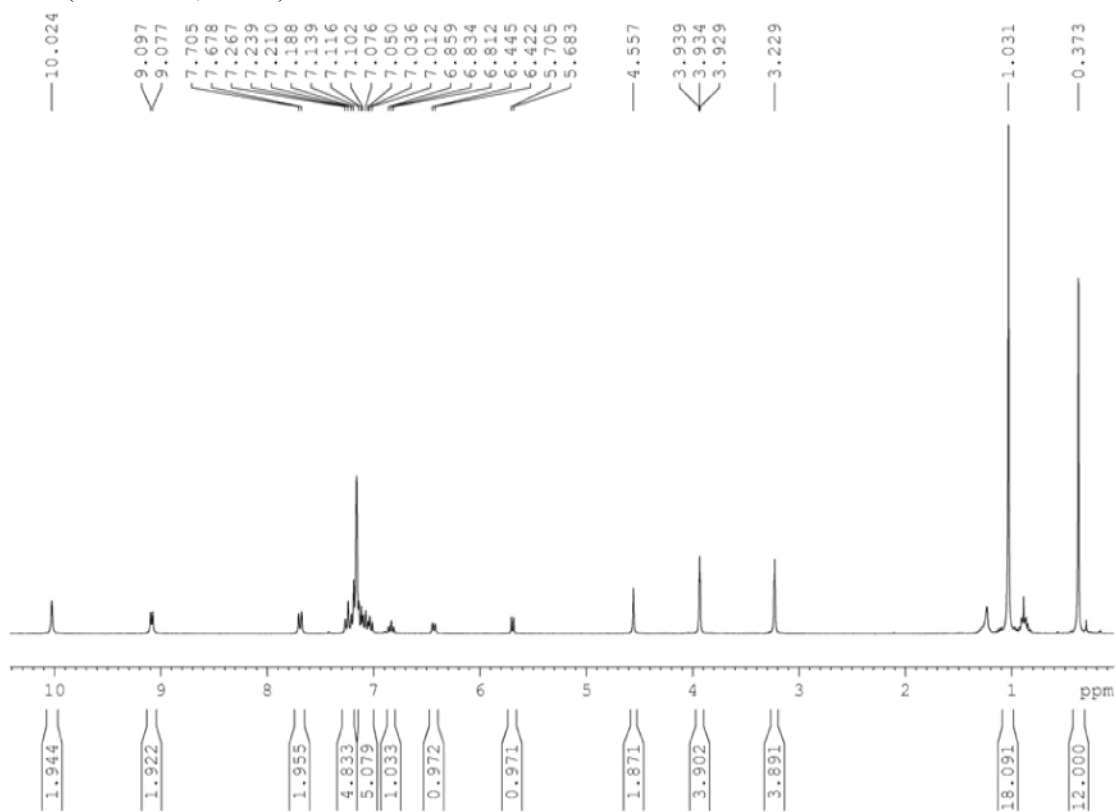
¹H NMR (500 MHz, C₆D₆): Peaks for hexanes (1.23 and 0.88 ppm) are present in this spectrum.



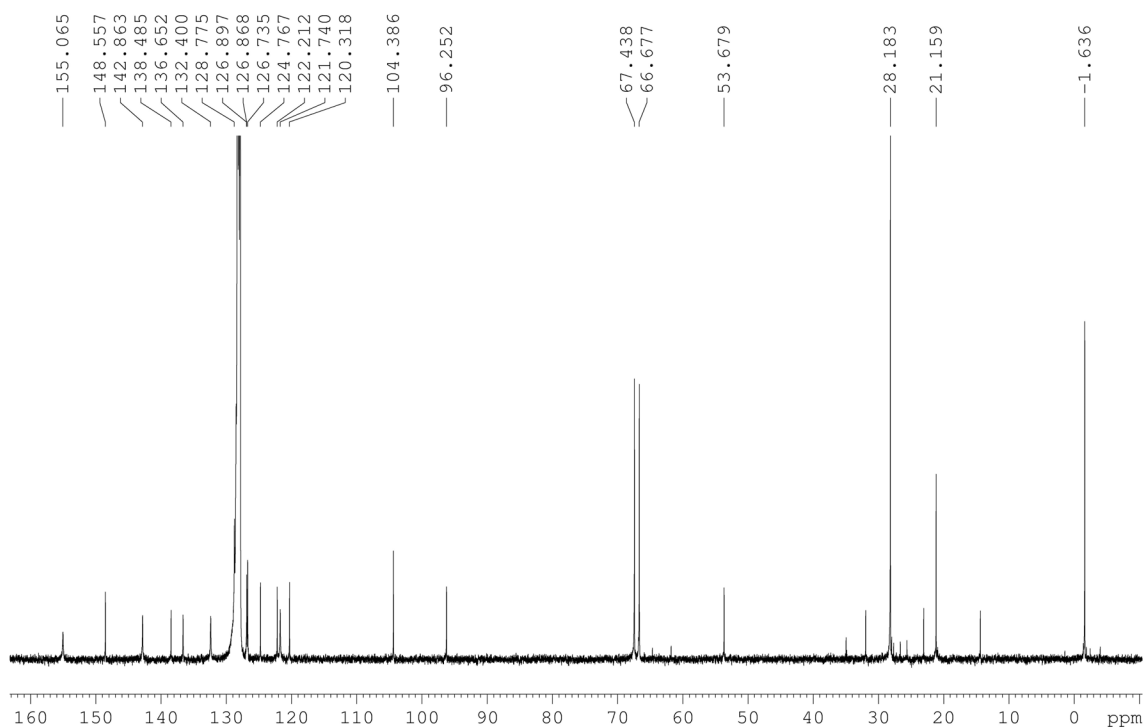
¹³C NMR (126 MHz, C₆D₆): Peaks for hexanes (35.0, 32.0, 29.4, 25.6, 23.1, and 14.4 ppm) are present in this spectrum.



$4^{\text{Lu}}\text{-(iqn)}_2$
 ^1H NMR (500 MHz, C_6D_6)

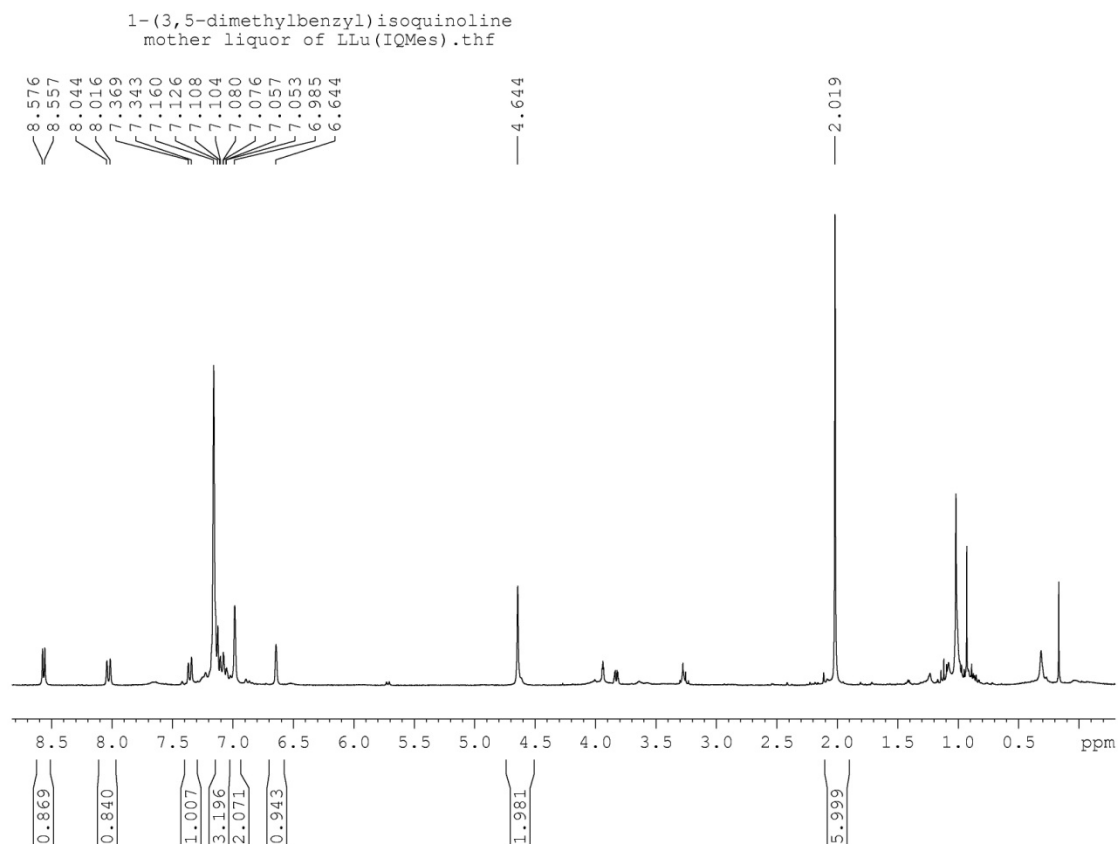


^{13}C NMR (126 MHz, C_6D_6)

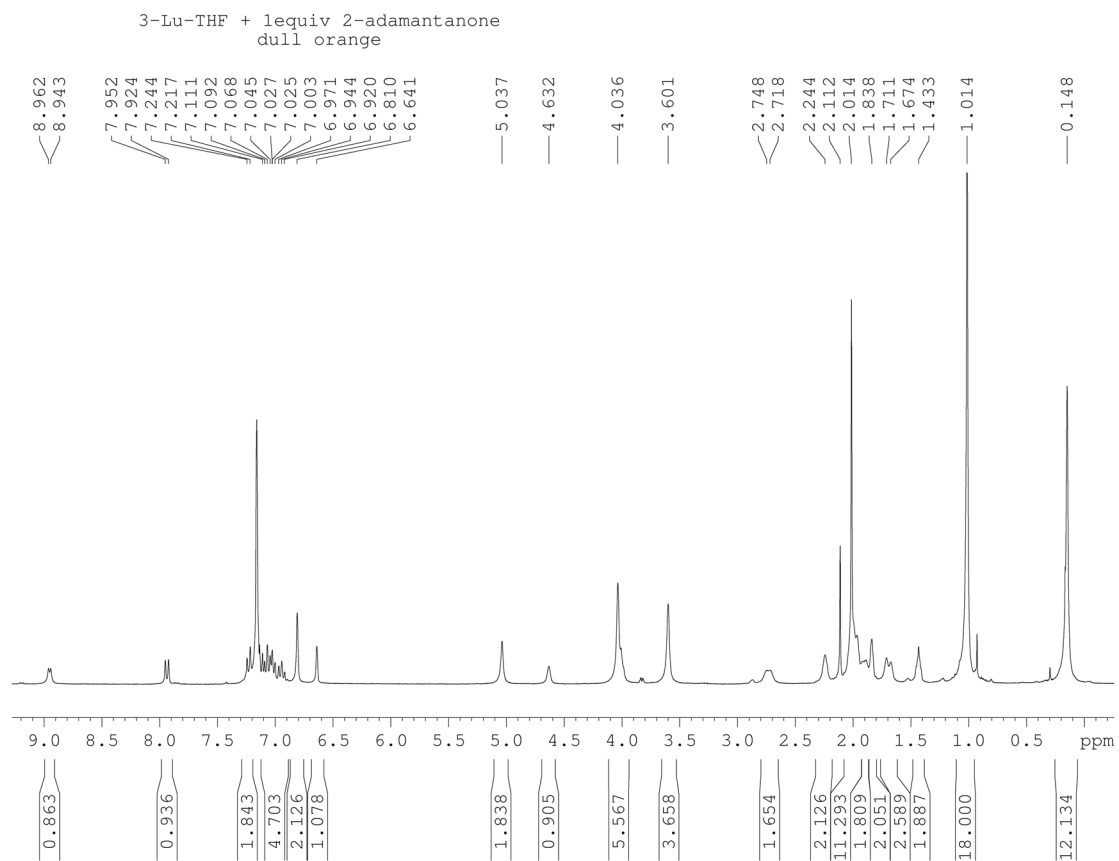


5^{Ar} (Ar = 3,5-dimethylxylyl)

¹H NMR (300 MHz, C₆D₆): The ¹H NMR spectrum shown also contains some **4^{Lu}-(iqn)₂**, as well as peaks for the free ligand (3.83, 0.92, and 0.16 ppm).

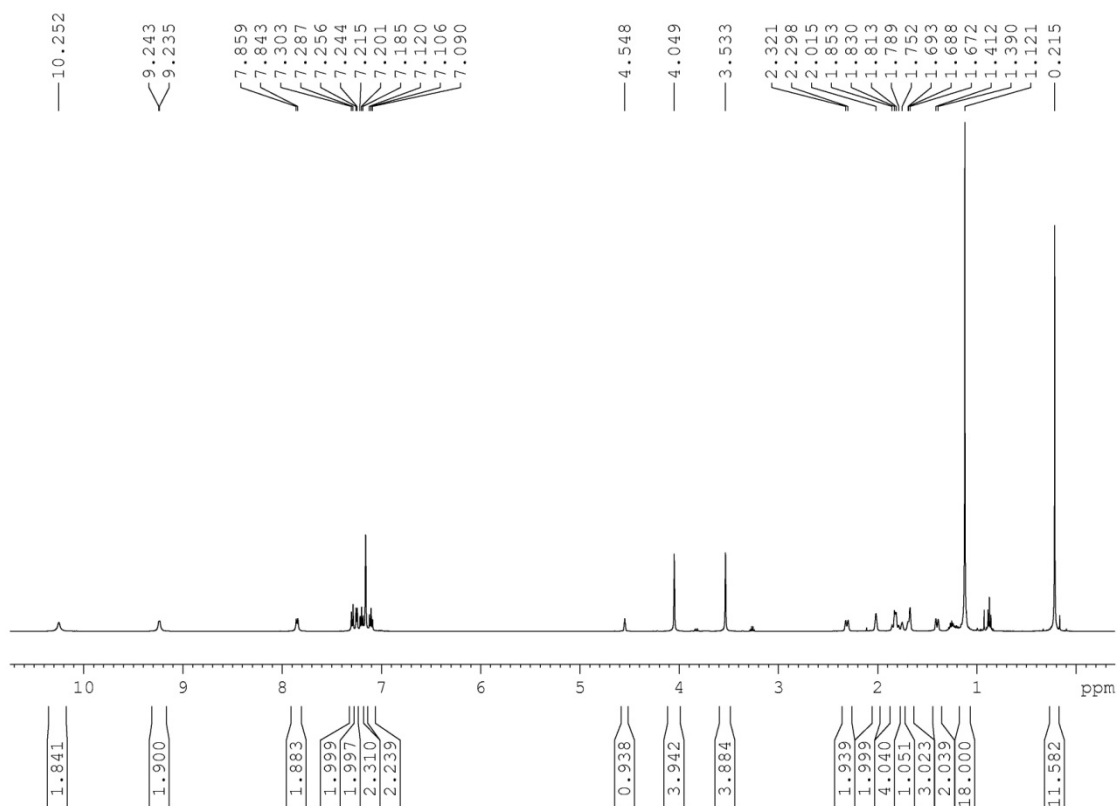


6-Lu-ign^{Ar}
¹H NMR (300 MHz, C₆D₆)

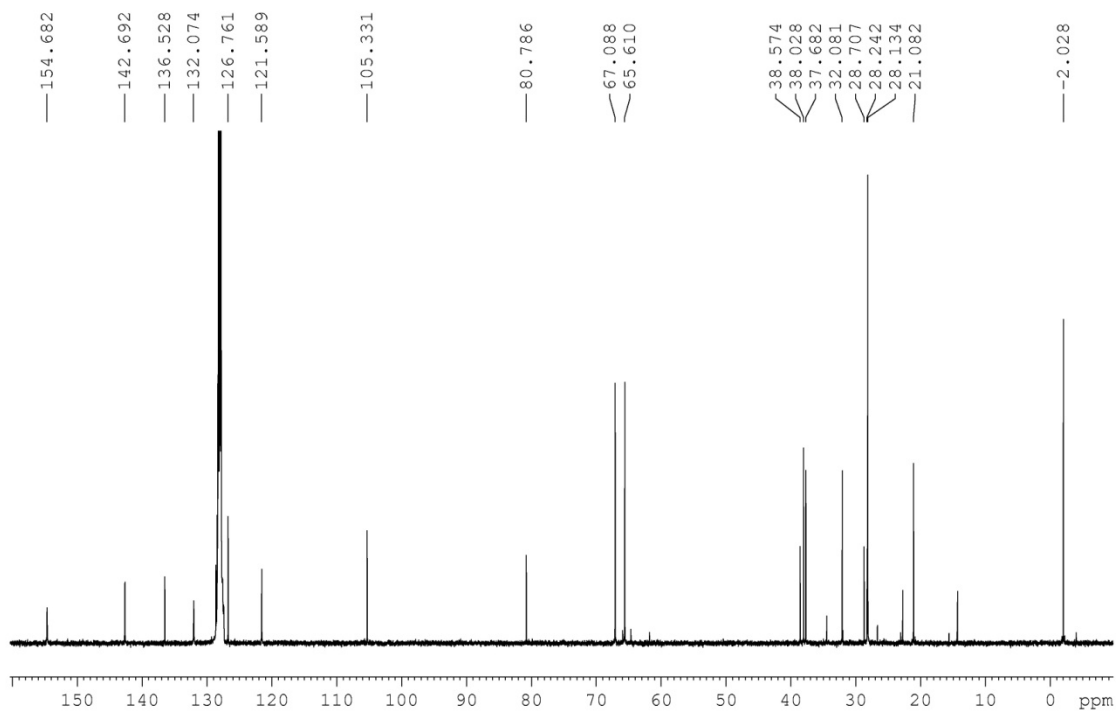


$6^{\text{Lu}}\text{-(iqn)}_2$
 ^1H NMR (500 MHz, C_6D_6)

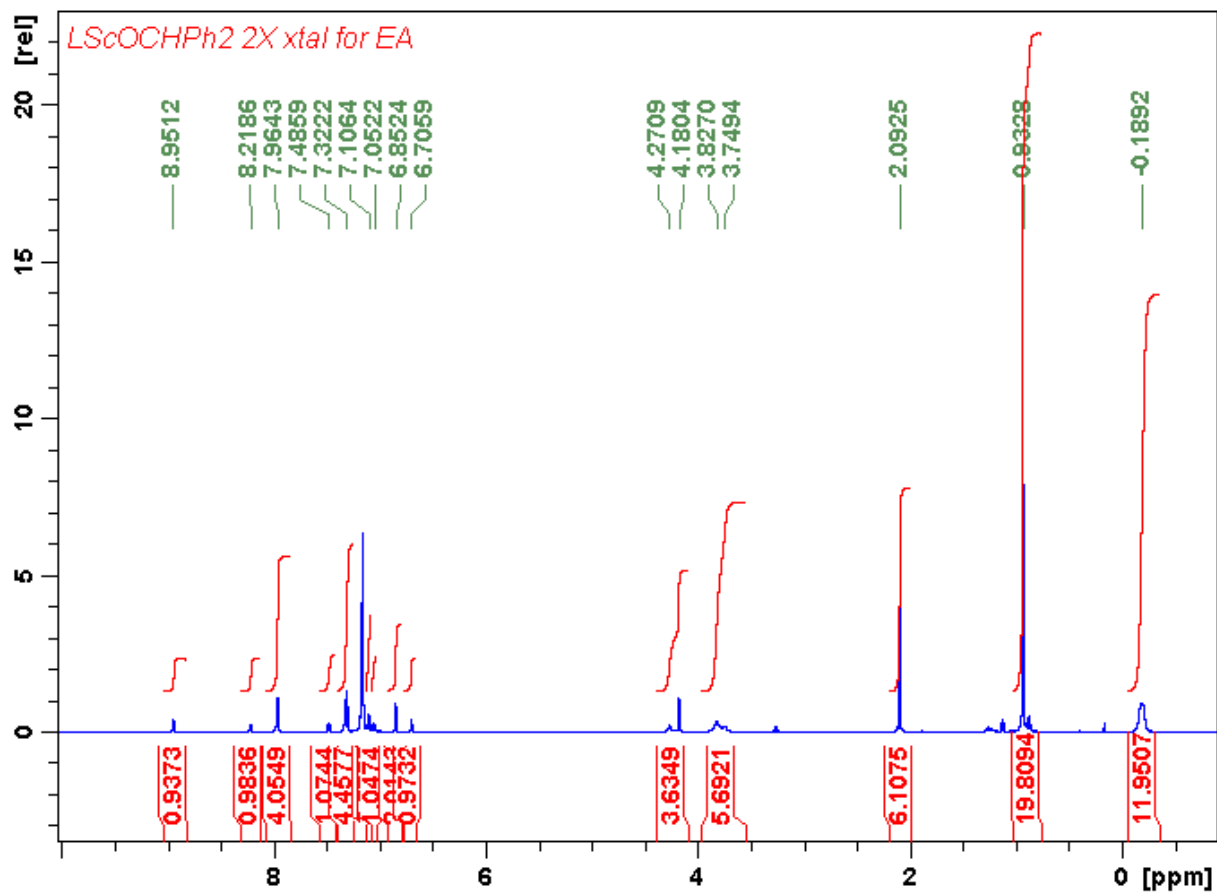
LLu(IQ)2 (adamantoxide) crystallized x4



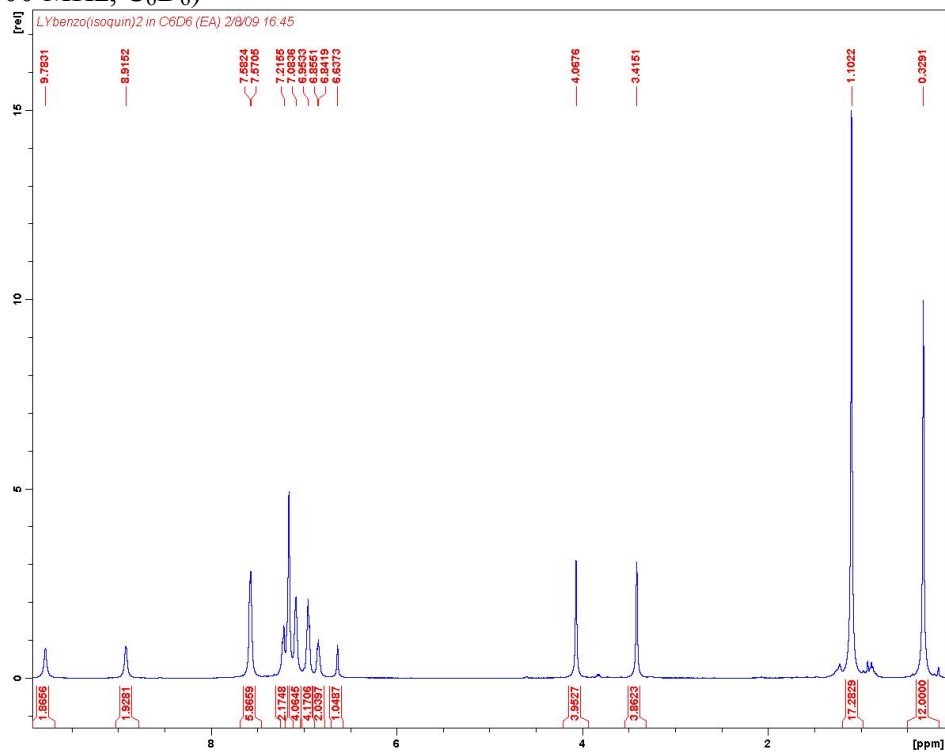
^{13}C NMR (126 MHz, C_6D_6)



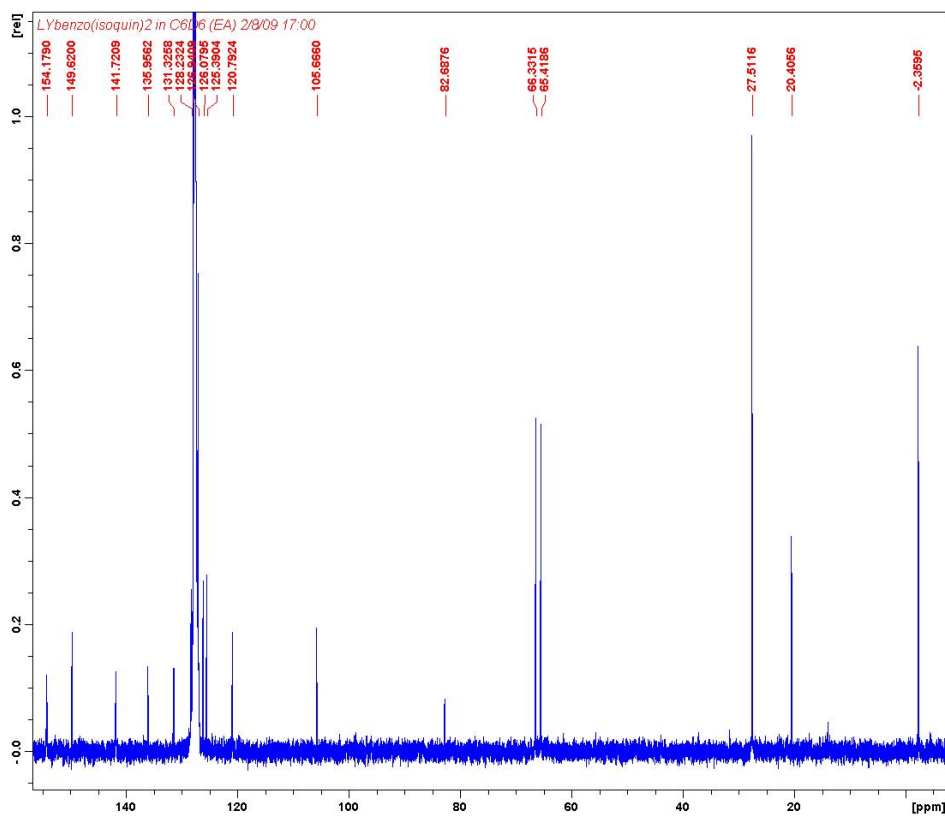
$7^{\text{Sc}}\text{-iqn}^{\text{Me}}$
 ^1H NMR (500 MHz, C_6D_6)



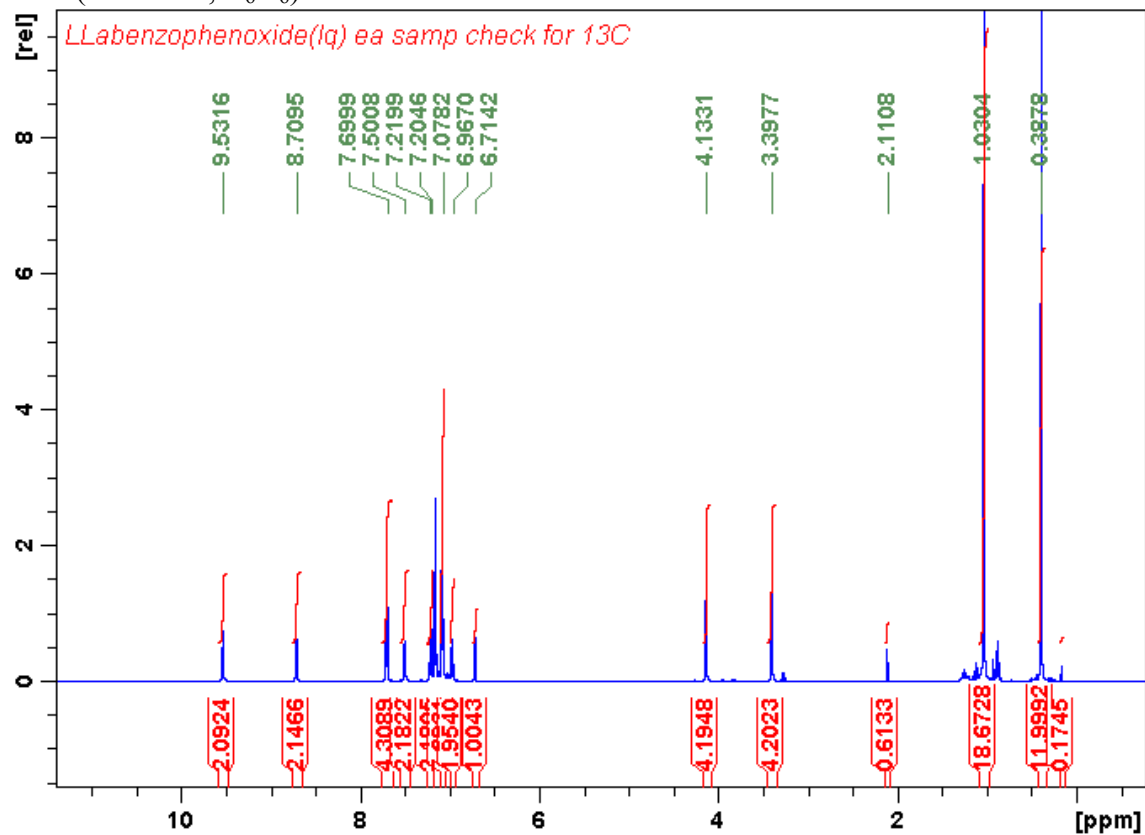
7^Y-(iqn)₂
¹H NMR (500 MHz, C₆D₆)



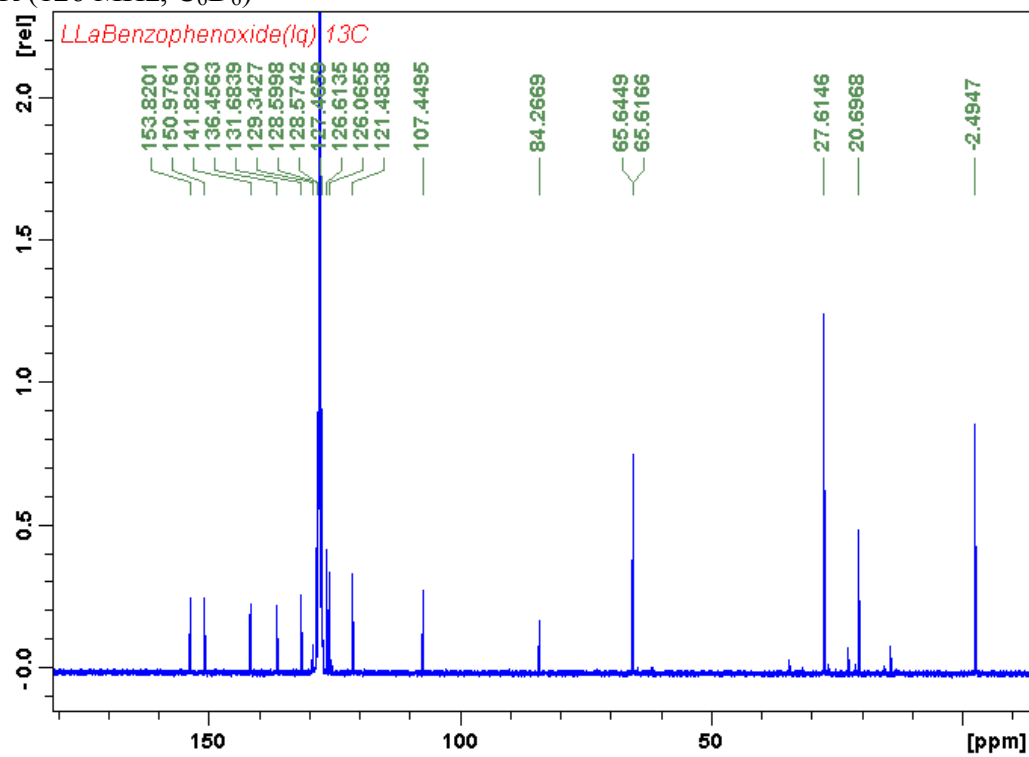
¹³C NMR (126 MHz, C₆D₆)



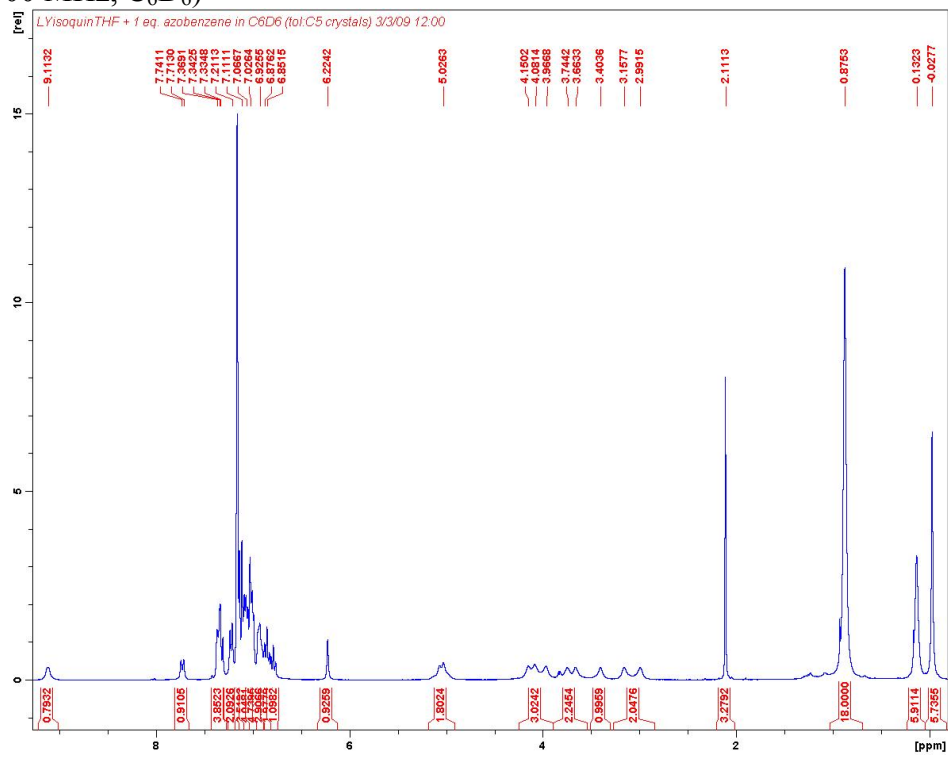
$7^{\text{La}}\text{-(iqn)}_2$
 ^1H NMR (500 MHz, C_6D_6)



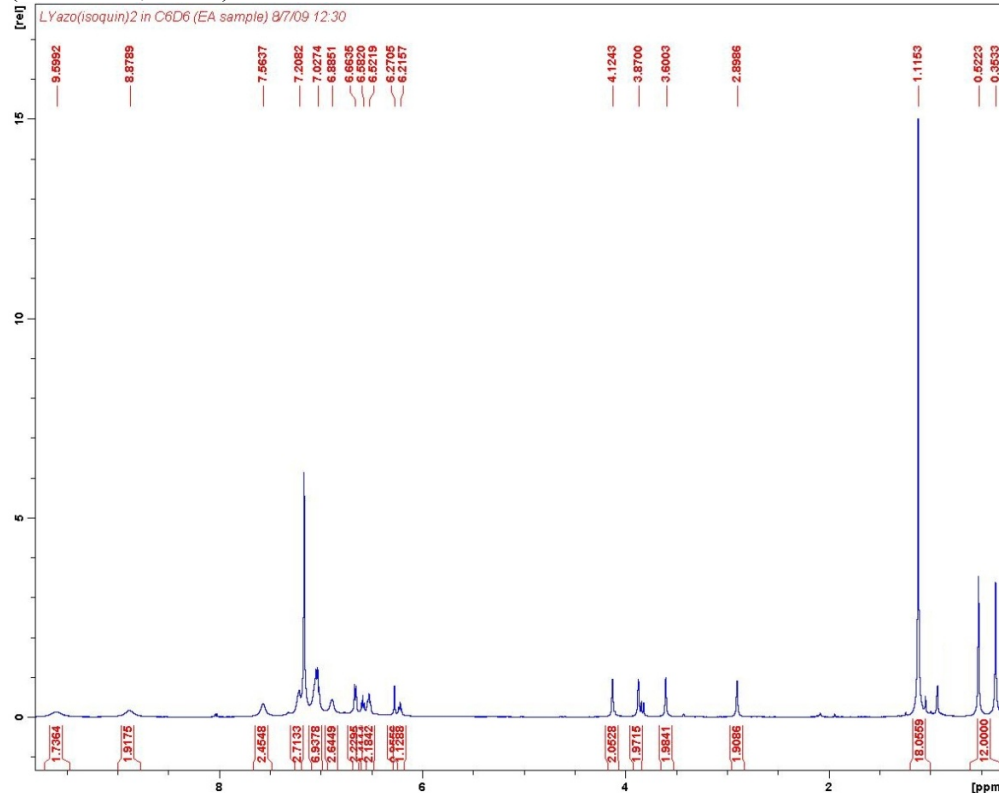
^{13}C NMR (126 MHz, C_6D_6)



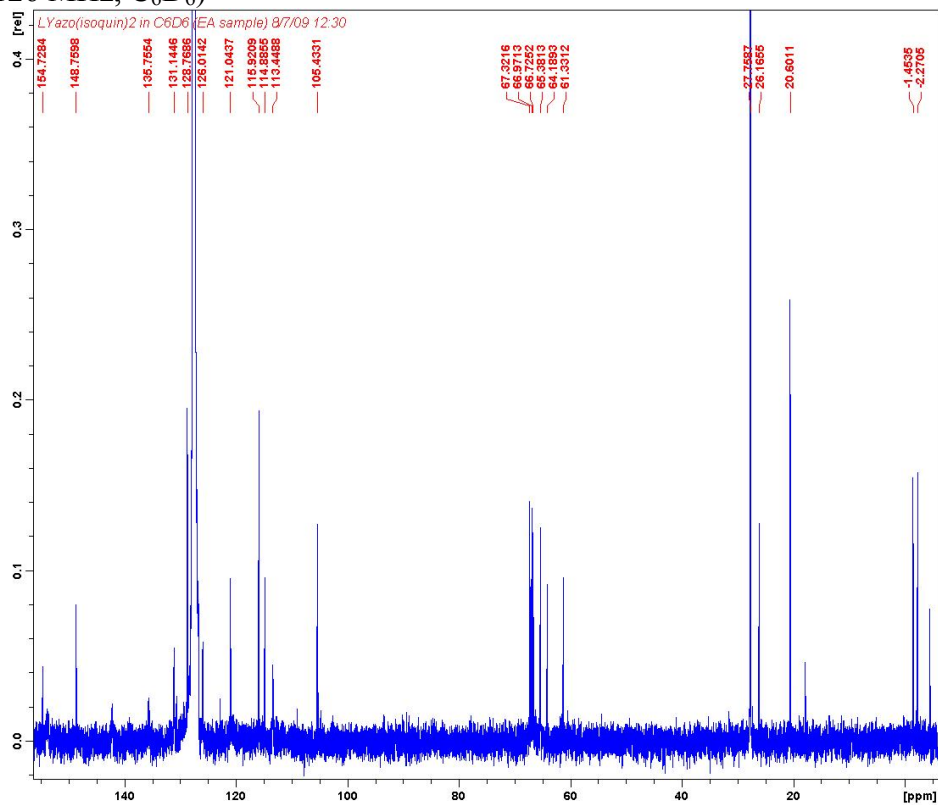
8^y
¹H NMR (300 MHz, C₆D₆)



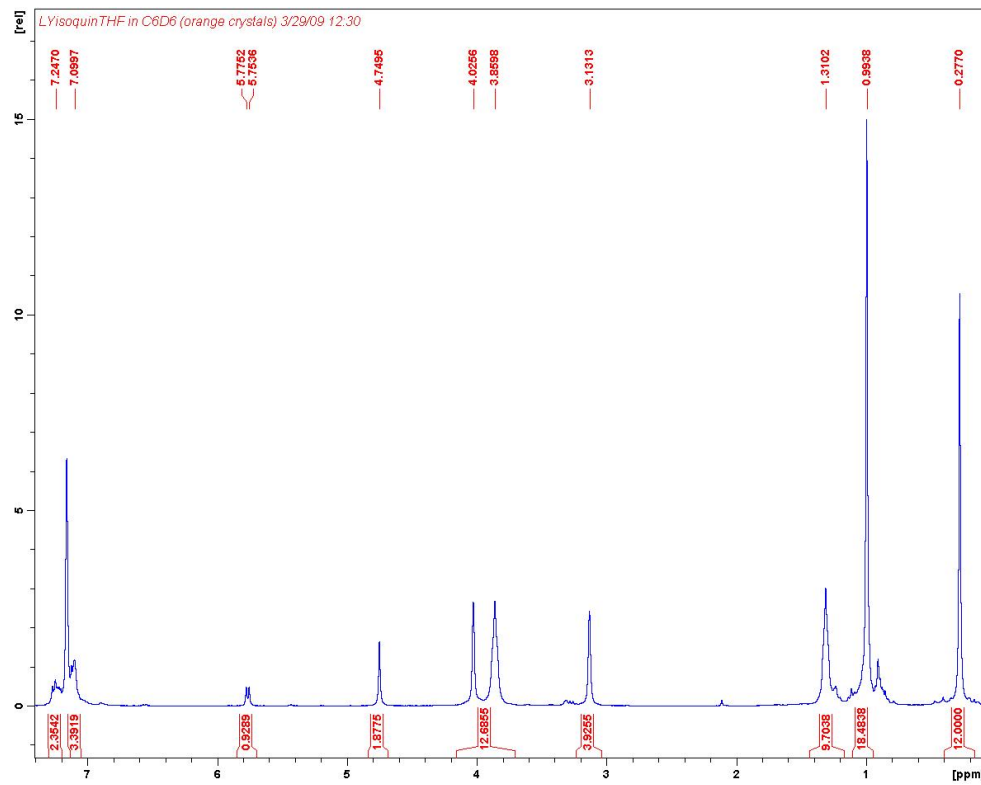
8^Y-(iqn)₂
¹H NMR (500 MHz, C₆D₆)



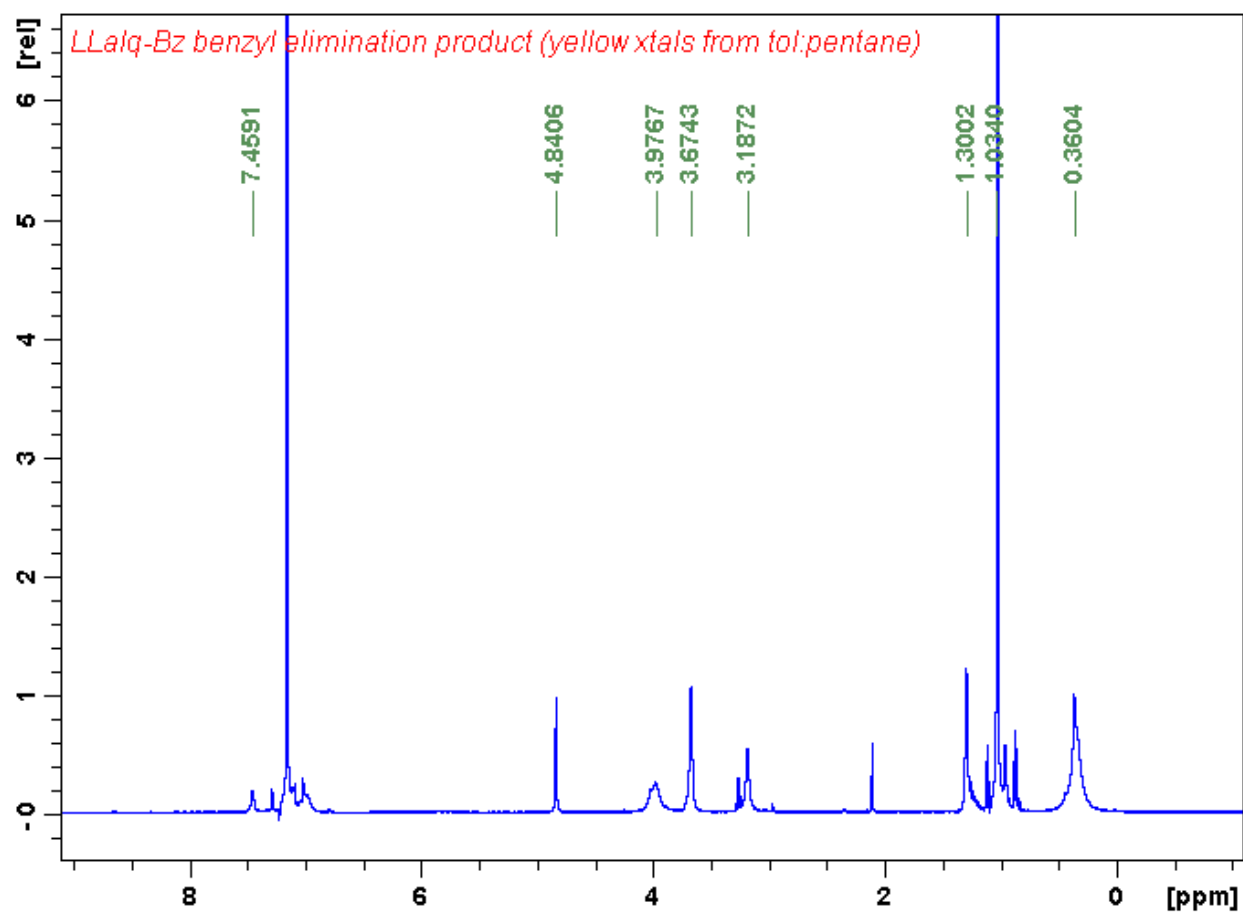
¹³C NMR (126 MHz, C₆D₆)



4^Y-(THF)₂
¹H NMR (300 MHz, C₆D₆)

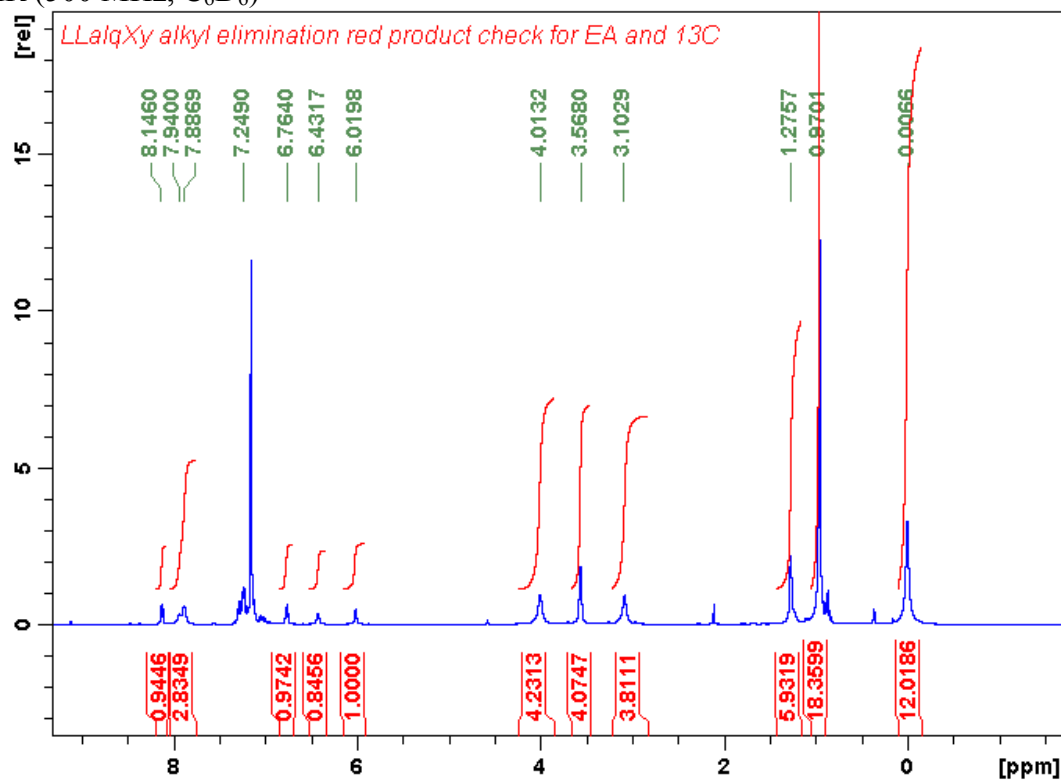


$4^{\text{La}}\text{-(THF)}_2$
 ^1H NMR (300 MHz, C_6D_6)

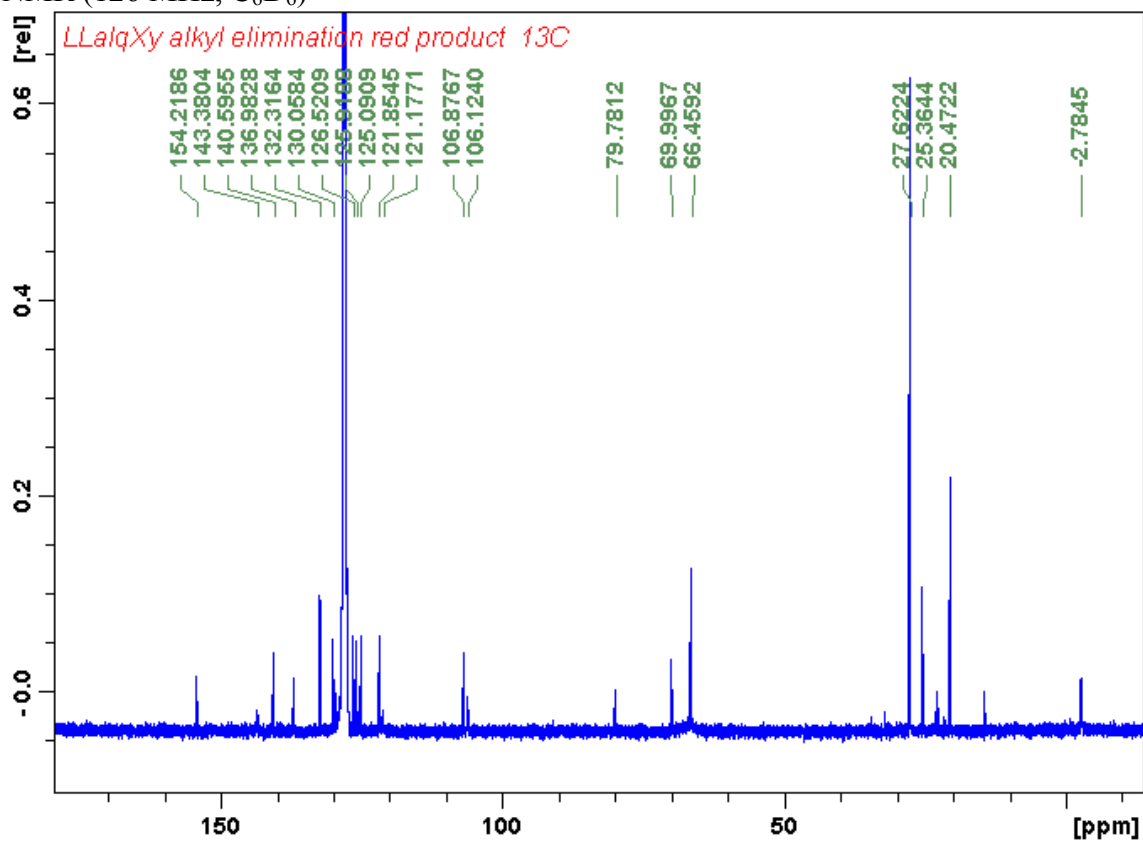


9^{La}

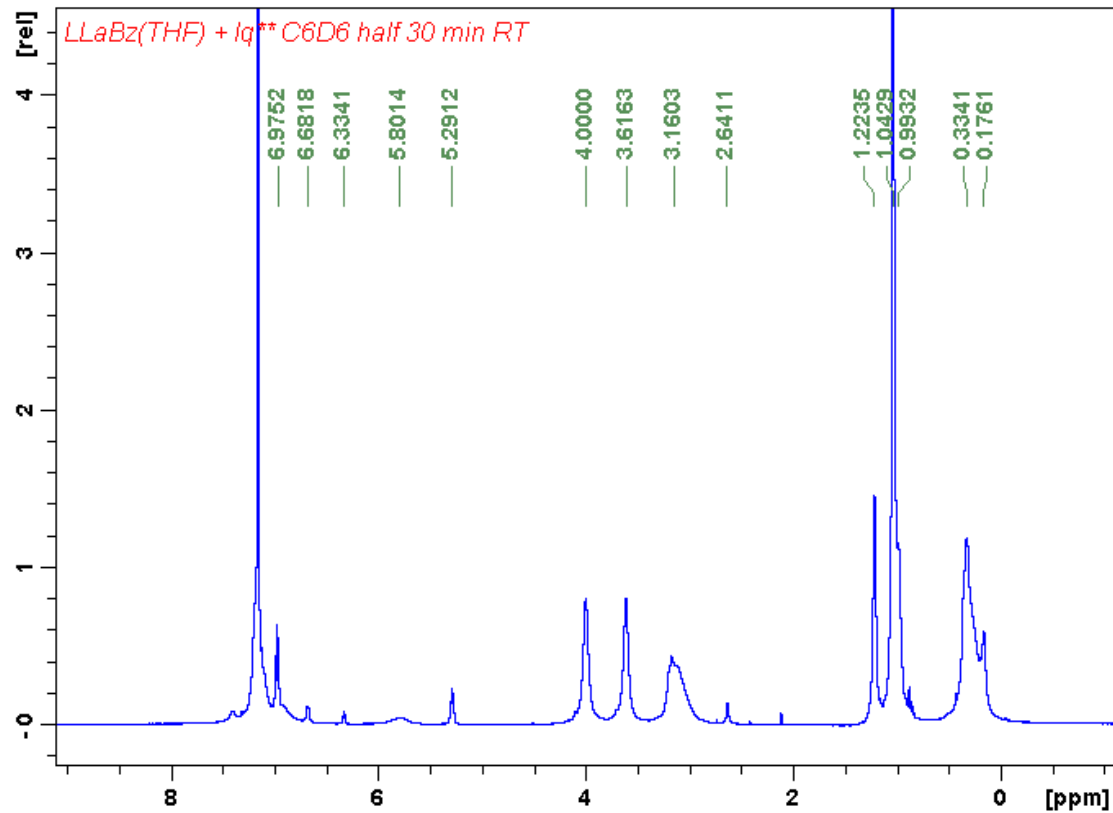
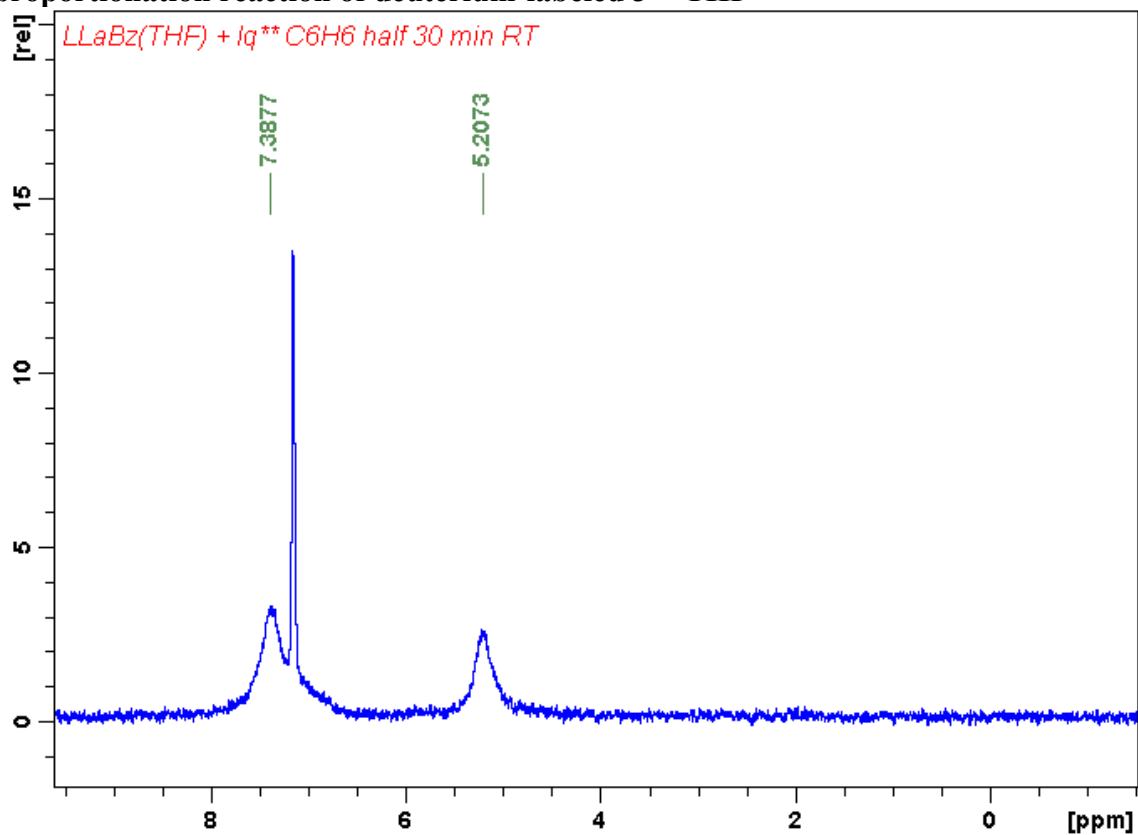
¹H NMR (500 MHz, C₆D₆)

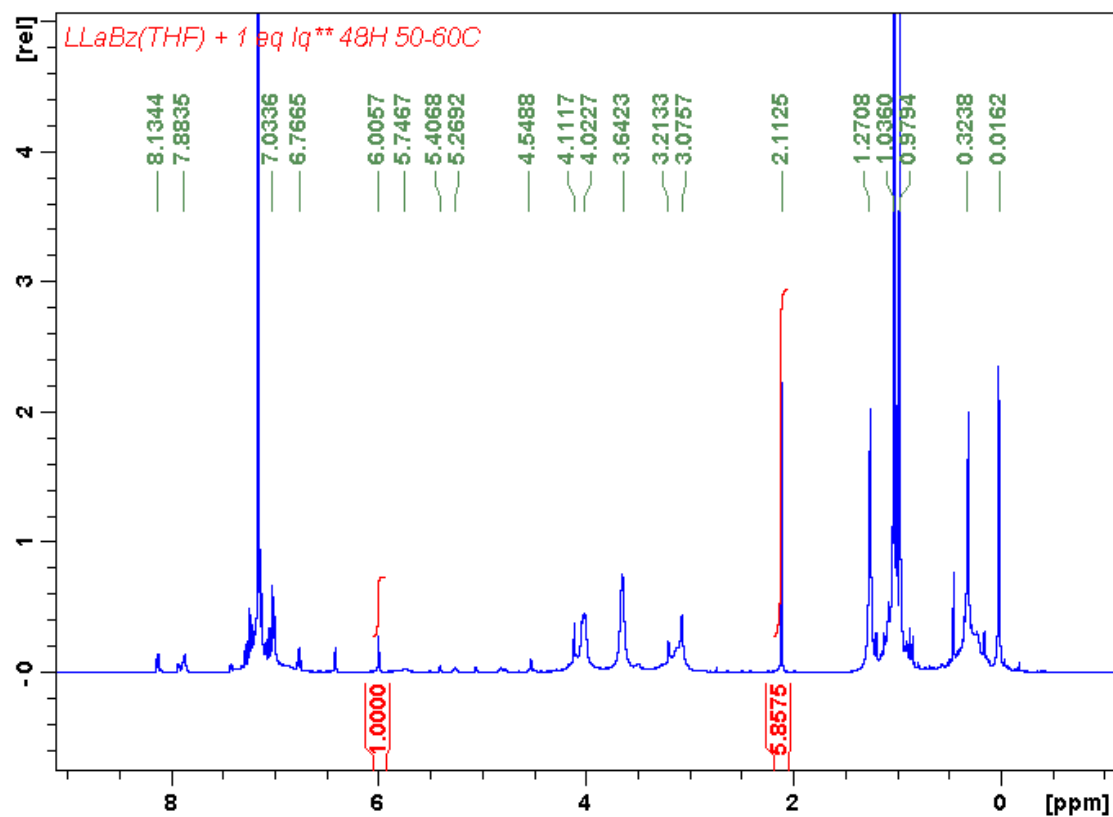
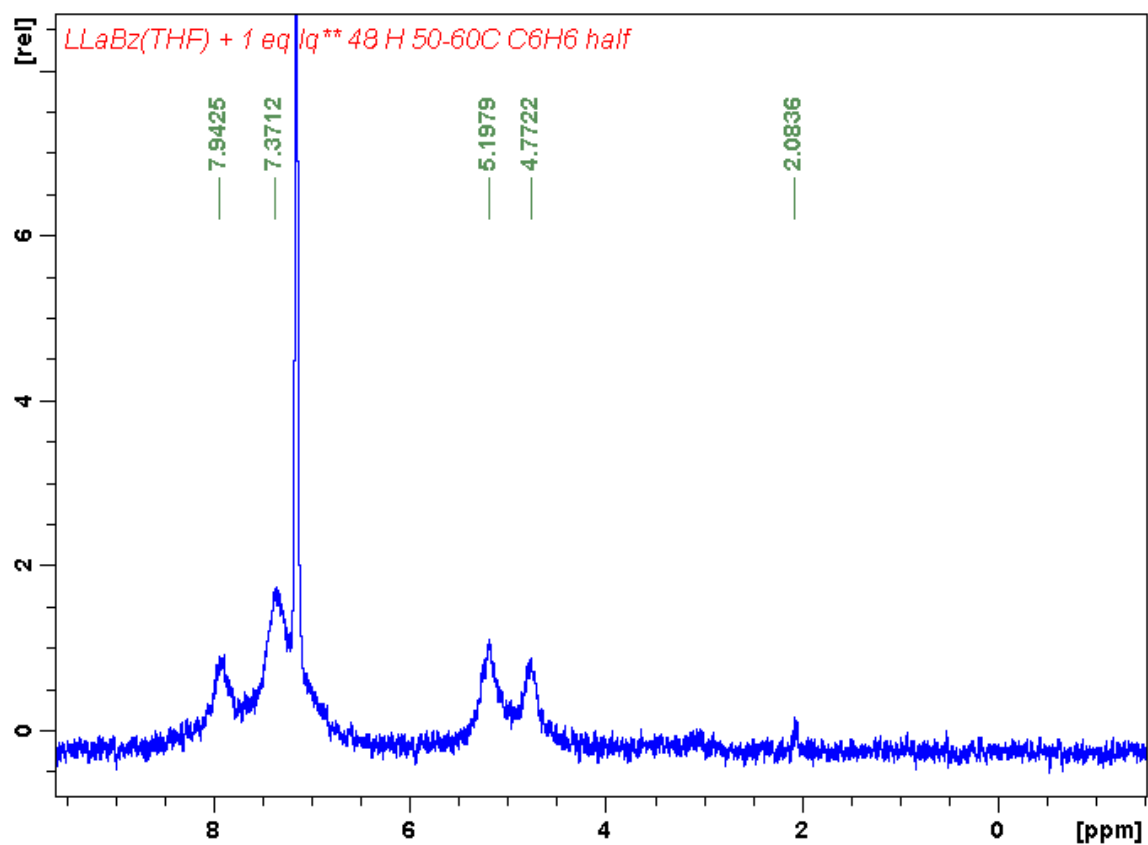


¹³C NMR (126 MHz, C₆D₆)



Disproportionation reaction of deuterium-labeled 3^{La}-THF





X-ray crystal structures

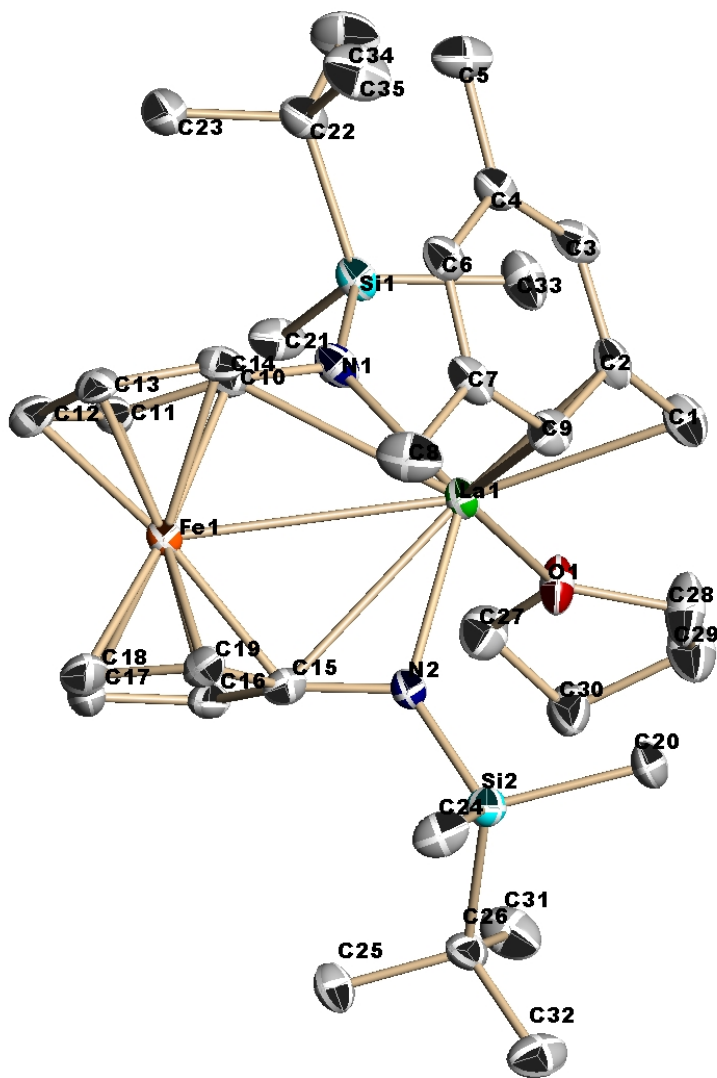


Figure SX1. Thermal-ellipsoid (50% probability) representation of **1'^{La}-THF**. Hydrogen atoms were omitted for clarity.

2^{Sc}

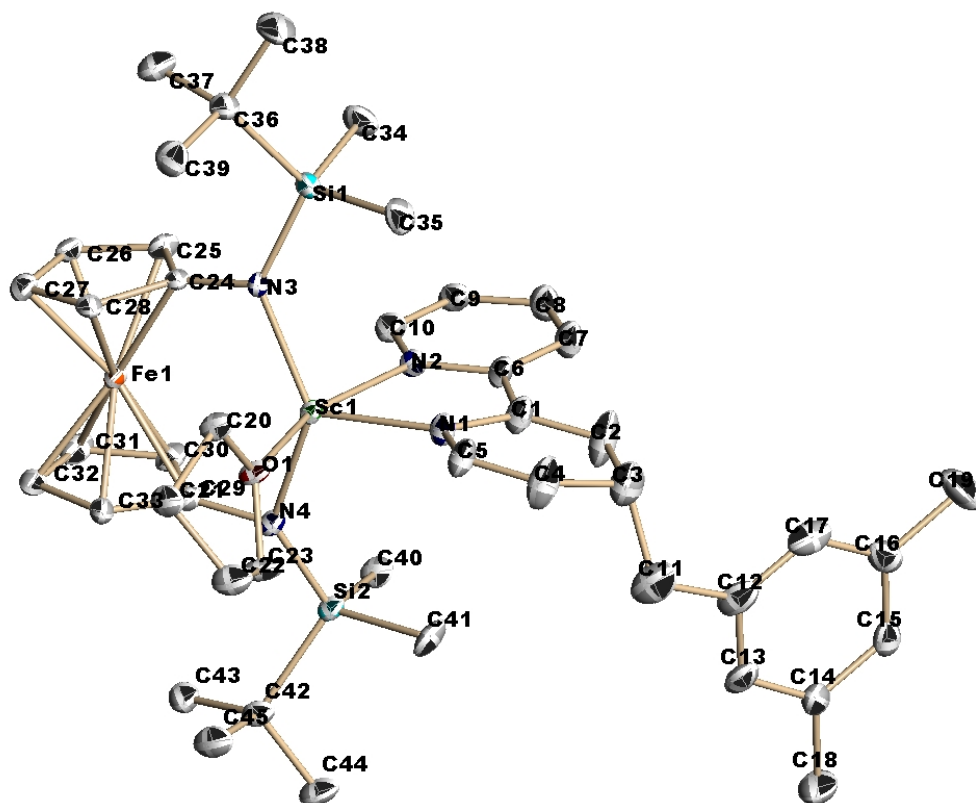


Figure SX2. Thermal-ellipsoid (50% probability) representation of 2^{Sc} . Hydrogen atoms were omitted for clarity.

$3^Y\text{-iqn}^{\text{Me}}$

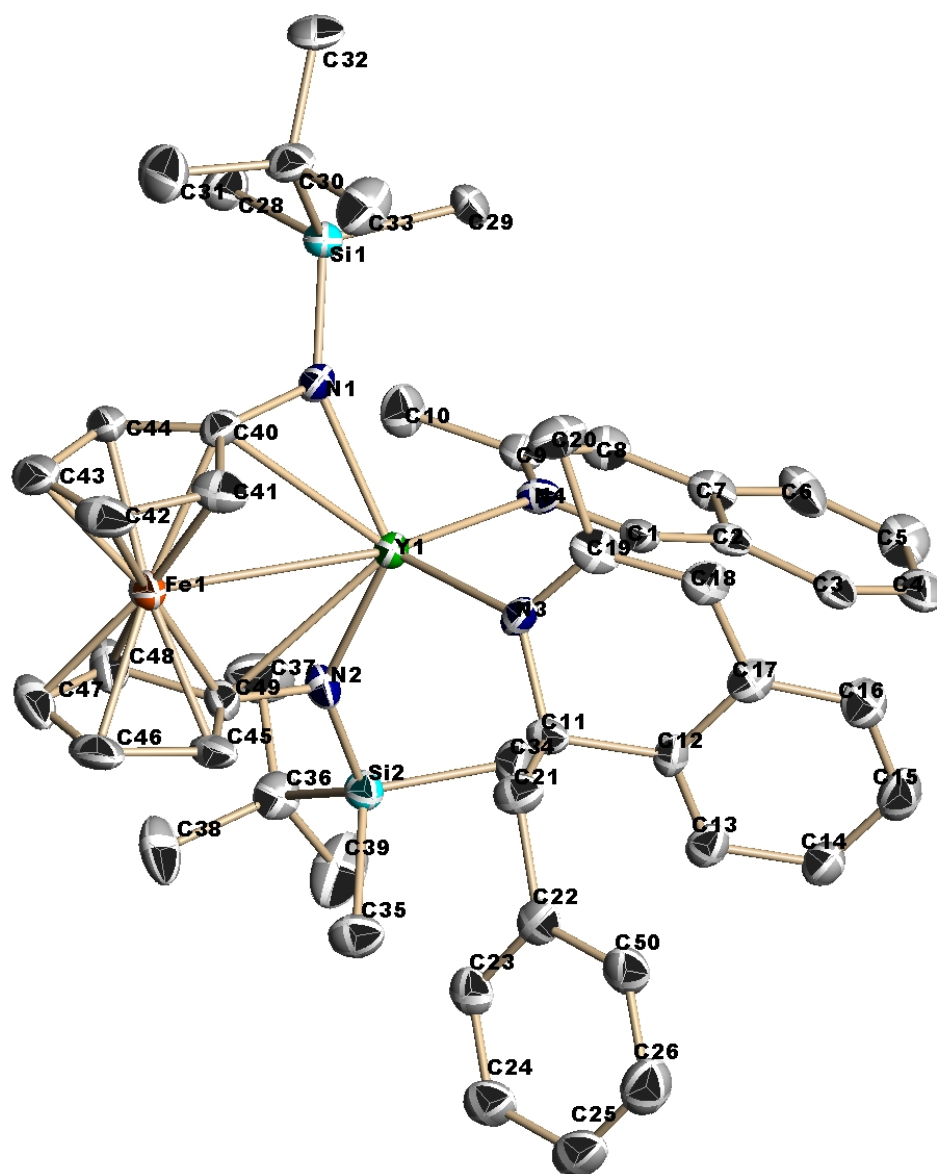


Figure SX3. Thermal-ellipsoid (50% probability) representation of $3^Y\text{-iqn}^{\text{Me}}$. Hydrogen atoms were omitted for clarity.

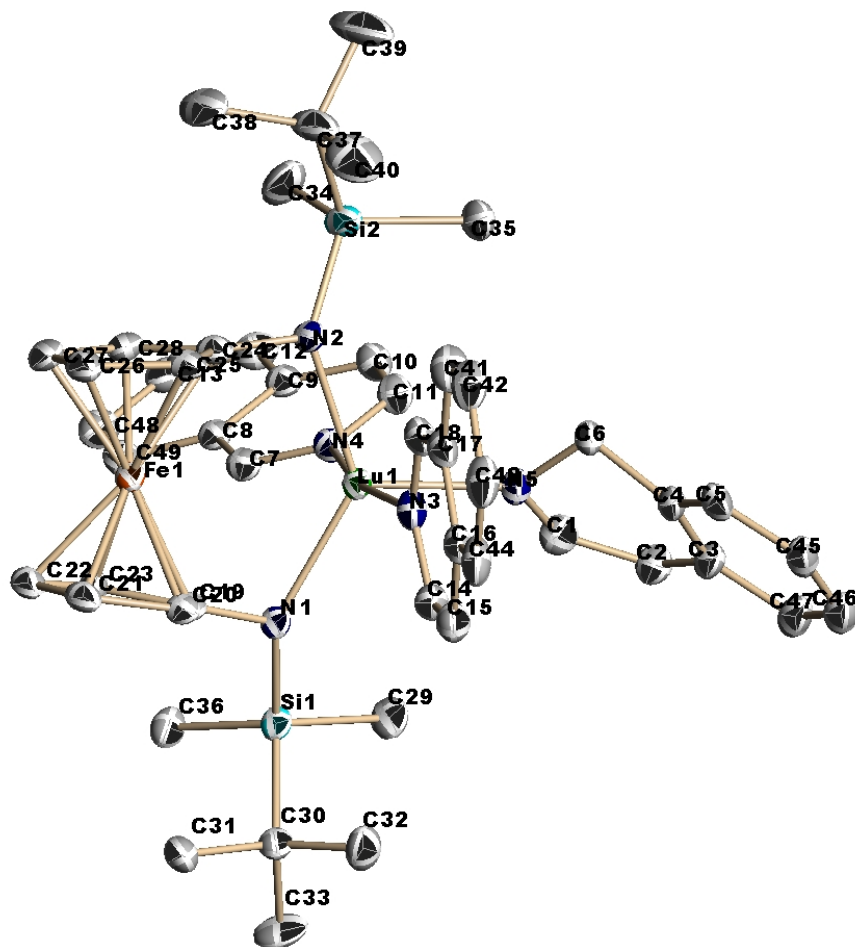
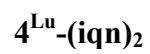


Figure SX4. Thermal-ellipsoid (50% probability) representation of $4^{\text{Lu}}\text{-(iqn)}_2$. Hydrogen atoms were omitted for clarity.

4^Y-1,5-(py)₂

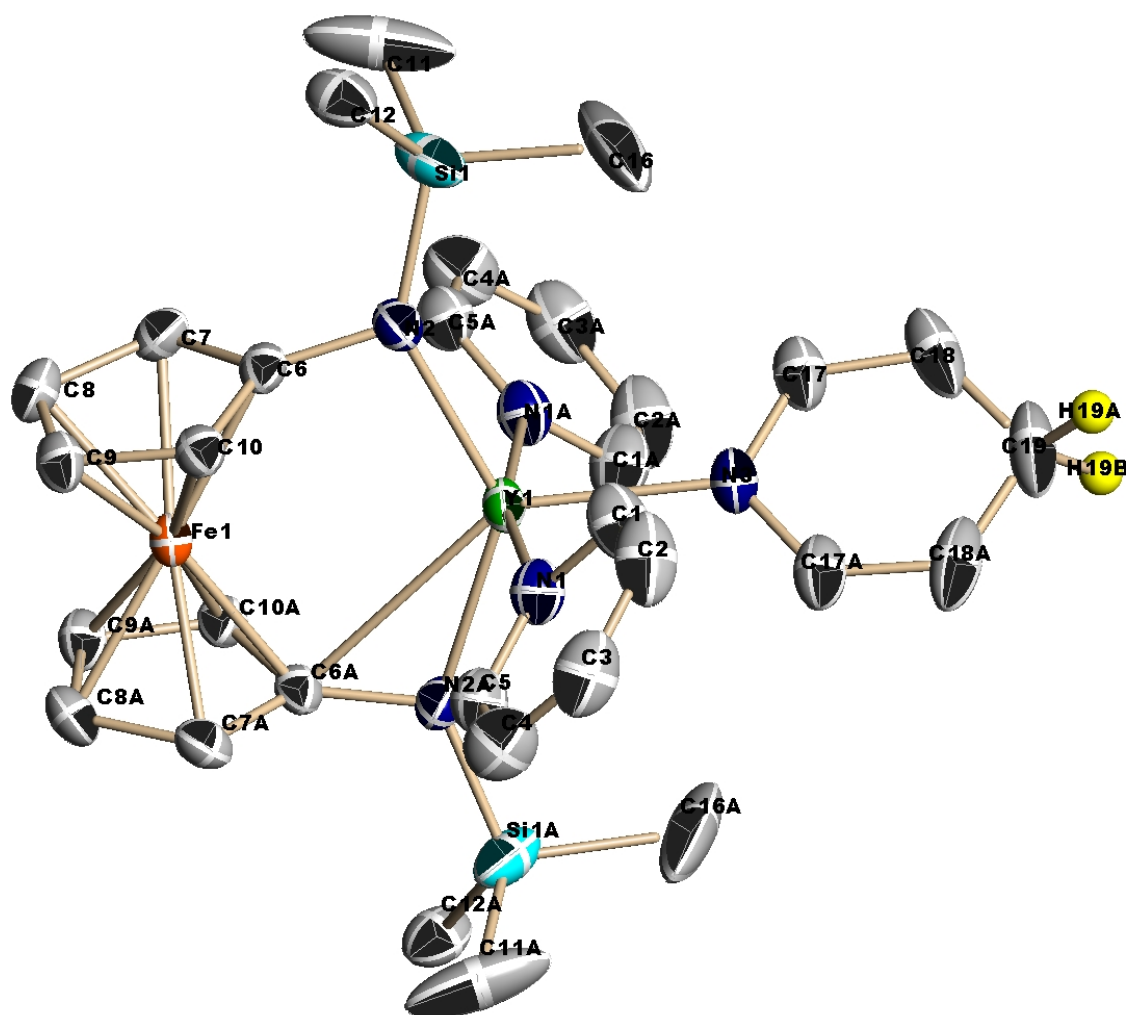


Figure SX5. Thermal-ellipsoid (50% probability) representation of **4^Y-1,5-(py)₂**. Irrelevant hydrogen atoms were omitted for clarity.

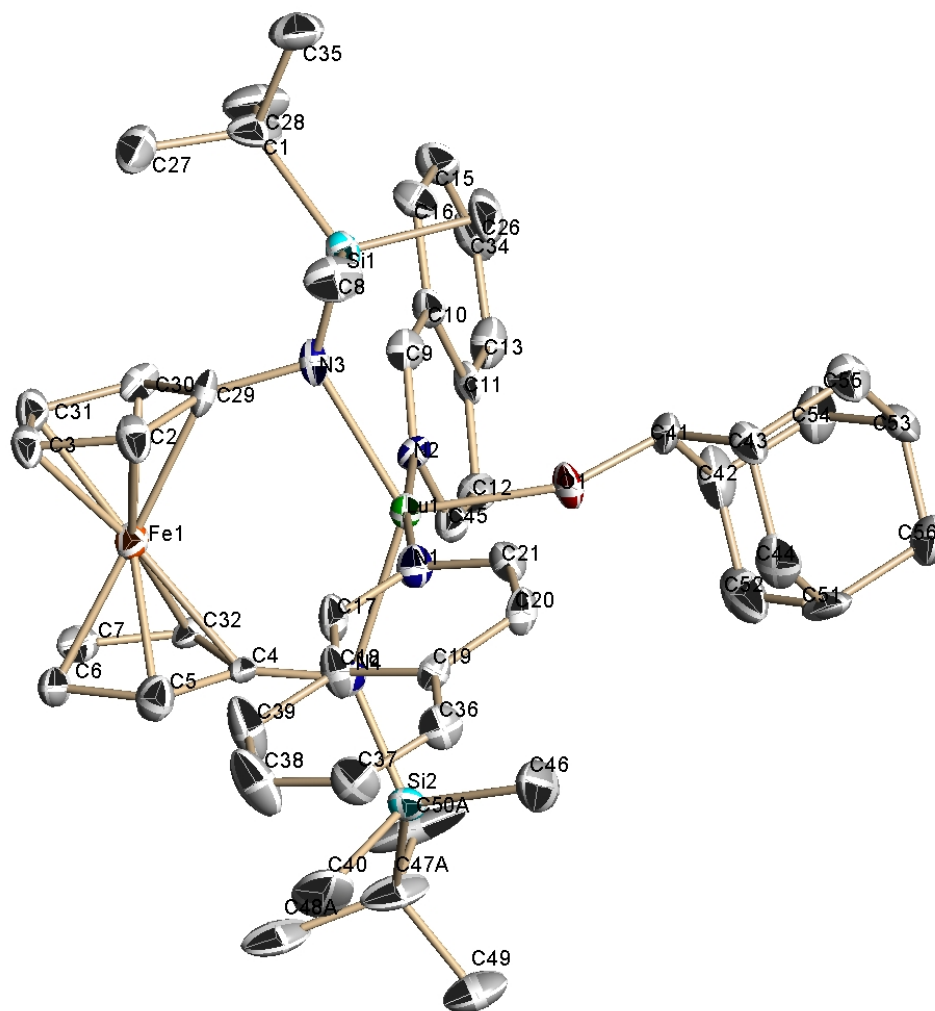
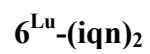


Figure SX6. Thermal-ellipsoid (50% probability) representation of $6^{\text{Lu}}\text{-(iqn)}_2$. Hydrogen atoms and disordered counterparts were omitted for clarity.

8^Y

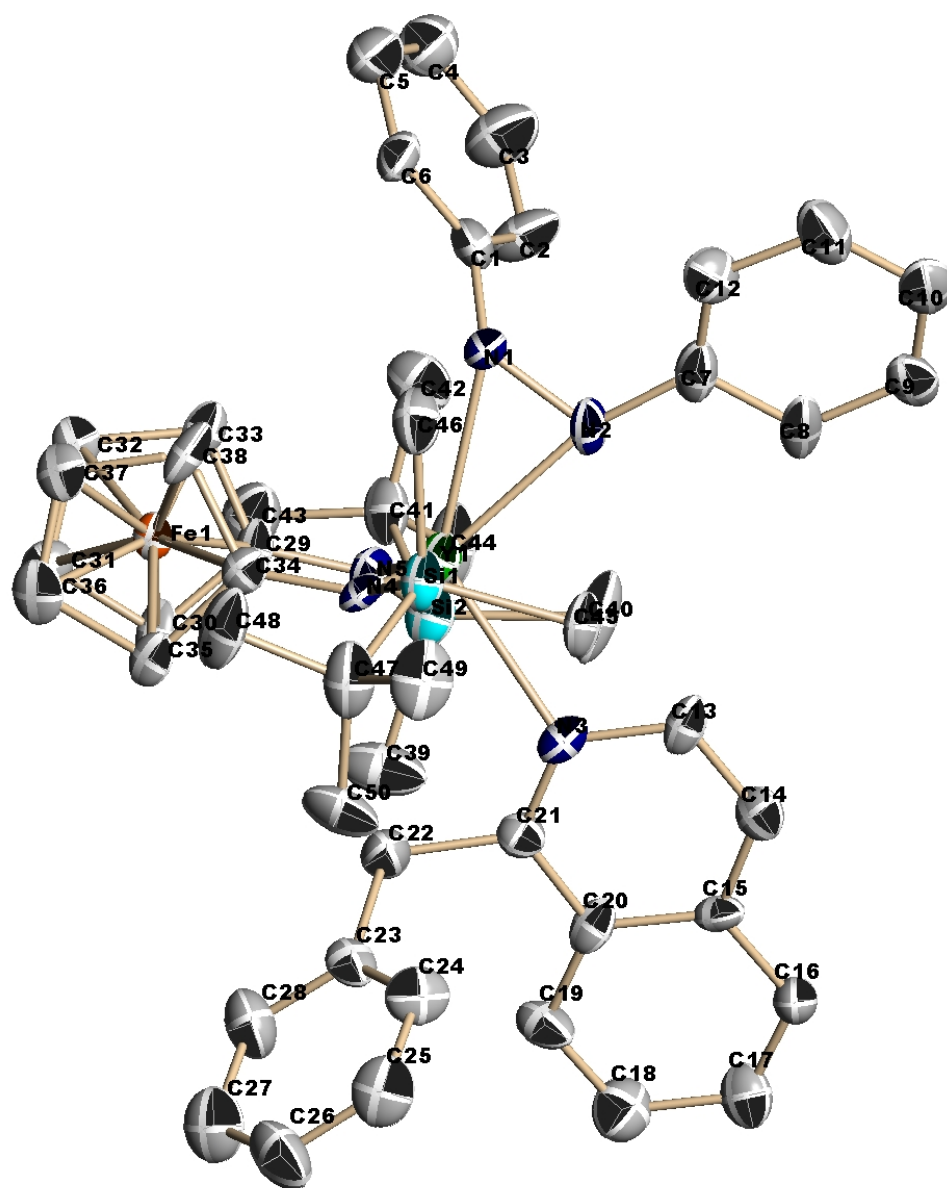


Figure SX7. Thermal-ellipsoid (50% probability) representation of **8^Y**. Hydrogen atoms were omitted for clarity.

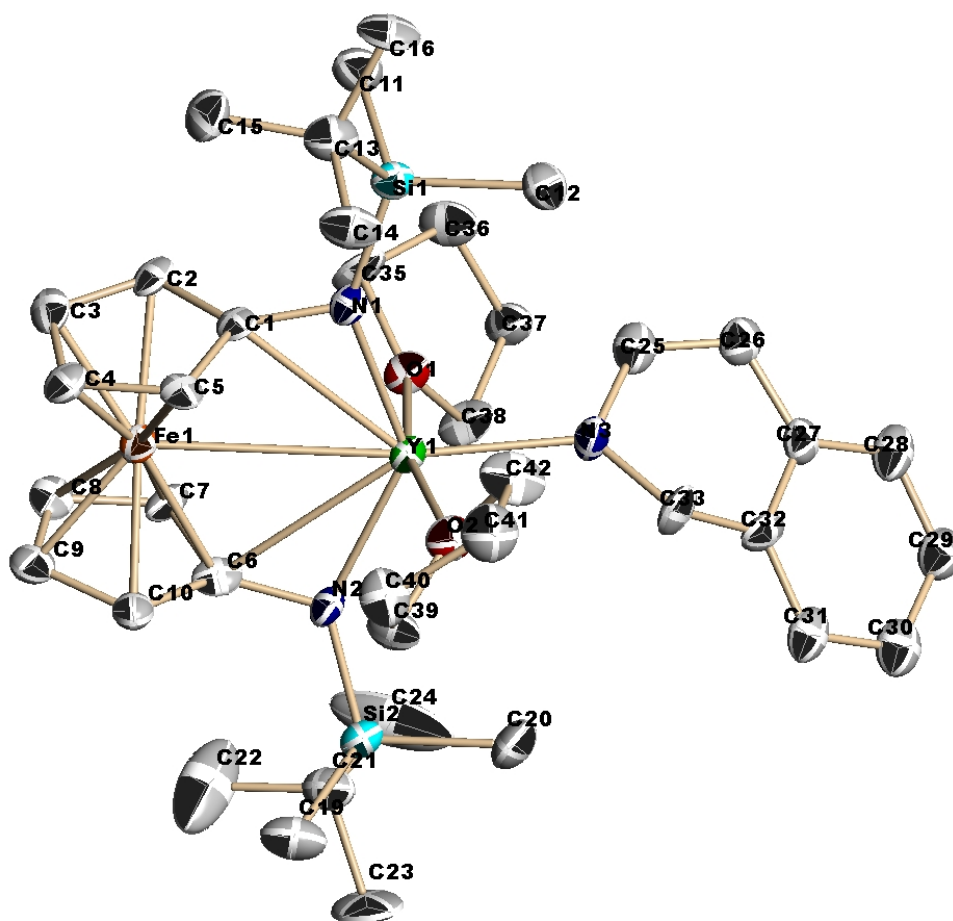


Figure SX8. Thermal-ellipsoid (50% probability) representation of $4^Y-(\text{THF})_2$. Hydrogen atoms were omitted for clarity.

9^{La}

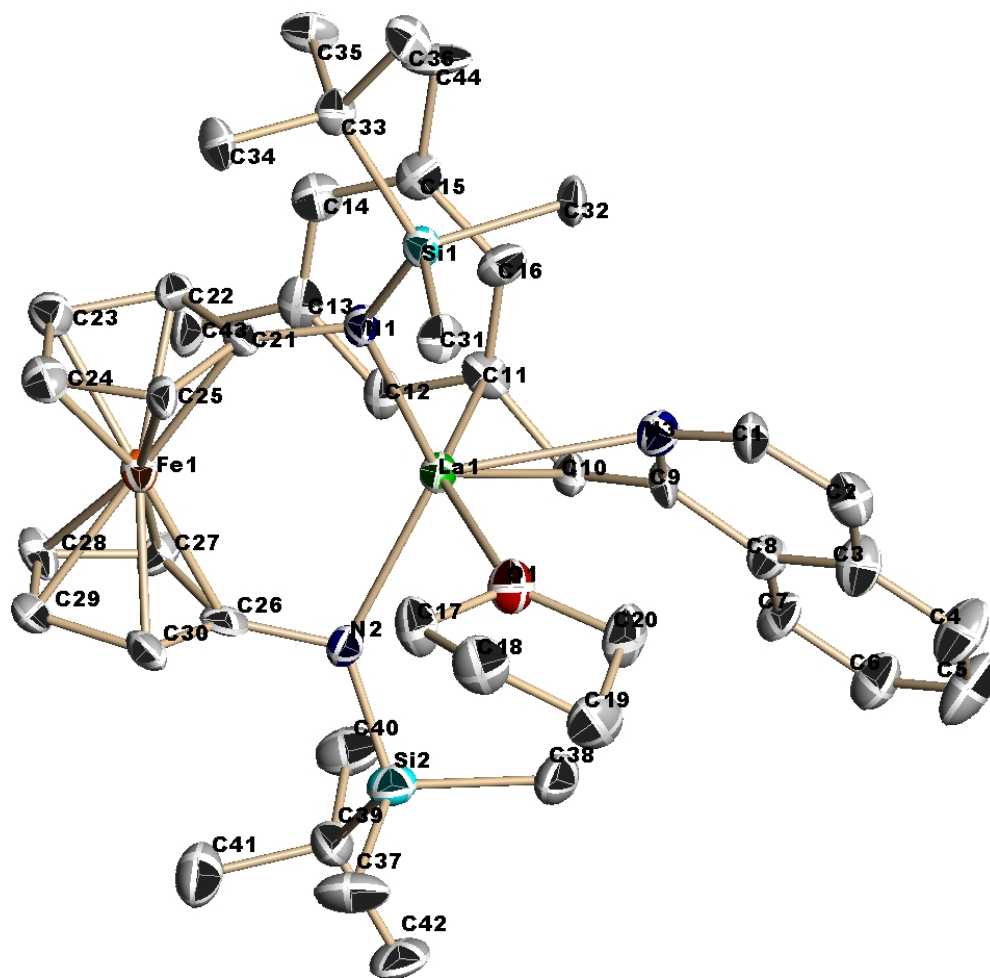
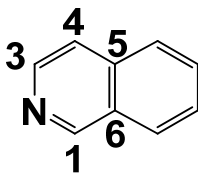


Figure SX9. Thermal-ellipsoid (50% probability) representation of **9^{La}**. Hydrogen atoms were omitted for clarity.

Computational details

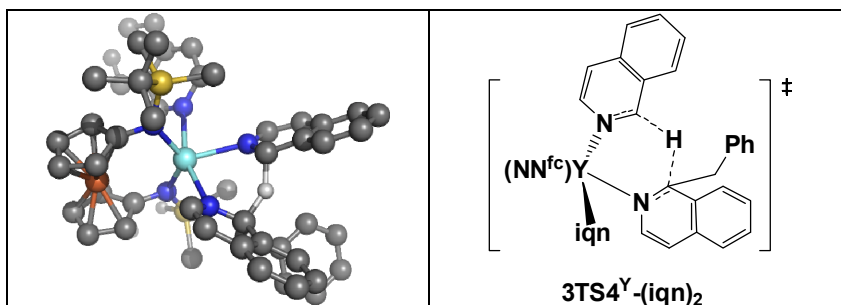
Comparison of metrical parameters



Complex	Parameter	Jaguar	Experimental
3^Y-py (compared to 3^Y-iqn^{Me})	Y-N1(py-amide)	2.26 Å	2.28 Å
	Y-N2 (py)	2.49 Å	2.47 Å
	N1-C1	1.47 Å	1.47 Å
	N1-C3	1.37 Å	1.38 Å
	C3-C4	1.37 Å	1.37 Å
	C4-C5	1.44 Å	1.44 Å
	C5-C6	1.35 Å	1.42 Å
	C6-C1	1.51 Å	1.52 Å
	N2-C1'	1.34 Å	1.33 Å
	N2-C3'	1.34 Å	1.38 Å
	Y-N _{amide}	2.24 Å	2.23 Å
	Y-N _{amide}	2.24 Å	2.23 Å
	N1YN2	98.0°	92.6°
	N _{amide} YN _{amide}	132.7°	128.8°
4^Y-(iqn)₂ (compared to 4^Y-(THF)₂)	Y-N1(py-amide)	2.30 Å	2.29 Å
	N1-C1	1.47 Å	1.47 Å
	N1-C3	1.37 Å	1.37 Å
	C3-C4	1.37 Å	1.36 Å
	C4-C5	1.45 Å	1.44 Å
	C5-C6	1.42 Å	1.42 Å
	C6-C1	1.51 Å	1.51 Å
	Y-N _{amide}	2.26 Å	2.25 Å
	Y-N _{amide}	2.28 Å	2.26 Å
	N _{amide} YN _{amide}	128.8°	144.0°

Transition Structures

	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \\ \text{N} \end{array} \right]^{\ddagger}$ <p>1TS3^Y-(py)</p>
	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \quad \\ \text{py} \quad \text{N} \end{array} \right]^{\ddagger}$ <p>1TS3^Y-(py)₂</p>
	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \quad \\ \text{N} \quad \text{N} \end{array} \right]^{\ddagger}$ <p>3'TS4^Y-(py)</p>
	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \quad \\ \text{py} \quad \text{N} \end{array} \right]^{\ddagger}$ <p>3'TS4^Y-(py)₂</p>
	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \quad \\ \text{py} \quad \text{N} \end{array} \right]^{\ddagger}$ <p>3'TS4^Y-1,5-(py)₂</p>
	$\left[\begin{array}{c} \text{Ph} \\ \\ (\text{NN}^{\text{fc}})\text{Y} \cdots \text{H} \\ \quad \\ \text{iqn} \quad \text{N} \end{array} \right]^{\ddagger}$ <p>3'TS4^Y-(iqn)₂</p>



XYZ Coordinates

1^Y-py

Y1	6.4549609075	8.1019044745	17.3107626128
Si2	8.4779477950	5.9994001516	14.9639833934
Si3	5.1701703407	11.3446762830	18.6346071648
N4	8.1799952040	7.0870327616	16.2925919976
N5	6.3539343783	10.1093216805	18.3023945360
N6	5.4766313410	8.9842832871	15.1624043827
C7	4.3174092726	8.6391316502	14.5727890784
H8	3.7186041459	7.8877315722	15.0780785740
C9	3.8921396628	9.2072502637	13.3742222876
C10	4.6951736466	10.1671989528	12.7613659750
C11	5.8980963509	10.5279577319	13.3693092197
H12	6.5544775210	11.2709553411	12.9288856194
C13	6.2489117573	9.9138803492	14.5665911808
H14	7.1741785356	10.1684796103	15.0754642174
C15	5.4878141117	6.4913456771	18.8926383851
H16	6.1184229189	5.6051620169	18.9903854778
H17	5.2530759799	6.9371586566	19.8609546852
C18	4.3515436817	6.3336018392	18.0005551060
C19	3.1989727193	7.1686445986	18.0857591590
H20	3.1242723174	7.8698029126	18.9142724506
C21	2.1400931547	7.0518055597	17.1873384930
H22	1.2644839304	7.6842488450	17.3156045706
C23	2.1837114919	6.1272203191	16.1365673741
H24	1.3475090395	6.0256502328	15.4511315561
C25	3.3215158631	5.3235815853	16.0020570871
H26	3.3779260327	4.5940604541	15.1972060043
C27	9.9769154282	6.5354820045	13.9265789121
H28	9.8277677832	7.5306202888	13.4910775439
H29	10.1594831688	5.8358121644	13.1015203262
H30	10.8890378332	6.5744137551	14.5324917730
C31	6.9527507055	5.9796759067	13.8385047433
H32	6.8001670433	6.9482090449	13.3494393334
H33	6.0369350126	5.7311452318	14.3866127981
H34	7.0765966953	5.2277356873	13.0494999611
C35	8.8020245164	4.2293132671	15.5699133573
H36	9.6454839706	4.2004955261	16.2693497056
H37	9.0369626940	3.5508612453	14.7406010175
H38	7.9286545783	3.8239934214	16.0947526296
C39	3.6974955878	11.1038485588	17.4655865743
H40	3.2764499578	10.0943610500	17.5314636949
H41	3.9763597294	11.2842274769	16.4216276663
H42	2.8967673310	11.8091476317	17.7192076503
C43	4.5393110899	11.2501091028	20.4230138056
H44	4.0324093555	10.2967202482	20.6133644131
H45	3.8294566701	12.0557593536	20.6469932307
H46	5.3653523728	11.3292117654	21.1389244690
C47	5.8710532053	13.0885886059	18.3603229428
H48	6.1829030599	13.2349361903	17.3195544511
H49	6.7459899279	13.2695478221	18.9947482566
H50	5.1274570331	13.8598018523	18.5965582311
C51	9.2245478265	7.3743485122	17.1836801070
C52	9.4364277497	6.7747643906	18.4826823981
H53	8.7911755034	6.0278261793	18.9250585023
C54	10.6339548288	7.3014439372	19.0452044616
H55	11.0490879311	7.0491943031	20.0119394619
C56	11.1697678247	8.2541168914	18.1246334628

H57	12.0605898622	8.8492330947	18.2762805467
C58	10.2928664337	8.3268614844	17.0035751779
H59	10.4069562014	8.9662451987	16.1388662427
C60	7.8908384178	9.4182799747	20.2096404354
H61	7.2087600682	8.7552828882	20.7239713381
C62	9.2124482934	9.7577731978	20.6158943658
H63	9.7315564647	9.3734908749	21.4839084499
C64	9.7510692705	10.6611633997	19.6483520513
H65	10.7490652180	11.0791589417	19.6586343536
C66	8.7653957852	10.8676297716	18.6400794566
H67	8.8669745567	11.4880637030	17.7599692035
C68	7.5746344922	10.1347308138	18.9937151363
C69	4.3868680612	5.4333427792	16.8949568962
H70	5.2436953824	4.7707156596	16.7910018292
Fe71	9.3045236297	8.8565082182	18.7590139973
X72	7.4429323912#	8.8222676116#	19.8756721182#
X73	9.4323965759#	6.7166823157#	18.0189394693#
H74	4.3901689105	10.6275000187	11.8259339660
H75	2.9488703903	8.8969720101	12.9370448967

1^Y-(py)₂

Y1	6.9679458895	8.5820127385	16.5084350768
Si2	9.1657876233	5.9984227966	15.0927490887
Si3	5.1204018707	11.2536483060	18.4119604152
N4	8.8339266164	7.3605302012	16.1236961226
N5	6.4012513743	10.1319198528	18.0389283238
N6	5.5009801086	8.9024679872	14.4272852973
C7	4.1946003869	8.5918894521	14.5514893075
H8	3.8709574806	8.2270280064	15.5201794816
C9	3.2940753959	8.6982270576	13.4942289469
C10	3.7578321943	9.1336694722	12.2552099608
C11	5.1105793908	9.4465738980	12.1165588584
H12	5.5194691233	9.7833710310	11.1694633027
C13	5.9419264872	9.3201097040	13.2234893896
H14	6.9975141467	9.5580755690	13.1580937916
C15	5.6235955470	6.5865390186	17.0909727162
H16	5.8822322495	5.8071755930	16.3623554296
H17	6.2335156786	6.4001684714	17.9918254923
C18	4.1876286882	6.5582005540	17.4238666103
C19	3.6860415306	7.1229912802	18.6214913024
H20	4.3906792628	7.5553804336	19.3286003733
C21	2.3258803953	7.1367977559	18.9162941807
H22	1.9870407646	7.5764083988	19.8523647999
C23	1.3953666127	6.5880386822	18.0275134013
H24	0.3339424325	6.5982398774	18.2593904398
C25	1.8624768271	6.0139748653	16.8442729059
H26	1.1605107511	5.5604284439	16.1468999734
C27	10.9658228731	6.0289072413	14.4784759095
H28	11.1746380600	6.9165969254	13.8688781992
H29	11.1997650677	5.1475453084	13.8688635377
H30	11.6657487407	6.0399354994	15.3222413222
C31	8.0127283571	6.1224783503	13.5898887312
H32	8.1920917876	7.0375343361	13.0124773295
H33	6.9575785346	6.1096246070	13.8864763843
H34	8.1713708290	5.2745617106	12.9128979028
C35	8.8819429143	4.3228629785	15.9364690198
H36	9.5470142529	4.1961607244	16.7982247087
H37	9.0731695335	3.4896932196	15.2489591335
H38	7.8518651194	4.2310228115	16.2984474676
C39	3.8385679925	11.1995969857	17.0161143236
H40	3.3274795663	10.2311841587	16.9911354149
H41	4.2799275632	11.3792704644	16.0284732744
H42	3.0734897158	11.9687702727	17.1752145124
C43	4.2430373632	10.8586748015	20.0462088064
H44	3.7290509150	9.8932999977	19.9921101452
H45	3.4954629302	11.6234354401	20.2905204279
H46	4.9531979873	10.8136666221	20.8796778235
C47	5.7769289337	13.0364846157	18.5561156985
H48	6.2151486440	13.3966779883	17.6174498601
H49	6.5549370495	13.1067388485	19.3249410394
H50	4.9763562891	13.7331377388	18.8342139120
C51	9.5837076376	7.5151270095	17.2978805059
C52	9.4396248190	6.7664626944	18.5261567002
H53	8.6973809298	5.9975112337	18.6920797193
C54	10.4434510167	7.1847410650	19.4446898985
H55	10.5853409142	6.8083994068	20.4491239328
C56	11.1981285552	8.2274248343	18.8263947960
H57	12.0117121593	8.7768835364	19.2813595058

C58	10.6572634101	8.4506357180	17.5277754008
H59	11.0022524338	9.1844336619	16.8133319684
C60	7.4786376059	9.1403131293	20.1206494695
H61	6.7209710739	8.4038084193	20.3516078354
C62	8.6416068301	9.4280200774	20.8887879787
H63	8.9465311371	8.9256458004	21.7972486540
C64	9.3657562475	10.4630748698	20.2212084528
H65	10.3131807342	10.8789592939	20.5378649932
C66	8.6488495039	10.8089566404	19.0404905192
H67	8.9346889413	11.5549174982	18.3116037018
C68	7.4367990728	10.0269756248	18.9817602854
C69	3.2268954989	5.9954748505	16.5510874300
H70	3.5704453256	5.5157770425	15.6355198778
Fe71	9.2251774094	8.7957164038	19.0127992769
H72	3.0807190231	9.2246310524	11.4106337380
H73	2.2539025204	8.4342579311	13.6523277195
N74	8.2390069309	10.5117173548	15.1668500878
C75	9.7860389171	12.5761631925	14.0936547725
C76	9.4275211412	10.2555553203	14.5870863323
C77	7.8194434013	11.7894633548	15.2184564984
C78	8.5578213587	12.8487257123	14.6963946511
C79	10.2278496137	11.2549790184	14.0366305488
H80	9.7282327381	9.2114155100	14.6001300111
H81	6.8682041098	11.9574575625	15.7126826185
H82	8.1781308753	13.8626927621	14.7706620872
H83	11.1796359809	10.9970919871	13.5830341370
H84	10.3897610022	13.3797430521	13.6811276310

1TS3^Y-(py)

Y1	6.9796186962	8.9291900127	16.428447489 0
Si2	9.4741371922	6.7651019042	14.7175191078
Si3	5.9101986693	12.0761349158	18.0059519260
N4	8.7429803999	7.6425991804	16.0479806522
N5	6.8036745711	10.5671229183	17.8931207109
N6	5.3185301972	9.1708763623	14.8755359578
C7	4.3295797691	8.6390228698	15.7450475281
H8	4.1274410290	9.2842532169	16.6039090233
C9	3.1283802800	8.0945084550	15.1131376521
C10	3.1206616095	7.8278142533	13.7782751267
C11	4.2497193665	8.1491513891	12.9630650001
H12	4.2570959936	7.9503283967	11.8977998401
C13	5.2824428627	8.8270308533	13.5555892990
H14	6.1246829563	9.1825267275	12.9654184993
C15	5.1077759048	7.1320669981	16.8705115911
H16	5.6876265719	6.5157728124	16.1720881541
H17	5.7383885083	7.4067438191	17.7402606030
C18	3.9494376268	6.4034428014	17.4263359993
C19	3.3695229433	6.7959962226	18.6484542151
H20	3.8092243498	7.6200200018	19.2073907290
C21	2.2503961911	6.1422319908	19.1573768500
H22	1.8271511550	6.4607933396	20.1067051920
C23	1.6784321535	5.0759662605	18.4582741709
H24	0.8100555184	4.5605804548	18.8589982791
C25	2.2380851358	4.6766247283	17.2437473817
H26	1.8050911841	3.8456928810	16.6926746088
C27	11.3503140538	7.0300809751	14.6543247574
H28	11.6003903113	8.0904256757	14.5326615974
H29	11.7974359141	6.4837646581	13.8150345100
H30	11.8356755490	6.6788210457	15.5715383640
C31	8.7105108505	7.4094353611	13.1099605525
H32	8.8710196843	8.4880076380	12.9872593330
H33	7.6338440221	7.2144310528	13.0547820519
H34	9.1733745468	6.9158775268	12.2471945496
C35	9.1439129790	4.9039826261	14.8665703620
H36	9.5130463056	4.5145650026	15.8222017158
H37	9.6395131035	4.3395789972	14.0677266233
H38	8.0714551062	4.6835318904	14.8137809471
C39	5.4095420436	12.5845180867	16.2552595053
H40	4.8958957629	11.7804449502	15.7172904533
H41	6.2860083971	12.8717927206	15.6621757795
H42	4.7371413483	13.4500464487	16.2835413631
C43	4.3585525256	11.8607430993	19.0769101131
H44	3.6644142177	11.1352005998	18.6365337648
H45	3.8156495185	12.8059507335	19.1977535306
H46	4.6194241686	11.5011355901	20.0789748355
C47	6.9698337783	13.4447770856	18.7775355138
H48	7.8638540000	13.6455990512	18.1765285300
H49	7.3018077652	13.1775089658	19.7867184139

H50	6.4035298841	14.3807950085	18.8533952265
C51	9.2405283029	7.3899180941	17.3423726002
C52	8.6604306740	6.5055142184	18.3279514336
H53	7.7562354725	5.9291258032	18.1853140614
C54	9.4981496636	6.4843042748	19.4790004784
H55	9.3215695187	5.9215518864	20.3858212770
C56	10.5960438991	7.3645638051	19.2370505202
H57	11.3940689863	7.5872400348	19.9327000345
C58	10.4253784250	7.9418473740	17.9458204282
H59	11.0736289265	8.6681242490	17.4753060963
C60	7.0339488623	9.1616224211	20.0042909205
H61	6.0640884895	8.6824041915	19.9834656476
C62	8.0295660292	9.0026808949	21.0095179109
H63	7.9694064612	8.3490918810	21.8694079699
C64	9.1390799122	9.8317438959	20.6612842918
H65	10.0669974047	9.9119796887	21.2116560022
C66	8.8326889048	10.4901440024	19.4353012314
H67	9.4741869082	11.1710152278	18.8926599630
C68	7.5069578119	10.1113204246	19.0235032385
C69	3.3571315774	5.3327405224	16.7311861110
H70	3.7886356350	5.0089819739	15.7875579044
Fe71	8.8245899155	8.4221129929	19.1862564877
H74	2.2290568679	7.4063742121	13.3197124917
H75	2.2618398476	7.8995728007	15.7333225638

1TS3^Y-(py)₂

Y1	7.0450187383	9.0242334874	16.2901862613
Si2	9.2498805078	6.4109396350	14.8638655881
Si3	5.5482382806	11.7730307792	18.2657804974
N4	8.6938390768	7.5162192825	16.1003735946
N5	6.6370533527	10.4336535866	17.9641892530
N6	5.3321076998	9.2209159225	14.7201568270
C7	4.3399963924	8.6391767463	15.5311718390
H8	4.0789977530	9.2414702539	16.4013994621
C9	3.2209074172	7.9926222769	14.8635936872
C10	3.2966284782	7.7107721167	13.5315593438
C11	4.4359323971	8.1098239423	12.7695507284
H12	4.5133121852	7.8994015173	11.7088675672
C13	5.3911330406	8.8613176486	13.4070354185
H14	6.2434727201	9.2580680052	12.8580433318
C15	6.1811050200	7.1362344512	16.7774457085
H16	5.7664636910	6.4936909562	16.1116192928
H17	5.7983947098	7.4673322385	17.6304163298
C18	3.9978508959	6.4593711635	17.3278264429
C19	3.3659848732	6.9421465644	18.4934962270
H20	3.7882639276	7.8032996020	19.0076938935
C21	2.2212093556	6.3332379317	19.0004626756
H22	1.7610516205	6.7237903496	19.9048794586
C23	1.6682967947	5.2215748899	18.3587228492
H24	0.7796317369	4.7413818787	18.7587882675
C25	2.2767370052	4.7320343592	17.2020959126
H26	1.8611094675	3.8640992241	16.6957812442
C27	11.1465742687	6.4093186240	14.7395459165
H28	11.5350309105	7.3900501969	14.4395747584
H29	11.4943103690	5.6776886692	14.0002166458
H30	11.6079115584	6.1522246782	15.6996922360
C31	8.5420698973	6.9637248601	13.1959085296
H32	8.8530416126	7.9830567697	12.9379199938
H33	7.4471420554	6.9292396755	13.1731119792
H34	8.9034195136	6.3016933781	12.3996705891
C35	8.6931930975	4.6282890510	15.2011081602
H36	9.0547029147	4.2762714933	16.1738920424
H37	9.0725617329	3.9377802243	14.4379189103
H38	7.5999320061	4.5464473579	15.2085724251
C39	4.9353471339	12.4559321603	16.6080472331
H40	4.5524617737	11.6737230049	15.9433726944
H41	5.7380606161	12.9856092967	16.0820928874
H42	4.1244899334	13.1751942300	16.7738245784
C43	4.0472908787	11.2368969540	19.2990600313
H44	3.4534041927	10.4740093090	18.7817716402
H45	3.3835341407	12.0830485238	19.5156183465
H46	4.3625107723	10.8128620382	20.2595359052
C47	6.4246089366	13.1728674911	19.1995982516
H48	7.2754068460	13.5631505632	18.6292068501
H49	6.8070768547	12.8309177181	20.1675206253
H50	5.7395934150	14.0076715374	19.3906645886
C51	9.1787638609	7.2928326988	17.4033909592
C52	8.5991776310	6.4369206576	18.4115876387

H53	7.6767483211	5.8841616075	18.2949241234
C54	9.4495362600	6.4265729165	19.5538609990
H55	9.2735552521	5.8855957365	20.4740986153
C56	10.5528023016	7.2936757095	19.2892889768
H57	11.3576989276	7.5237630460	19.9747705163
C58	10.3769717681	7.8429486255	17.9865615583
H59	11.0374851988	8.5450018611	17.4954074392
C60	6.9878099729	9.0291508686	20.0666220586
H61	6.0521025335	8.4865397449	20.0614237634
C62	8.0087694317	8.9375059361	21.0552413980
H63	7.9984585257	8.2926537630	21.9239506540
C64	9.0729840775	9.8093198516	20.6714279810
H65	10.0075048861	9.9404974968	21.2006765998
C66	8.7080046404	10.4342778239	19.4442002852
H67	9.2975907503	11.1484827379	18.8852312521
C68	7.3915518494	9.9874474118	19.0660079551
C69	3.4216832840	5.3421351626	16.6912472591
H70	3.8906335022	4.9446924487	15.7946446182
Fe71	8.7868129071	8.3594250488	19.2299735662
H72	2.4665253236	7.2109367757	13.0374535239
H73	2.3488307878	7.7275052551	15.4486451565
N74	8.3071581625	10.6142105546	14.8075063898
C75	9.7513689841	12.5132374431	13.3681339962
C76	9.6520556184	10.5569247465	14.7508666210
C77	7.6742477593	11.6031172536	14.1473987713
C78	8.3586943766	12.5703939606	13.4171112763
C79	10.4098384324	11.4876545958	14.0463618651
H80	10.1062082992	9.7255775772	15.2817294482
H81	6.5906614963	11.5990877398	14.2156963320
H82	7.8067901006	13.3486361190	12.9004625677
H83	11.4914106540	11.4028373795	14.0295591189
H84	10.3145880205	13.2546612779	12.8087049301

3^Y

Y1	6.9179775130	8.4506931575	16.4741129739
Si2	10.0642947812	8.5230184048	14.5143124229
Si3	6.3550892753	11.9383301259	17.6798748151
N4	8.9687367401	7.9335321779	15.7334270086
N5	6.5814225977	10.2153247929	17.8137973253
N6	5.2360276605	7.1985903874	15.7071435422
C7	3.8841043223	7.2635207000	16.3042238162
H8	3.8617031600	8.1217630094	16.9936736746
C9	2.8339280382	7.4478619005	15.2297445012
C10	3.0126900459	6.8288386404	14.0423699899
C11	4.2636903156	6.1635609065	13.7481240157
H12	4.3972309858	5.5901685141	12.8376565494
C13	5.3275869010	6.4406673989	14.5563145002
H14	6.3360516169	6.1358159827	14.2694179799
C15	3.6215231475	5.9855650135	17.1755149576
H16	3.6011509249	5.1224635124	16.5019936911
H17	4.4860465646	5.8583930868	17.8408346037
C18	2.3528073740	6.0588957754	17.9910663646
C19	2.3677277112	6.5822887298	19.2925056443
H20	3.3133671866	6.8941930484	19.7321395434
C21	1.1956249108	6.6982556477	20.0405247923
H22	1.2362109991	7.1036664716	21.0483305929
C23	-0.0239559022	6.2886908565	19.4987195106
H24	-0.9382883994	6.3743478208	20.0793408338
C25	-0.0552938404	5.7617614158	18.2062252800
H26	-0.9982885168	5.4344193626	17.7758049998
C27	11.5221653154	9.5203653907	15.2090544912
H28	11.1810377570	10.3474025320	15.8423186555
H29	12.1209010356	9.9501293857	14.3969699681
H30	12.1932397825	8.8943631927	15.8079630513
C31	9.0110115090	9.6575596690	13.4196284379
H32	8.6483685033	10.5323139146	13.9753465503
H33	8.1427024451	9.1291252543	13.0065370772
H34	9.5868453721	10.0402212416	12.5691691912
C35	10.7609036744	7.1003853739	13.4774504330
H36	11.3266747407	6.3985588440	14.1014403200
H37	11.4364730729	7.4633046835	12.6934824842
H38	9.9570074123	6.5348455699	12.9933552928
C39	5.9925781800	12.2526371788	15.8469085388
H40	5.1203338496	11.6815998431	15.5060312288
H41	6.8464938272	11.9845364134	15.2112212330
H42	5.7782848083	13.3109917891	15.6593532910
C43	4.8931883528	12.5235010217	18.7312325106
H44	3.9672101648	12.0193624661	18.4337950929

H45	4.7330189623	13.6043780367	18.6375501099
H46	5.0596555072	12.3066197888	19.7928998542
C47	7.8863990510	12.9388793010	18.1891781362
H48	8.7725920103	12.6385529323	17.6180920708
H49	8.1163049419	12.8119415091	19.2533333115
H50	7.7291045084	14.0106996968	18.0180995910
C51	9.2785628310	7.2806875408	16.9197376216
C52	8.4940749876	6.1856194892	17.4697995026
H53	7.7091528169	5.6595823409	16.9372348980
C54	9.0324455858	5.8105056177	18.7389941128
H55	8.6775423800	5.0048273707	19.3667737187
C56	10.1222455890	6.6855985168	19.0193163730
H57	10.7286021977	6.6745334569	19.9146386348
C58	10.2346538860	7.6210004141	17.9468497364
H59	10.9364346356	8.4402565488	17.8897279299
C60	6.4144256620	8.3300340932	19.4721546623
H61	5.4544747404	7.9432021735	19.1524023234
C62	7.1840172962	7.8514579335	20.5742640038
H63	6.9512606921	6.9926452637	21.1881377268
C64	8.3157061783	8.7086851400	20.7142422927
H65	9.1039725846	8.6011201804	21.4465825752
C66	8.2618952592	9.6936951117	19.6833618187
H67	9.0000201521	10.4608467677	19.4968527779
C68	7.0386175603	9.5274657796	18.9343378134
C69	1.1200312830	5.6481465515	17.4620527283
H70	1.0867992666	5.2378824358	16.4565001098
Fe71	8.3684501585	7.7581322075	18.8862290331
X72	7.6452000000#	8.6790000000#	19.8064000000#
X73	9.6258000000#	6.7812000000#	17.9226000000#
H74	2.2466413311	6.8810771950	13.2711856427
H75	1.9392366481	8.0205767910	15.4538600095

3^Y-py

Y1	6.9175271451	8.9854972034	16.2043990043
Si2	9.6249265232	7.1618215265	14.4272697698
Si3	5.1441549321	11.6443968469	18.1573795437
N4	8.8543998087	7.9309478804	15.7904822003
N5	6.2329712707	10.3092850038	17.8802322901
N6	5.2416235999	7.7440213610	15.3531969400
N7	7.0149616643	10.7131307987	14.4078463608
C8	6.0867524342	10.7577038018	13.4307918376
H9	5.3357490831	9.9722804026	13.4403090080
C10	6.0874065221	11.7473302493	12.4516307422
C11	7.0805634277	12.7249755077	12.4834887000
C12	8.0438919482	12.6801270743	13.4922483431
H13	8.8346264706	13.4204028535	13.5529033792
C14	7.9747414548	11.6584820931	14.4324978296
H15	8.7043037892	11.5839212092	15.2345744808
C16	4.0257494249	7.4757723513	16.1496636650
H17	4.0952387564	8.0701856839	17.0712746070
C18	2.7868082824	7.8738920698	15.3760896325
C19	2.7706055800	7.6672604740	14.0392925774
C20	3.9741073138	7.2504906933	13.3540275683
H21	3.9627234210	6.9769754552	12.3044928282
C22	5.1567092407	7.3719768363	14.0333292168
H23	6.1071663102	7.2561960456	13.5095808910
C24	4.0021373933	5.9697760885	16.5877707524
H25	3.8054750391	5.3619393078	15.6983289803
H26	5.0120813742	5.7198807954	16.9369542823
C27	3.0025598505	5.6774971009	17.6791240850
C28	3.4071125665	5.6568010735	19.0227274874
H29	4.4598710234	5.7970980061	19.2614666384
C30	2.4893085815	5.4444543788	20.0518130741
H31	2.8283958409	5.4293258246	21.0847363417
C32	1.1405179237	5.2457316312	19.7547935107
H33	0.4226796951	5.0779783053	20.5533799824
C34	0.7226465527	5.2567169602	18.4229612611
H35	-0.3253074807	5.0964453678	18.1819036168
C36	11.5155638185	7.1914253223	14.5839031262
H37	11.8992105884	8.2173442305	14.6240708884
H38	11.9935611624	6.6883457978	13.7346135515
H39	11.8447138308	6.6809180677	15.4960411369
C40	9.1389394184	8.1124627825	12.8593255094
H41	9.4810112645	9.1527381395	12.9020399735
H42	8.0561091448	8.1222595443	12.6906280910
H43	9.5978945601	7.6489425201	11.9781717605
C44	9.0852002318	5.3511791650	14.2337235614
H45	9.3200608347	4.7703605651	15.1335100091

H46	9.5893396086	4.8652888006	13.3892448655
H47	8.0042227233	5.2735264171	14.0679527705
C48	4.2236299877	12.0030171802	16.5409682855
H49	3.6912952945	11.1175851516	16.1742466995
H50	4.9027890755	12.3421047217	15.7504921413
H51	3.4809724724	12.7955180837	16.6928904993
C52	3.8861006532	11.2468279776	19.5200179313
H53	3.2645076475	10.3847480849	19.2531427241
H54	3.2171131888	12.0957378096	19.7067688907
H55	4.3871285848	11.0097532283	20.4657042074
C56	6.0824445738	13.2131490771	18.6794065269
H57	6.7806233150	13.5376121655	17.8985082515
H58	6.6662899498	13.0392393827	19.5909155696
H59	5.3989067122	14.0468379746	18.8819137906
C60	9.1632113026	7.4788244134	17.0815015447
C61	8.4980932006	6.4144342746	17.8045643812
H62	7.6777351075	5.8261981583	17.4144358971
C63	9.1451673604	6.2345051689	19.0607559114
H64	8.8738982501	5.5145158773	19.8213443908
C65	10.1950135474	7.1988079293	19.1533494391
H66	10.8520695395	7.3386402550	20.0011834423
C67	10.1847898297	7.9820032728	17.9633943680
H68	10.8419107474	8.8087484479	17.7315214149
C69	6.4480451341	8.5743152032	19.7210399541
H70	5.5388682913	8.0244859459	19.5186388903
C71	7.3634874756	8.3339532917	20.7839042831
H72	7.3027125327	7.5345665137	21.5099736838
C73	8.4048660274	9.3081396137	20.6967984782
H74	9.2691862524	9.3705507441	21.3441479475
C75	8.1354690757	10.1435646948	19.5746239356
H76	8.7425830917	10.9687772833	19.2273011324
C77	6.8908896539	9.7304349111	18.9737566953
C78	1.6441477560	5.4683891270	17.3966441230
H79	1.3115573417	5.4748504433	16.3622453717
Fe80	8.3758131058	8.1510876809	18.9919317067
X81	7.64520000000#	8.67900000000#	19.80640000000#
X82	9.62580000000#	6.78120000000#	17.92260000000#
H83	5.3205128037	11.7453819024	11.6844077131
H84	7.1053887632	13.5103369679	11.7336036179
H85	1.8724796920	7.8724421828	13.4591144510
H86	1.9247268467	8.2628996073	15.9101775187

3^Y-(py)₂

Y1	7.1083128717	8.9341720801	15.8359336663
Si2	4.3018252350	7.0515651138	14.2354842463
Si3	10.2825441668	10.2493211646	17.3600459989
N4	5.8250025111	7.2301580751	15.0561395623
N5	9.0883164616	9.0680008850	16.9003446869
N6	5.6275149161	9.7669785099	17.3985088718
N7	6.7044047488	11.1539101734	14.6042794868
C8	6.8338321737	11.3308239917	13.2731755267
H9	7.1217420021	10.4555532072	12.7014517303
C10	6.6157641367	12.5524217333	12.6475601028
C11	6.2529090774	13.6496778095	13.4304341736
C12	6.1133691391	13.4761715354	14.8044470839
H13	5.8255031282	14.2966727316	15.4531601377
C14	6.3361278366	12.2155292110	15.3544832108
H15	6.2186811044	12.0365025725	16.4192762015
C16	5.9539118219	10.1447035370	18.7909311664
H17	7.0304192997	9.9929483808	18.9312334266
C18	5.5930373880	11.5950535829	19.0328774784
C19	4.4431729502	12.0625533968	18.4857939837
C20	3.7239670951	11.2597928199	17.5278440510
H21	2.7601437124	11.5674900853	17.1367465768
C22	4.3983034456	10.1941868715	16.9799664967
H23	4.0030375688	9.7036845991	16.0898583995
C24	5.2196723317	9.1755795512	19.7838657656
H25	4.1421687989	9.3159457451	19.6463167087
H26	5.4606730152	8.1515727330	19.4752311355
C27	5.6005707291	9.3756068346	21.2301346867
C28	6.5682175711	8.5611286431	21.8369969329
H29	7.0081676455	7.7450028659	21.2675520032
C30	6.9640739275	8.7670893673	23.1591763208
H31	7.7148447370	8.1196690464	23.6058103179
C32	6.3940253408	9.7975669608	23.9074298440
H33	6.6988636462	9.9605950652	24.9380049517
C34	5.4221642125	10.6112360149	23.3226830921
H35	4.9651912366	11.4116095657	23.8998163424

C36	4.3045814584	5.5437982975	13.0750009990
H37	5.0490739457	5.6416747633	12.2753083555
H38	3.3263947895	5.4053052868	12.5984887572
H39	4.5346860871	4.6246184484	13.6257910021
C40	4.0339344258	8.6024505672	13.1705347788
H41	4.8147907578	8.7004451323	12.4061731680
H42	4.0272837723	9.5252151667	13.7617779645
H43	3.0722918366	8.5460073562	12.6466243346
C44	2.8325354626	6.8338821899	15.4185229317
H45	2.9736304559	5.9501588568	16.0519300487
H46	1.8913967379	6.6983723271	14.8712742020
H47	2.7135634984	7.6950718580	16.0848701150
C48	9.7954706472	11.9270378084	16.6183686032
H49	8.8492877853	12.2884941648	17.0359335708
H50	9.6904545691	11.8982799929	15.5271825333
H51	10.5622466153	12.6758045439	16.8508330693
C52	10.4378818966	10.4549306060	19.2395155119
H53	9.4957594102	10.7888474146	19.6883531394
H54	11.2102358875	11.1901264911	19.4975275611
H55	10.7120883226	9.5087067142	19.7196425816
C56	12.0118940191	9.7874802754	16.7097161444
H57	12.0456010901	9.7370295803	15.6147281020
H58	12.3227070114	8.8069021025	17.0883321342
H59	12.7658259161	10.5173083823	17.0299261128
C60	6.2786617909	6.1581802827	15.8409657108
C61	5.9362872947	5.8865608070	17.2190532169
H62	5.2981370889	6.5159735069	17.8235284523
C63	6.5397936194	4.6583306567	17.6124980747
H64	6.4680620984	4.1965171993	18.5883424907
C65	7.2965756101	4.1658770644	16.5053622132
H66	7.8994649282	3.2673260345	16.4996408251
C67	7.1673362834	5.0964173255	15.4347141782
H68	7.6339462201	5.0187474189	14.4625807676
C69	8.8524508814	7.2042510056	18.6146150997
H70	8.2967779425	7.7548966346	19.3602116135
C71	9.3184614557	5.8635277888	18.7202775432
H72	9.1485927245	5.1931414427	19.5521077440
C73	10.0059030281	5.5386919428	17.5104057379
H74	10.4472205420	4.5804936182	17.2694049560
C75	9.9605398530	6.6804582364	16.6592647389
H76	10.3837663344	6.7580141267	15.6670750880
C77	9.2807198458	7.7509321331	17.3493368429
C78	5.0286799947	10.4004415143	22.0009851940
H79	4.2701353243	11.0363430175	21.5538707799
Fe80	8.0349052619	5.9906114325	17.1105283962
X81	9.5965786397	6.7660183385	17.7085235310
X82	6.8869134234	5.2345503229	16.3173261884
H83	6.7301646703	12.6372917258	11.5718100743
H84	6.0777796132	14.6197471068	12.9737912514
H85	4.0957221037	13.0720822803	18.7032378841
H86	6.2106413728	12.2044399908	19.6867197975
X87	7.7702623614	7.3628483361	16.4311568116
C88	10.1468925463	7.8504139487	11.4528829580
C89	8.9205292044	7.2194101697	11.6536763900
C90	8.1443153543	7.5930101069	12.7492988076
N91	8.5280997419	8.5436411673	13.6226521300
C92	9.7154949777	9.1465209148	13.4233695274
C93	10.5521904759	8.8339980028	12.3556799256
H94	10.7786489937	7.5782340398	10.6120085761
H95	8.5676394393	6.4443316374	10.9808514241
H96	7.1902972319	7.1252181194	12.9755955474
H97	10.0006655460	9.8907798251	14.1590965264
H98	11.5025950646	9.3459859481	12.2443448584

3'TS4^Y-(py)₂

Y1	7.1395351685	9.1229354852	16.4179951510
Si2	9.6742334314	7.8712966525	13.9991200609
Si3	5.5937308587	10.7798285202	19.4594891571
N4	8.9850895929	8.1521988553	15.5768729915
N5	6.6841334101	9.7608560566	18.5486365988
N6	5.6827845035	7.2603570269	15.9617155605
N7	5.6297300894	10.0830070675	14.7417101741
C8	5.0005576843	9.1909455753	13.8754981786
H9	5.5922679678	8.3033432005	13.6568694216
C10	4.2237209815	11.8608649290	13.8966679490
H11	3.9218441247	12.9005128972	13.9588198634
C12	5.1674551304	11.3583262574	14.7694551387
H13	5.6266120986	12.0058565833	15.5099258764

C14	4.2763980255	7.4390787411	15.7761410424
H15	4.2224679466	8.2910629115	14.7759767147
C16	5.5697563578	5.0605145021	14.9345971752
H17	6.1014806403	4.1779247394	14.5969974682
C18	6.2541625398	6.1244382138	15.4725253252
H19	7.3361560987	6.0935010213	15.5548696696
C20	3.6580844719	8.3078513222	16.8981791568
H21	3.9312485909	7.8425764802	17.8509668363
H22	4.1460896972	9.2891698568	16.8848778801
C23	2.1583480561	8.4808043952	16.8259684434
C24	1.5633798906	9.3233969274	15.8755616887
H25	2.1896630865	9.8870040860	15.1900670857
C26	0.1761965132	9.4428039299	15.7955357103
H27	-0.2657869506	10.0986380772	15.0496272146
C28	-0.6441353116	8.7263495739	16.6688621726
H29	-1.7251128921	8.8197973410	16.6057245189
C30	-0.0653796845	7.8912433237	17.6246002662
H31	-0.6938741660	7.3301632104	18.3114406769
C32	11.1806131791	8.9866076024	13.6795221306
H33	10.9087394047	10.0482667171	13.7120691812
H34	11.6328123283	8.7866091721	12.7003191753
H35	11.9535170754	8.8242987635	14.4397177657
C36	8.3633934663	8.2350143324	12.6768987884
H37	7.8875653626	9.2154398281	12.7955318445
H38	7.5736081810	7.4753159512	12.6914632664
H39	8.8178510597	8.2139654233	11.6788740997
C40	10.2416195531	6.0740260878	13.7731875887
C41	4.6937205337	11.9733615229	18.2917641099
H42	4.0832054193	11.4654803584	17.5383803987
H43	5.3943255074	12.6376163498	17.7717539741
H44	4.0183568258	12.6108682939	18.8755149305
C45	4.3060173395	9.7748446551	20.4273950971
H46	3.5869473228	9.2849733067	19.7625370463
H47	3.7377842680	10.4136091198	21.1145257401
H48	4.7884897430	8.9940268448	21.0266088117
C49	6.5097786916	11.8576330988	20.7347567233
C50	9.7185941863	7.6889314964	16.6843160043
C51	9.6699460495	6.3670151289	17.2628293969
H52	9.0208329964	5.5680466182	16.9329849911
C53	10.6223555387	6.2882112700	18.3177003346
H54	10.8063242866	5.4266851306	18.9460207887
C55	11.2511713790	7.5645475437	18.4401739607
H56	11.9973786147	7.8367026777	19.1749226032
C57	10.6879397579	8.4268390076	17.4551645828
H58	10.9437287989	9.4643085331	17.2877997326
C59	7.2681759477	7.4804793559	19.5250297788
H60	6.4785979599	6.9054331380	19.0592648401
C61	8.2432228454	6.9922216405	20.4420373968
H62	8.3438509553	5.9692904419	20.7787811053
C63	9.0901561041	8.0828035205	20.8054982156
H64	9.9456205634	8.0288910613	21.4658272240
C65	8.6476070860	9.2372442931	20.0974360059
H66	9.0909062156	10.2223233499	20.1455604568
C67	7.4794769979	8.8941267556	19.3233618945
C68	1.3230056740	7.7710303349	17.6997472246
H69	1.7675909907	7.1125728297	18.4425423918
Fe70	9.2216765780	7.7319650099	18.7798478696
X72	8.1366987575#	8.2503194829#	20.0588701930#
X73	10.2664009961#	7.1481695343#	17.6442418973#
C74	3.7251913834	11.0020655290	12.8832019990
C75	4.1339664349	9.6931868372	12.8486956433
C76	8.6754315910	12.1227734731	17.1254657897
N77	8.2438498558	11.4360675183	16.0509239576
C78	8.5648838038	11.8971099272	14.8277637893
C79	9.3217790324	13.0477067064	14.6307530781
H80	8.3796082259	11.7111560918	18.0857354880
H81	8.1926108748	11.3196148264	13.9871123214
H82	9.5536638109	13.3776730781	13.6233613836
C83	9.7681163742	13.7541545613	15.7481326149
C84	9.4380923273	13.2836508597	17.0178919580
C85	3.5128201405	6.2487126855	15.3750515964
C86	4.1448132516	5.1282054080	14.9312750051
H87	9.7611784376	13.8028434643	17.9142749729
H88	10.3613926377	14.6563271111	15.6294416564
H89	3.0426853423	11.3855206791	12.1289527220
H90	3.7834323589	9.0087333692	12.0821993440
H91	5.7989628096	12.4894227239	21.2815843652
H92	7.0419349160	11.2477183643	21.4723862997
H93	7.2436146582	12.5238213053	20.2645493958
H94	10.6978395466	5.9276311727	12.7865061165
H95	10.9845215447	5.7900575730	14.5264392051

H96	9.4031576389	5.3729705700	13.8565962731
H97	2.4299645042	6.3065986782	15.3980098139
H98	3.5611196344	4.2694945132	14.6055691225

3'TS4^Y-1,5-(py)₂

Y1	7.1980524448	8.3429648717	16.8015650875
Si2	9.8445734824	6.3563453172	14.8428052474
Si3	5.8954529668	8.9969365687	20.3148398942
N4	9.1309461745	7.5248728151	15.9442506827
N5	6.9529475455	9.0852994442	18.9162898057
N6	5.1493592653	7.6893116455	15.5720309069
N7	7.1940692821	10.3786651050	15.4032326232
C8	7.0852072931	9.7943320579	14.1634002318
H9	7.9723958091	9.2609145630	13.8279719469
C10	5.9597413417	9.8423965144	13.3832451395
C11	4.7594343432	10.4364477660	13.9300319703
C12	5.0209650261	11.3747109374	15.0078551507
H13	4.2825400367	12.1154563063	15.2974974019
C14	6.1766900184	11.2387053067	15.7315158127
H15	6.3439646285	11.8423732262	16.6208489169
C16	3.8696104677	8.2407826722	15.3131386061
H17	4.1292770892	9.3342572054	14.5399551394
C18	2.9596479211	7.4290711855	14.5029078513
C19	3.4030661272	6.3366567425	13.8199567697
C20	4.7546324778	5.9098465900	13.9615661988
H21	5.1453092592	5.0425197736	13.4423923762
C22	5.5388647057	6.6085703997	14.8461576129
H23	6.5536121691	6.2661516207	15.0331083716
C24	3.2746846042	8.9731701708	16.5336359234
H25	3.3528232493	8.2812186365	17.3745122681
H26	3.9146564739	9.8325754307	16.7700132323
C27	1.8336438274	9.4152711663	16.4022249113
C28	1.4664768100	10.5417483967	15.6513464655
H29	2.2335037051	11.1328428651	15.1607956461
C30	0.1287167040	10.9172996285	15.5269210848
H31	-0.1323309269	11.7937519956	14.9393098617
C32	-0.8716455416	10.1750740757	16.1562896052
H33	-1.9136270792	10.4681551649	16.0601364584
C34	-0.5222728431	9.0560377381	16.9124594112
H35	-1.2919730675	8.4725352960	17.4110296720
C36	11.0072068269	5.1379772015	15.7311159571
H37	11.8717718821	5.6404134397	16.1756908562
H38	11.3887332249	4.3916787539	15.0233964893
H39	10.4872475558	4.5956715985	16.5302123214
C40	10.8561079158	7.2289093881	13.4930184008
H41	11.6171909741	7.8870948179	13.9253172692
H42	10.2170259272	7.8452822921	12.8494180072
H43	11.3696341563	6.5030396501	12.8506735519
C44	8.5647416937	5.2676932002	13.9602739447
H45	7.9650724144	4.6624369456	14.6496424711
H46	9.1132830057	4.5663297874	13.3192618367
H47	7.8859670106	5.8314263471	13.3128140946
C48	5.5483088872	10.7304630696	21.0036063303
H49	5.0240688040	11.3475869605	20.2644465034
H50	6.4756616564	11.2501388769	21.2686258826
H51	4.9230143218	10.6863353705	21.9035834617
C52	4.2261483373	8.2026829596	19.8974910846
H53	3.7211096603	7.9314697510	20.8327641432
H54	4.3246679346	7.2862485983	19.3060765771
H55	3.5673208660	8.8927269996	19.3640664214
C56	6.6275997940	7.9505287881	21.7270678201
H57	5.8919652246	7.8376338484	22.5333603810
H58	7.5223721555	8.4066246732	22.1619036776
H59	6.8975161532	6.9445306232	21.3836498242
C60	10.1218981195	8.3658640830	16.5122106730
C61	11.0884166257	8.0141689123	17.5260321674
H62	11.1310805752	7.0651746523	18.0423789013
C63	11.9825276719	9.1080621808	17.7129911933
H64	12.8043423163	9.1457470830	18.4156710849
C65	11.5639488082	10.1686614282	16.8533378729
H66	12.0114547486	11.1519758318	16.7945031942
C67	10.4228841752	9.7246448761	16.1294428322
H68	9.8426665838	10.3042782778	15.4263990837
C69	9.2455334193	9.2578972868	20.0471314327
H70	9.2726889614	8.2865913705	20.5199474708
C71	10.2361111793	10.2763661992	20.1596480649
H72	11.1600600005	10.2084200362	20.7183808282
C73	9.8250934910	11.3809348533	19.3538658215

H74	10.3826318161	12.2943125514	19.1943526565
C75	8.5741735609	11.0497619839	18.7612414293
H76	8.0030201383	11.6752225700	18.0903659153
C77	8.1752162797	9.7364968995	19.2033340162
C78	0.8166006828	8.6824242707	17.0311720360
H79	1.0804124431	7.8078509586	17.6215821107
Fe80	10.0631433104	9.6845185277	18.1937643704
H81	5.9430576266	9.3510797579	12.4152535823
H82	3.9503140815	10.6689878141	13.2351192787
H83	2.7156078822	5.7720626065	13.1941209399
H84	1.9286275287	7.7551546569	14.4214382149
N85	6.8586125027	5.9533277639	17.7989973929
C86	6.7047771918	3.5296747449	19.1771426581
C87	5.7105384272	5.2533605948	17.8391452459
C88	7.9313868699	5.4533115152	18.4402116999
C89	7.8982702740	4.2503714813	19.1399943815
C90	5.5905507627	4.0405743232	18.5135594188
H91	4.8718152998	5.6877667850	17.3044798810
H92	8.8399874825	6.0429723207	18.3715363515
H93	8.7912006138	3.8909925587	19.6411487241
H94	4.6419592583	3.5135329658	18.5138527440
H95	6.6450938153	2.5865945681	19.7130805356

4^Y-(py)₂

Y1	7.1980524448	8.3429648717	16.8015650875
Si2	9.8445734824	6.3563453172	14.8428052474
Si3	5.8954529668	8.9969365687	20.3148398942
N4	9.1309461745	7.5248728151	15.9442506827
N5	6.9529475455	9.0852994442	18.9162898057
N6	5.1493592653	7.6893116455	15.5720309069
N7	7.1940692821	10.3786651050	15.4032326232
C8	7.0852072931	9.7943320579	14.1634002318
H9	7.9723958091	9.2609145630	13.8279719469
C10	5.9597413417	9.8423965144	13.3832451395
C11	4.7594343432	10.4364477660	13.9300319703
C12	5.0209650261	11.3747109374	15.0078551507
H13	4.2825400367	12.1154563063	15.2974974019
C14	6.1766900184	11.2387053067	15.7315158127
H15	6.3439646285	11.8423732262	16.6208489169
C16	3.8696104677	8.2407826722	15.3131386061
H17	4.1292770892	9.3342572054	14.5399551394
C18	2.9596479211	7.4290711855	14.5029078513
C19	3.4030661272	6.3366567425	13.8199567697
C20	4.7546324778	5.9098465900	13.9615661988
H21	5.1453092592	5.0425197736	13.4423923762
C22	5.5388647057	6.6085703997	14.8461576129
H23	6.5536121691	6.2661516207	15.0331083716
C24	3.2746846042	8.9731701708	16.5336359234
H25	3.3528232493	8.2812186365	17.3745122681
H26	3.9146564739	9.8325754307	16.7700132323
C27	1.8336438274	9.4152711663	16.4022249113
C28	1.4664768100	10.5417483967	15.6513464655
H29	2.2335037051	11.1328428651	15.1607956461
C30	0.1287167040	10.9172996285	15.5269210848
H31	-0.1323309269	11.7937519956	14.9393098617
C32	-0.8716455416	10.1750740757	16.1562896052
H33	-1.9136270792	10.4681551649	16.0601364584
C34	-0.5222728431	9.0560377381	16.9124594112
H35	-1.2919730675	8.4725352960	17.4110296720
C36	11.0072068269	5.1379772015	15.7311159571
H37	11.8717718821	5.6404134397	16.1756908562
H38	11.3887332249	4.3916787539	15.0233964893
H39	10.4872475558	4.5956715985	16.5302123214
C40	10.8561079158	7.2289093881	13.4930184008
H41	11.6171909741	7.8870948179	13.9253172692
H42	10.2170259272	7.8452822921	12.8494180072
H43	11.3696341563	6.5030396501	12.8506735519
C44	8.5647416937	5.2676932002	13.9602739447
H45	7.9650724144	4.6624369456	14.6496424711
H46	9.1132830057	4.5663297874	13.3192618367
H47	7.8859670106	5.8314263471	13.3128140946
C48	5.5483088872	10.7304630696	21.0036063303
H49	5.0240688040	11.3475869605	20.2644465034
H50	6.4756616564	11.2501388769	21.2686258826
H51	4.9230143218	10.6863353705	21.9035834617
C52	4.2261483373	8.2026829596	19.8974910846
H53	3.7211096603	7.9314697510	20.8327641432
H54	4.3246679346	7.2862485983	19.3060765771

H55	3.5673208660	8.8927269996	19.3640664214
C56	6.6275997940	7.9505287881	21.7270678201
H57	5.8919652246	7.8376338484	22.5333603810
H58	7.5223721555	8.4066246732	22.1619036776
H59	6.8975161532	6.9445306232	21.3836498242
C60	10.1218981195	8.3658640830	16.5122106730
C61	11.0884166257	8.0141689123	17.5260321674
H62	11.1310805752	7.0651746523	18.0423789013
C63	11.9825276719	9.1080621808	17.7129911933
H64	12.8043423163	9.1457470830	18.4156710849
C65	11.5639488082	10.1686614282	16.8533378729
H66	12.0114547486	11.1519758318	16.7945031942
C67	10.4228841752	9.7246448761	16.1294428322
H68	9.8426665838	10.3042782778	15.4263990837
C69	9.2455334193	9.2578972868	20.0471314327
H70	9.2726889614	8.2865913705	20.5199474708
C71	10.2361111793	10.2763661992	20.1596480649
H72	11.1600600005	10.2084200362	20.7183808282
C73	9.8250934910	11.3809348533	19.3538658215
H74	10.3826318161	12.2943125514	19.1943526565
C75	8.5741735609	11.0497619839	18.7612414293
H76	8.0030201383	11.6752225700	18.0903659153
C77	8.1752162797	9.7364968995	19.2033340162
C78	0.8166006828	8.6824242707	17.0311720360
H79	1.0804124431	7.8078509586	17.6215821107
Fe80	10.0631433104	9.6845185277	18.1937643704
H81	5.9430576266	9.3510797579	12.4152535823
H82	3.9503140815	10.6689878141	13.2351192787
H83	2.7156078822	5.7720626065	13.1941209399
H84	1.9286275287	7.7551546569	14.4214382149
N85	6.8586125027	5.9533277639	17.7989973929
C86	6.7047771918	3.5296747449	19.1771426581
C87	5.7105384272	5.2533605948	17.8391452459
C88	7.9313868699	5.4533115152	18.4402116999
C89	7.8982702740	4.2503714813	19.1399943815
C90	5.5905507627	4.0405743232	18.5135594188
H91	4.8718152998	5.6877667850	17.3044798810
H92	8.8399874825	6.0429723207	18.3715363515
H93	8.7912006138	3.8909925587	19.6411487241
H94	4.6419592583	3.5135329658	18.5138527440
H95	6.6450938153	2.5865945681	19.7130805356

4^Y-1,5-(py)₂

Y1	6.9925542054	9.3037728979	16.2678351113
Si2	8.4953415851	6.1877992695	14.8249798332
Si3	4.6473077450	11.2401386008	18.4669233234
N4	8.1391358397	7.3869543490	16.0411580746
N5	6.0043844580	10.2190733220	18.0674298425
N6	4.9489251440	8.6459842496	15.0206600793
N7	7.6212342704	10.8465118113	14.7527873317
C8	7.1264998534	12.1581549614	14.7590484836
H9	6.5208600693	12.4111753586	15.6290764063
C10	7.3480140815	13.0855735738	13.8081167603
C11	8.2040039970	12.8222259490	12.5899293995
C12	8.7177713117	11.4013594125	12.6382498459
H13	9.3649465804	11.0552172566	11.8354900259
C14	8.4296467940	10.5546590802	13.6447336709
H15	8.8451347006	9.5478716911	13.6392093035
C16	4.1146195589	7.6818320267	15.4788499290
C17	2.9768828473	7.3184543660	14.7566305904
C18	2.6986215202	7.9583335923	13.5499029534
C19	3.5614124936	8.9491647964	13.0855962408
H20	3.3806936542	9.4706503074	12.1519328169
C21	4.6774012086	9.2628683102	13.8528496848
H22	5.3876836311	10.0248884007	13.5438144167
C23	4.5088052033	7.0443266387	16.8011718300
H24	5.5156008128	6.6217832930	16.6735386007
H25	4.6124408744	7.8549577310	17.5371566930
C26	3.5734383569	5.9846639269	17.3393819005
C27	2.4746081381	6.3380567711	18.1347853090
H28	2.2957714698	7.3857542699	18.3655148696
C29	1.6151078150	5.3620291413	18.6391376965
H30	0.7723131674	5.6537936162	19.2596412618
C31	1.8423570571	4.0143541858	18.3551789799
H32	1.1770711850	3.2528665531	18.7523571930
C33	2.9331975000	3.6498185416	17.5649363926
H34	3.1215084952	2.6024249174	17.3452675466
C35	10.3312196251	6.1963725907	14.3486957687

H36	10.6277834241	7.1582334961	13.9141143106
H37	10.5598925681	5.4133545868	13.6151813229
H38	10.9663465699	6.0223424170	15.2251479476
C39	7.4497380375	6.5620619505	13.2893023066
H40	7.6520270266	7.5597130067	12.8829934909
H41	6.3765526082	6.4958111540	13.5008083446
H42	7.6717510851	5.8368733675	12.4967994551
C43	8.0710225775	4.4326662382	15.4214878425
H44	8.6169081679	4.1804418091	16.3380970001
H45	8.3310753166	3.6814226954	14.6658702148
H46	7.0008304181	4.3262698750	15.6371777969
C47	3.5985666979	11.4776994659	16.9061304798
H48	3.1760692075	10.5314288746	16.5493917890
H49	4.1739629909	11.9195195393	16.0848244759
H50	2.7592510135	12.1519668834	17.1144906186
C51	3.5486637435	10.4642859060	19.8110369901
H52	3.1425591034	9.4954754601	19.4951452951
H53	2.7002147670	11.1147506471	20.0557471362
H54	4.1107659945	10.2962760920	20.7367438959
C55	5.2083825296	12.9358431157	19.1039663294
H56	5.7750632828	13.4813705624	18.3411271104
H57	5.8565362432	12.8317114951	19.9816785884
H58	4.3548776158	13.5592450473	19.3969489068
C59	8.8357926480	7.3229301632	17.2588812633
C60	8.5248353517	6.5125538408	18.4105093623
H61	7.6706529078	5.8535419811	18.4901638895
C62	9.5336650471	6.7086426281	19.3977571814
H63	9.5706373507	6.2382498417	20.3715242837
C64	10.4582277880	7.6779553107	18.9007537942
H65	11.3161080900	8.0676191430	19.4321031556
C66	10.0243124283	8.0710996034	17.6026224351
H67	10.5133574385	8.7807712230	16.9483770567
C68	6.8070696538	8.8946848095	20.0996049866
H69	5.9757542511	8.2092544320	20.1949786850
C70	7.9408210867	8.9715807066	20.9597645649
H71	8.1343260864	8.3381622797	21.8153977992
C72	8.8083370157	9.9911611892	20.4605826507
H73	9.7695831405	10.2654397952	20.8740989764
C74	8.2014776174	10.5524130407	19.3002710415
H75	8.5925065689	11.3613746825	18.6964012787
C76	6.9255795630	9.9079573318	19.0802834284
C77	3.7911582539	4.6284689272	17.0614543020
H78	4.6438503787	4.3364431442	16.4527032705
Fe79	8.5688445041	8.4970467290	19.0561477889
X80	7.4485514733#	9.2180815429#	19.9500246693#
X81	9.4372550481#	7.0617150118#	18.2127131289#
H82	6.9106952164	14.0735829884	13.9323501464
H83	1.8159344651	7.6833703419	12.9790666000
H84	2.3255741145	6.5437489897	15.1441659323
H86	9.0433301277	13.5406159072	12.5390957820
H87	7.6359310515	13.0059018828	11.6591907558

3^y-(iqn)₂

Y1	6.9910071738	9.1863378093	16.3304913237
Si2	9.8287031289	8.3314812553	14.0667692201
Si3	5.4410453238	11.0617258732	19.2114263355
N4	8.8903290405	8.2484551483	15.5341307921
N5	6.5418537542	9.9419314494	18.4413245722
N6	5.6079892112	7.3794708879	15.8243222106
N7	5.5546640899	10.2789003911	14.4571750320
C8	5.0310171408	9.4331845092	13.5759063814
H9	5.2618144908	8.3835746301	13.7281908277
C10	4.4381264898	12.1005937303	13.3351394178
H11	4.2243738233	13.1638939431	13.2878370679
C12	5.2498868234	11.6098343545	14.3266855457
H13	5.6794517628	12.2652856195	15.0749680256
C14	4.1857054601	7.1036182222	16.1291733808
C15	4.0226132783	5.7096042202	16.6895956812
C16	4.7103148636	4.7203467851	16.0789275105
C17	5.7100078694	5.0620334232	15.0931973148
H18	6.2357636250	4.2980091232	14.5299810584
C19	6.1782974546	6.3530549270	15.1082668538
H20	7.1188964423	6.5919051742	14.6205806453
C21	3.5856698907	8.2017103425	17.0277802011
H22	4.1117752369	8.2058021775	17.9868243815
H23	3.7812850269	9.1734931338	16.5551932933
C24	2.0954104127	8.0619200804	17.2576814221
C25	1.1784032021	8.3841864487	16.2457976933

H26	1.5481805524	8.7436775131	15.2875885254
C27	-0.1951432083	8.2522795001	16.4489662808
H28	-0.8857533060	8.5104011813	15.6498743728
C29	-0.6855413461	7.7961234336	17.6748843017
H30	-1.7556278191	7.6972765972	17.8361322108
C31	0.2134933430	7.4728063102	18.6910996939
H32	-0.1529180139	7.1195971861	19.6518252230
C33	11.3157691933	9.5121400640	14.2281768587
H34	10.9824829333	10.5313201690	14.4502608999
H35	11.9109055131	9.5531646462	13.3081592736
H36	11.9857420234	9.2011528470	15.0373291711
C37	8.6737691007	9.0267890054	12.7234626915
H38	8.2018739105	9.9616006530	13.0457267601
H39	7.8735477585	8.3210746573	12.4718119988
H40	9.2239065257	9.2438720347	11.8011963848
C41	10.5292724894	6.6261823549	13.4471946261
C42	4.5699980439	12.0201177221	17.8198538530
H43	4.1872349489	11.3455084235	17.0470909925
H44	5.2430521409	12.7427924578	17.3427842385
H45	3.7128076343	12.5805996237	18.2087269696
C46	4.1358690711	10.1519228509	20.2562251857
H47	3.3799208814	9.6735215638	19.6257448666
H48	3.6087867692	10.8295746593	20.9380734867
H49	4.6007382126	9.3693835423	20.8670544557
C50	6.2343962749	12.3977051264	20.3945065035
C51	9.4093742064	7.5808243984	16.6556366589
C52	8.9956089434	6.2891439916	17.1561983819
H53	8.1833786326	5.7018508023	16.7499173750
C54	9.8363972586	5.9275485563	18.2468953549
H55	9.7630278397	5.0200423378	18.8318942474
C56	10.7538906616	6.9986241546	18.4750491245
H57	11.5001587403	7.0392938126	19.2578002090
C58	10.4727632345	8.0249305250	17.5268126486
H59	10.9906477243	8.9693687223	17.4343030265
C60	6.8621262938	7.6455832974	19.4942027775
H61	6.0253912387	7.1401349144	19.0309361237
C62	7.7778761937	7.0740153656	20.4224776118
H63	7.7626965114	6.0550286930	20.7844993992
C64	8.7527089150	8.0644415416	20.7483975492
H65	9.6003013859	7.9294190909	21.4074201428
C66	8.4437471063	9.2432502651	20.0089675585
H67	8.9977871232	10.1710221478	20.0418555684
C68	7.2344952627	9.0204429040	19.2492546590
C69	1.5879430456	7.6048554748	18.4820457317
H70	2.2784661501	7.3546767971	19.2835608397
Fe71	8.8160353159	7.6464208893	18.7348858276
H72	4.5852182559	3.6807501362	16.3782770950
H73	3.3266964108	5.5242539205	17.5026229224
X74	7.8115906248	8.7810945849	18.8848746782
X75	8.2124535633	8.2052504317	20.0656050477
X76	10.3332827995	7.1101037737	17.6426285704
C77	3.8667870565	11.2153084754	12.3832093304
C78	4.1813257998	9.8295388173	12.5150583161
C79	3.6297417716	8.8870695509	11.6086710035
C80	2.7936544658	9.3129493945	10.6027633954
C81	2.4817062261	10.6890394323	10.4682322987
C82	3.0036952090	11.6236187267	11.3352179376
H83	3.8709215465	7.8350431032	11.7301284746
H84	2.3647702271	8.5958024602	9.9093656649
H85	1.8171120402	11.0072518353	9.6697944972
H86	2.7572391101	12.6761528912	11.2298897421
C87	9.4304340257	5.5444846305	13.4061308635
H88	8.5866646271	5.8359788333	12.7687177327
H89	9.8325620811	4.6053524497	12.9981164331
H90	9.0363260741	5.3252002124	14.4024053315
C91	11.0918457447	6.7988199022	12.0170617428
H92	10.3144805269	7.0846312294	11.2992451860
H93	11.8854984953	7.5537018357	11.9690331396
H94	11.5259680632	5.8519788590	11.6635423887
C95	11.6729862249	6.1310606579	14.3611347621
H96	12.0689116579	5.1739948837	13.9897979843
H97	12.5108846545	6.8371028278	14.3894081383
H98	11.3376982934	5.9682198386	15.3899139679
C99	5.1923771854	13.5121353067	20.6511393105
H100	4.9472799501	14.0676170953	19.7393289708
H101	4.2555012612	13.1196071596	21.0637004199
H102	5.5846325667	14.2379915201	21.3786890324
C103	7.4835095993	13.0486057621	19.7701561797
H104	7.2727273464	13.4921347858	18.7891202203
H105	7.8661887349	13.8536299747	20.4150647868
H106	8.2937757203	12.3262866588	19.6359982468

C107	6.6172801414	11.7865307689	21.7610473135
H108	7.0532647977	12.5561083194	22.4157240349
H109	5.7448412682	11.3772561501	22.2819723143
H110	7.3514348920	10.9807921595	21.6671970651
C111	9.2726036878	11.5409609267	16.9846582423
N112	8.4021723191	11.4561846590	15.9893257283
C113	8.5872010726	12.2802266323	14.9129416744
C114	9.6164622467	13.1843940647	14.8216510275
H115	9.1068957261	10.8766315185	17.8284991535
H116	7.8649992364	12.1779592998	14.1102338074
H117	9.7120598242	13.8113837131	13.9405371071
C118	10.5676429775	13.2812036394	15.8709421708
C119	10.3849842159	12.4206243862	16.9948253400
C120	11.3111035493	12.4571003690	18.0696456759
C121	12.3836502947	13.3173973014	18.0229185500
C122	12.5661907378	14.1730609187	16.9077966013
C123	11.6797390855	14.1613019541	15.8540780917
H124	11.1630379400	11.7965476635	18.9196565434
H125	13.0977824354	13.3442297166	18.8406854749
H126	13.4202192042	14.8443847547	16.8871237847
H127	11.8251178165	14.8162299445	14.9992390583
H128	3.6286142279	7.1494359022	15.1622135164

3'TS4^Y-(iqn)₂

Y1	7.1197299985	9.1494622401	16.4240510935
Si2	9.7129028497	8.0629077080	13.9992100721
Si3	5.4780951670	10.8428322915	19.3829073507
N4	8.9350196536	8.0916296518	15.5665674657
N5	6.6741890981	9.8606743266	18.5530543631
N6	5.6788922946	7.2200584599	16.0226873491
N7	5.6171862430	10.0209870527	14.7248828548
C8	4.9908682611	9.0869314631	13.9172437684
H9	5.5945638655	8.2023126226	13.7161375917
C10	4.1804961604	11.7473012328	13.8054239696
H11	3.8706517328	12.7875961439	13.8205374428
C12	5.1308163595	11.3022990696	14.6834282015
H13	5.5827542110	11.9915224027	15.3899392315
C14	4.2736404710	7.3872032021	15.8662407075
H15	4.2129473246	8.2284171084	14.8573851733
C16	3.5033485578	6.2063583188	15.4723387277
C17	4.1315881055	5.0991458706	14.9819570057
C18	5.5520642485	5.0531582960	14.9338786538
H19	6.0850942890	4.1910597094	14.5488765793
C20	6.2453808614	6.1122602032	15.4796704261
H21	7.3279940203	6.0991125188	15.5109708203
C22	3.6734182191	8.2703127779	16.9793472273
H23	3.9556223818	7.8118014339	17.9323627975
H24	4.1710825920	9.2451109821	16.9500735616
C25	2.1749085758	8.4612982774	16.9311289850
C26	1.5727291985	9.2986136789	15.9805701055
H27	2.1912282061	9.8389260281	15.2699517848
C28	0.1869302331	9.4477285473	15.9369120549
H29	-0.2602040033	10.0993494160	15.1906458806
C30	-0.6235861584	8.7678980008	16.8478156136
H31	-1.7033493539	8.8871907488	16.8149052008
C32	-0.0374185263	7.9373623709	17.8025601553
H33	-0.6584020225	7.4057058310	18.5189462731
C34	11.1427729493	9.3186863743	13.9144809004
H35	10.7686096907	10.3394159705	14.0493704036
H36	11.6673725543	9.2836277544	12.9524582209
H37	11.8835438142	9.1330975944	14.7000638676
C38	8.4093894480	8.5628723717	12.7116663226
H39	7.8295350809	9.4360130562	13.0291979186
H40	7.6996861039	7.7506090603	12.5171066580
H41	8.8847202294	8.8163637221	11.7575832625
C42	10.4436065471	6.3411410139	13.4625532521
C43	4.5571640553	11.8850533506	18.0905703873
H44	4.1514402240	11.2917042068	17.2673958493
H45	5.2008072862	12.6606007012	17.6588105784
H46	3.7069928208	12.3917987306	18.5600055491
C47	4.2159679459	9.7575840995	20.3088622520
H48	3.4998432565	9.2997604617	19.6197590897
H49	3.6360922578	10.3351580501	21.0379348911
H50	4.7164641138	8.9490811187	20.8534711038
C51	6.1656092626	12.1114651509	20.6958951466
C52	9.6286662370	7.6001921329	16.6837959229
C53	9.4604583299	6.3093400248	17.3117089779
H54	8.7334765708	5.5639285365	17.0241070895

C55	10.4151197811	6.1737787604	18.3592428793
H56	10.5253342396	5.3180176625	19.0121974599
C57	11.1612789713	7.3880971875	18.4351063192
H58	11.9393914959	7.6109932449	19.1531209083
C59	10.6664816611	8.2694395658	17.4313553870
H60	11.0218955403	9.2703300457	17.2275934422
C61	7.2195489329	7.6067945151	19.6053530904
H62	6.3972893788	7.0407178631	19.1888894520
C63	8.2045775884	7.1219561385	20.5123116726
H64	8.2784900807	6.1116474665	20.8910011858
C65	9.1059370188	8.1915033062	20.7948478704
H66	9.9801590818	8.1339194675	21.4297587605
C67	8.6840540666	9.3282745017	20.0469042983
H68	9.1644446845	10.2960186936	20.0517995348
C69	7.4693761806	9.0030689530	19.3349340334
C70	1.3493803518	7.7860789523	17.8407523954
H71	1.8000368371	7.1333962966	18.5851728390
Fe72	9.1562707840	7.7455240183	18.7893962033
H73	3.5464047554	4.2408360074	14.6584303457
H74	2.4217040336	6.2567738768	15.5350529232
X75	7.8115906248#	8.7810945849#	18.8848746782#
X76	8.2124535633#	8.2052504317#	20.0656050477#
X77	10.3332827995#	7.1101037737#	17.6426285704#
C78	3.6413137676	10.8484116221	12.8231566201
C79	4.0873544710	9.5003015108	12.8540344025
C80	3.6238353643	8.5827666757	11.8940237909
C81	2.7234525129	8.9839707250	10.9185188781
C82	2.2730463227	10.3151933059	10.8874511827
C83	2.7248164931	11.2343680212	11.8217655588
H84	3.9710499160	7.5528847520	11.9347381505
H85	2.3649356008	8.2715940329	10.1808518156
H86	1.5659951058	10.6262255314	10.1227575127
H87	2.3794568520	12.2642977536	11.7889631761
C88	9.4203805239	5.2011388164	13.6491740345
H89	8.4705766563	5.4038984452	13.1398541380
H90	9.8150231939	4.2602089494	13.2374263271
H91	9.2018402449	5.0240196073	14.7066185114
C92	10.8193370861	6.4086091484	11.9631261158
H93	9.9432178570	6.5671847088	11.3245094941
H94	11.5382390959	7.2080101120	11.7480371380
H95	11.2849423979	5.4638224206	11.6459900097
C96	11.7184055180	5.9978522017	14.2654508953
H97	12.1274606062	5.0304049061	13.9375613498
H98	12.5062298093	6.7459096129	14.1215133136
H99	11.5214406087	5.9221436996	15.3395403829
C100	5.0417639694	13.1145732201	21.0499838391
H101	4.7621662980	13.7419054508	20.1971409649
H102	4.1336883302	12.6147878726	21.4071197078
H103	5.3751115010	13.7875521092	21.8533970227
C104	7.3579710471	12.9157865461	20.1416050063
H105	7.1057419326	13.4369203186	19.2098042858
H106	7.6807425213	13.6801364766	20.8637600142
H107	8.2211957280	12.2758365829	19.9371310307
C108	6.5913275552	11.4035910689	22.0014831390
H109	6.9551233012	12.1390635118	22.7345023526
H110	5.7520494077	10.8741749794	22.4659746566
H111	7.3914857214	10.6754425353	21.8411326375
C112	9.1469723877	11.7129866511	17.0048006319
N113	8.3558652588	11.3705354406	15.9990205639
C114	8.4819749364	12.0440043336	14.8142929181
C115	9.3954375797	13.0506944147	14.6244358823
H116	9.0080491745	11.1649698208	17.9320687387
H117	7.8105547197	11.7289866414	14.0231541864
H118	9.4569255301	13.5534496869	13.6642856173
C119	10.2711210133	13.4201846769	15.6794073758
C120	10.1359743875	12.7221385108	16.9181773288
C121	10.9884742883	13.0424427931	18.0066747299
C122	11.9463063334	14.0194523521	17.8640890760
C123	12.0827381764	14.7127225415	16.6352232255
C124	11.2648729204	14.4255366053	15.5651651583
H125	10.8745732824	12.5057215916	18.9444051552
H126	12.6038305334	14.2643572403	18.6928875692
H127	12.8457193022	15.4802990307	16.5397664249
H128	11.3741895785	14.9581518924	14.6243730985

4^Y-(iqn)₂

Y1	6.8924322440	9.3226592185	16.2992136194
Si2	9.6100420896	8.2827839154	14.0469488857

Si3	5.3722359449	11.0166273727	19.3192871263
N4	8.6835720281	8.1390236754	15.5302286544
N5	6.4335950348	9.9025204517	18.4681375947
N6	5.4658035551	7.1608344301	16.0390838984
N7	5.4723399401	10.0410161739	14.6381455024
C8	4.9080451679	9.1138065209	13.6364717026
H9	5.5135086739	8.2037857325	13.5971286015
C10	4.4396482980	11.8459757537	13.3668226959
H11	4.1400829377	12.8887594608	13.3419734870
C12	5.0272428038	11.3310798211	14.4889164966
H13	5.2152262872	11.9924191771	15.3345481931
C14	4.1668723431	7.0376727869	16.3976929461
C15	3.4489070260	5.8682987436	16.1283012300
C16	4.0697277161	4.8167064932	15.4611696110
C17	5.3973798071	4.9597213682	15.0626286555
H18	5.9205613843	4.1762223904	14.5243516331
C19	6.0514310543	6.1467437446	15.3700414208
H20	7.0790784341	6.3284030358	15.0748622327
C21	3.5407034523	8.2495817921	17.0585735885
H22	4.2162672174	8.5789856093	17.8575235983
H23	3.5498828561	9.0589111499	16.3163685552
C24	2.1432510142	8.0588343891	17.6011355408
C25	1.0318770028	8.5769934435	16.9254777037
H26	1.1782145804	9.1232583078	15.9962570818
C27	-0.2568336648	8.4060765764	17.4344192856
H28	-1.1069684122	8.8201026498	16.8989048004
C29	-0.4525516579	7.7113634652	18.6279813901
H30	-1.4548987271	7.5813057805	19.0269694556
C31	0.6473168867	7.1892371290	19.3113585481
H32	0.5043672741	6.6523968371	20.2454542341
C33	11.0839742299	9.4769312974	14.2312193180
H34	10.7337090296	10.4897831788	14.4584137274
H35	11.6693764656	9.5360083223	13.3057520053
H36	11.7672086904	9.1738229972	15.0314509831
C37	8.4672612597	8.9937528843	12.7149706817
H38	7.8594930840	9.8255726895	13.0848789367
H39	7.7707399453	8.2496708781	12.3140705246
H40	9.0570418034	9.3706995807	11.8716739221
C41	10.3244608060	6.5952945828	13.3927278787
C42	4.3677506730	11.9604901948	18.0171228078
H43	3.9480271434	11.2920808687	17.2597430656
H44	4.9697720989	12.7165320057	17.4998660547
H45	3.5288626944	12.4834355858	18.4888487452
C46	4.1724280726	10.0626921300	20.4481922877
H47	3.4151463959	9.5212170360	19.8723292402
H48	3.6374187831	10.7348994614	21.1289605268
H49	4.7069503103	9.3301283964	21.0632739883
C50	6.2191694571	12.3590329328	20.4552886614
C51	9.2906780930	7.5388894024	16.6476345536
C52	8.9835619280	6.2454920621	17.2165572193
H53	8.2006789712	5.5830532190	16.8785523719
C54	9.8909822905	5.9738477873	18.2808305411
H55	9.9006397827	5.0842344590	18.8969374308
C56	10.7471711817	7.1057800265	18.4278724013
H57	11.5244587372	7.2225262911	19.1716374603
C58	10.3638879427	8.0727455831	17.4531038984
H59	10.8243375091	9.0382474750	17.3021420541
C60	6.8363515187	7.6239195054	19.5311089122
H61	5.9873942948	7.1027799946	19.1098548530
C62	7.7754580862	7.0850002933	20.4575848825
H63	7.7826785174	6.0749540786	20.8443115883
C64	8.7342366878	8.1007912279	20.7499998085
H65	9.5940401769	7.9954822815	21.3984460723
C66	8.3904763214	9.2580004311	19.9908931646
H67	8.9275078406	10.1958923373	19.9931397608
C68	7.1723706216	9.0011035831	19.2583166960
C69	1.9333727537	7.3630755932	18.8016845676
H70	2.7869835858	6.9615020429	19.3433858967
Fe71	8.7820435430	7.6423613793	18.7473600313
H72	3.5199490210	3.9043766169	15.2459736992
H73	2.4122298606	5.8002232460	16.4358926194
X74	7.8115906248	8.7810945849	18.8848746782
X75	8.2124535633	8.2052504317	20.0656050477
X76	10.3332827995	7.1101037737	17.6426285704
C77	4.4215701982	11.0593580456	12.1468083076
C78	4.7709805997	9.6933640043	12.2447624175
C79	4.8802797185	8.9138894757	11.0970871684
C80	4.6135905215	9.4577618902	9.8360027792
C81	4.2461883145	10.8007880568	9.7334743989
C82	4.1586610361	11.5959523880	10.8750167173
H83	5.1549192536	7.8637285648	11.1880680626

H84	4.6852920191	8.8374701382	8.9465614736
H85	4.0321567243	11.2326666420	8.7586128892
H86	3.8915731369	12.6466710247	10.7870495541
C87	9.2425528915	5.4954078830	13.3905566201
H88	8.3488923083	5.7947662732	12.8282765300
H89	9.6252392586	4.5757807517	12.9229369014
H90	8.9345893577	5.2362412395	14.4091446539
C91	10.8197518300	6.7932416993	11.9415797037
H92	10.0048734922	7.0633812595	11.2610831373
H93	11.5869996545	7.5730427442	11.8683763057
H94	11.2684800074	5.8637699258	11.5611247899
C95	11.5149524331	6.1138975151	14.2513929435
H96	11.9121738503	5.1656810366	13.8588264007
H97	12.3397713744	6.8353645213	14.2457031650
H98	11.2294200653	5.9423062948	15.2942130783
C99	5.1776461687	13.4613662474	20.7633045256
H100	4.8776858802	14.0109405417	19.8650423198
H101	4.2691017294	13.0580815055	21.2262214500
H102	5.5992175270	14.1930342054	21.4679244343
C103	7.4227174851	13.0220512779	19.7579470268
H104	7.1475646335	13.4631056554	18.7920161065
H105	7.8341962787	13.8310848378	20.3794222864
H106	8.2315564111	12.3089553954	19.5735833230
C107	6.6794430986	11.7644794840	21.8051557309
H108	7.1372513973	12.5460904204	22.4297706941
H109	5.8390507965	11.3500196996	22.3728321405
H110	7.4177745846	10.9669774374	21.6835732463
C111	9.2579710911	11.5712421621	16.9293853041
N112	8.2960309563	11.4464395297	16.0268756430
C113	8.2881304557	12.3073353897	14.9610245802
C114	9.2373708391	13.2859519234	14.7929679284
H115	9.2381295865	10.8709729030	17.7608361805
H116	7.4761463035	12.1746657667	14.2538051341
H117	9.1885427365	13.9431036107	13.9303875441
C118	10.2857916499	13.4304945177	15.7391750529
C119	10.2909862450	12.5359285462	16.8520086372
C120	11.3158911272	12.6262452318	17.8298703799
C121	12.3048265310	13.5731425270	17.7012888182
C122	12.3027074710	14.4626209286	16.5969871277
C123	11.3179417390	14.3984798998	15.6367183810
H124	11.3063760540	11.9399924582	18.6726263879
H125	13.0932404023	13.6442247183	18.4448221525
H126	13.0923725744	15.2038785642	16.5107983696
H127	11.3214324578	15.0818616504	14.7919855146
H128	3.8989747049	8.7956186479	13.9747823158

3^Y-(iqn)₂

Y1	6.9152128754	9.1429990420	16.3570950386
Si2	9.7429664346	8.4002585600	14.0243514688
Si3	5.4306828965	11.0574517612	19.2398011971
N4	8.8155265836	8.2647908187	15.4945126148
N5	6.5126569715	9.9214655749	18.4687063458
N6	5.5617960274	7.2923371840	15.9177345221
N7	5.4583781922	10.2249478824	14.5021386873
C8	4.9739810890	9.3888818470	13.5907120520
H9	5.1707675156	8.3341411740	13.7584788027
C10	4.4628363109	12.0700819609	13.3075974409
H11	4.2758942076	13.1382609667	13.2452548555
C12	5.1927542255	11.5620536494	14.3526840374
H13	5.5841088603	12.2069317788	15.1300296849
C14	4.1962518224	6.9265311257	16.3582577441
C17	5.6942301795	5.0065970316	15.0958912995
H18	6.1958668035	4.2917749286	14.4502521196
C19	6.1069166982	6.3126514355	15.1227584256
H20	6.9741133701	6.6110633826	14.5389237943
C21	3.6077006048	8.0325869643	17.2541082860
H22	3.9989446738	7.9422275364	18.2708452831
H23	3.9879677663	8.9881018542	16.8683563733
C24	2.0942146535	8.1310421802	17.2868217363
C25	1.3696089209	8.3764383694	16.1105778255
H26	1.8989789590	8.4612198327	15.1639022727
C27	-0.0171023918	8.5192392854	16.1355635361
H28	-0.5567666734	8.7092518798	15.2110012595
C29	-0.7118459233	8.4245404557	17.3428451020
H30	-1.7924940697	8.5379465168	17.3639420969
C31	-0.0062464285	8.1861956986	18.5210701944
H32	-0.5340580824	8.1129854775	19.4685325140
C33	11.2378426819	9.5662233673	14.2114438773

H34	10.9092498903	10.5725555852	14.4891959910
H35	11.8101480590	9.6513303607	13.2800464992
H36	11.9272891782	9.2179281197	14.9880613720
C37	8.5889966218	9.1540495681	12.7137793684
H38	8.1293357698	10.0807209369	13.0741078854
H39	7.7814309677	8.4676008924	12.4349255753
H40	9.1407619530	9.4013827886	11.8001195742
C41	10.4263536723	6.7139770462	13.3441949369
C42	4.5259016432	11.9812245678	17.8459111089
H43	4.1326744760	11.2904519860	17.0923165144
H44	5.1832007621	12.7012623025	17.3437264364
H45	3.6713818847	12.5414424187	18.2410055323
C46	4.1425743220	10.1713073646	20.3245707729
H47	3.3587807061	9.7207763051	19.7087367150
H48	3.6507658339	10.8548511293	21.0264595910
H49	4.6059274642	9.3711863114	20.9131309910
C50	6.2422810120	12.4209622584	20.3771932903
C51	9.3719034995	7.6005469288	16.5999078701
C52	8.9817851316	6.3056910567	17.1091279569
H53	8.1672110131	5.7110996745	16.7202623650
C54	9.8528019738	5.9478947750	18.1761009402
H55	9.8010940262	5.0382596176	18.7598361489
C56	10.7697016007	7.0236360659	18.3800608158
H57	11.5383649026	7.0673788673	19.1406157183
C58	10.4571764641	8.0487659235	17.4417488848
H59	10.9685618651	8.9952642449	17.3366711341
C60	6.9019281187	7.6394019762	19.5285502745
H61	6.0561944209	7.1168614424	19.1045996447
C62	7.8561693241	7.0881745836	20.4284011478
H63	7.8676819111	6.0711803149	20.7956753170
C64	8.8254231854	8.0949601367	20.7151020786
H65	9.6954592085	7.9788127347	21.3480664758
C66	8.4721446804	9.2641131900	19.9810675869
H67	9.0077914005	10.2029351544	19.9979469769
C68	7.2419008459	9.0184569381	19.2637115362
C69	1.3816031899	8.0421594291	18.4901509198
H70	1.9199080911	7.8617555645	19.4175658139
Fe71	8.8323316685	7.6624169714	18.6990500207
X74	7.8115906248#	8.7810945849#	18.8848746782#
X75	7.8141907543#	8.2095466747#	19.9846600312#
X76	9.8936068609#	6.9642143252#	17.6121184338#
C77	3.9456287899	11.1966797085	12.3146769894
C78	4.2143912577	9.8032968494	12.4694489790
C79	3.7169042720	8.8754059380	11.5178159121
C80	2.9786647238	9.3221735498	10.4464968418
C81	2.7115806682	10.7053710456	10.2903218327
C82	3.1813620360	11.6260319006	11.2007376094
H83	3.9254148576	7.8179338733	11.6523858070
H84	2.5947157569	8.6164152349	9.7160221401
H85	2.1252532002	11.0405978727	9.4392605468
H86	2.9711684858	12.6844618367	11.0776502645
C87	9.3130917153	5.6492167825	13.2674049055
H88	8.4785922190	5.9706329431	12.6316600143
H89	9.7037959752	4.7152503705	12.8371882779
H90	8.9078282465	5.4106142109	14.2549395846
C91	10.9927367974	6.9295979133	11.9214370902
H92	10.2212714383	7.2545422128	11.2137894574
H93	11.7983171353	7.6731389933	11.9020298800
H94	11.4125409676	5.9898880043	11.5332768209
C95	11.5637316669	6.1739535943	14.2407279261
H96	11.9497103891	5.2265687828	13.8357253288
H97	12.4093293662	6.8693852334	14.2941776916
H98	11.2264350025	5.9784637800	15.2631147357
C99	5.1975185167	13.5320240588	20.6377092193
H100	4.9260853161	14.0677286847	19.7214391319
H101	4.2739801248	13.1411644793	21.0806743130
H102	5.6017391792	14.2750805486	21.3409620688
C103	7.4710430069	13.0707721199	19.7128136544
H104	7.2342342623	13.4944420823	18.7289328801
H105	7.8605865174	13.8910022109	20.3340510588
H106	8.2851907252	12.3541489453	19.5735118642
C107	6.6618583092	11.8364641107	21.7446194144
H108	7.1044245938	12.6209096566	22.3768303545
H109	5.8057846361	11.4265385686	22.2916806560
H110	7.4022720098	11.0368040229	21.6471050509
C111	9.1833050683	11.4613572806	16.9898181901
N112	8.3013271180	11.4438895669	16.0020297064
C113	8.4861836154	12.3258962836	14.9724594324
C114	9.5252516546	13.2228799810	14.9225275056
H115	9.0217646545	10.7535367066	17.7973000212
H116	7.7552289264	12.2786054162	14.1725449195

H117	9.6200732288	13.9003660393	14.0786933374
C118	10.4876377558	13.2476663068	15.9661389456
C119	10.3063324225	12.3233121282	17.0385759256
C120	11.2444005688	12.2839412432	18.1032760417
C121	12.3254873269	13.1350421005	18.0980338936
C122	12.5053641051	14.0555711235	17.0352160724
C123	11.6090599248	14.1159891899	15.9914109937
H124	11.0987864445	11.5721297557	18.9112461628
H125	13.0481542401	13.1047272048	18.9082600687
H126	13.3656339866	14.7191945542	17.0467601346
H127	11.7535859422	14.8202964983	15.1765616897
H128	3.5756230663	6.8860701257	15.4379662070
C129	4.1536522966	5.5141417989	16.9357023349
C130	4.8336885144	4.5366260837	16.1637969255
C131	4.7413437666	3.1839989766	16.5376982398
C132	4.0147413778	2.8028932258	17.6640036299
C133	3.3811676716	3.7721230882	18.4449716814
C134	3.4554260916	5.1206586399	18.0762881945
H137	5.2640683234	2.4351794219	15.9458827465
H138	3.9499421422	1.7524472986	17.9380934381
H139	2.8150030516	3.4831341178	19.3268097076
H140	2.9279884985	5.8562919548	18.6738904901

3TS4^Y-(iqn)₂

Y1	7.0958508834	9.0707003015	16.4661135276
Si2	9.6179886998	8.1116235815	13.8904716375
Si3	5.5618752288	10.7317011588	19.4956552606
N4	8.8986296095	8.1113175224	15.4886442545
N5	6.7581997668	9.7855273542	18.6322940122
N6	5.5546354226	7.1629137037	16.2645322174
N7	5.5625056324	9.8744033798	14.7860610544
C8	4.9836872990	8.8616693576	14.0204819122
H9	5.6217549909	7.9770244052	13.9289314552
C10	4.2609600658	11.5199949472	13.5730674115
H11	3.9676280936	12.5587474639	13.4639438753
C12	5.1040890290	11.1477494459	14.5856507692
H13	5.4831711373	11.8910867067	15.2810242499
C14	4.1843518206	7.3120439484	15.9972540416
H15	4.1953958364	8.1625522436	14.9164084210
C18	5.5237070740	4.8550869061	15.5250996952
H19	6.0755754896	3.9358801556	15.3568946267
C20	6.1620094106	5.9748102126	15.9731742241
H21	7.2326217713	5.9628076938	16.1393882880
C22	3.5653475187	8.2267040729	17.0791242622
H23	3.6266360120	7.6454939378	18.0060252984
H24	4.2686776863	9.0552109103	17.2155092014
C25	2.1698400865	8.7955234410	16.9515477899
C26	1.8474030368	9.7654431184	15.9912314788
H27	2.6027934158	10.1106502581	15.2942010084
C28	0.5614075619	10.3001166523	15.9201812225
H29	0.3324189772	11.0462978393	15.1635798188
C30	-0.4251555434	9.8857599437	16.8168654827
H31	-1.4259756048	10.3060643666	16.7629278665
C32	-0.1146223410	8.9310243968	17.7853093981
H33	-0.8724248753	8.6030038252	18.4921250113
C34	11.0687694511	9.3433286136	13.8018885312
H35	10.7177963327	10.3671545466	13.9744903905
H36	11.5646853515	9.3246467745	12.8240609122
H37	11.8277195522	9.1244326040	14.5609640970
C38	8.2973035224	8.6686233482	12.6447050038
H39	7.7204427411	9.5271642892	13.0022989654
H40	7.5831623684	7.8700797390	12.4150056280
H41	8.7692221432	8.9627567819	11.7001404301
C42	10.2854950721	6.3854754192	13.2983567547
C43	4.6826364552	11.8120582938	18.2053210654
H44	4.2704517816	11.2245567606	17.3798141491
H45	5.3644518966	12.5567975004	17.7772679671
H46	3.8438076950	12.3534290266	18.6547849530
C47	4.2963138364	9.6112826927	20.3770055510
H48	3.5609876421	9.2042125568	19.6775387064
H49	3.7394966980	10.1471378394	21.1542097020
H50	4.7989190928	8.7647847402	20.8592378019
C51	6.2240719701	11.9415628263	20.8787257268
C52	9.6921085235	7.6855529315	16.5691547074
C53	9.7265746062	6.3723055349	17.1722632033
H54	9.1185155568	5.5292775724	16.8783701245
C55	10.7235053723	6.3535742774	18.1886587965
H56	10.9731284221	5.5102207033	18.8190333023

C57	11.2960246851	7.6581104860	18.2684997372
H58	12.0570384174	7.9754704426	18.9690842327
C59	10.6535529081	8.4773057980	17.2968953706
H60	10.8597028416	9.5205793541	17.1029265747
C61	7.3413827759	7.4704408381	19.5080994707
H62	6.5194929459	6.9285301459	19.0597104414
C63	8.3482123513	6.9289806668	20.3581229794
H64	8.4460205413	5.8917609400	20.6481917432
C65	9.2256455608	7.9906200667	20.7298223427
H66	10.1072951027	7.8971060790	21.3501371393
C67	8.7718291881	9.1799440507	20.0885701088
H68	9.2389782645	10.1517813148	20.1600419697
C69	7.5595855808	8.8900796953	19.3594355304
C70	1.1707259714	8.3921066048	17.8484777225
H71	1.4034561365	7.6422687004	18.6012374277
Fe72	9.2752522430	7.7294545293	18.6931475078
X75	7.8115906248#	8.7810945849#	18.8848746782#
X76	8.1366987575#	8.2503194829#	20.0588701930#
X77	10.2664009961#	7.1481695343#	17.6442418973#
C78	3.8133698305	10.5411899037	12.6210442615
C79	4.2081166983	9.1932932328	12.8258819482
C80	3.8325211363	8.2001535454	11.9051272436
C81	3.0685163209	8.5263907367	10.7943289248
C82	2.6678165993	9.8578648205	10.5897974758
C83	3.0340304470	10.8502905524	11.4854619024
H84	4.1408203024	7.1716658279	12.0782793746
H85	2.7790333161	7.7556551291	10.0858012429
H86	2.0681613168	10.1115873548	9.7194518360
H87	2.7285059689	11.8796952382	11.3178444923
C88	9.2263409279	5.2837050601	13.5078765873
H89	8.2894266466	5.5045695040	12.9825683284
H90	9.5928124664	4.3189747862	13.1269222494
H91	8.9840058041	5.1482732506	14.5657678094
C92	10.6144347239	6.4634854561	11.7891801583
H93	9.7270848558	6.6732454604	11.1818379487
H94	11.3615194832	7.2348787030	11.5669616870
H95	11.0281131115	5.5057748330	11.4405572959
C96	11.5771063254	5.9905612132	14.0489804849
H97	11.9475825883	5.0200593722	13.6862644826
H98	12.3794433514	6.7205739434	13.8918099151
H99	11.4185281122	5.8976495043	15.1275193173
C100	5.0870150889	12.9217392114	21.2548502564
H101	4.8262904432	13.5891467473	20.4265567649
H102	4.1723692727	12.4025688553	21.5637461827
H103	5.3970739647	13.5558094030	22.0983523857
C104	7.4262305424	12.7785268183	20.3994482533
H105	7.2077960802	13.3290725766	19.4761547030
H106	7.7112485430	13.5208708022	21.1599367230
H107	8.3050002245	12.1526343511	20.2148615996
C108	6.6276077235	11.1710963625	22.1557950400
H109	6.9768366741	11.8701756483	22.9303941382
H110	5.7831974582	10.6169059033	22.5796631445
H111	7.4335930127	10.4541154710	21.9726067054
C112	8.8821885390	11.8442240980	17.1190475112
N113	8.1836126516	11.3942638474	16.0864512208
C114	8.3643604288	11.9960360388	14.8692710884
C115	9.2353756563	13.0380549653	14.6730295708
H116	8.6899767276	11.3499597829	18.0667050346
H117	7.7693747814	11.5968893071	14.0560047936
H118	9.3397383732	13.4808041033	13.6867247579
C119	10.0136733708	13.5219989052	15.7577611621
C120	9.8256074189	12.8978613293	17.0288650058
C121	10.5851570152	13.3332811282	18.1462490674
C122	11.5003781253	14.3503130018	18.0015050076
C123	11.6866158137	14.9710158742	16.7412086533
C124	10.9608283114	14.5709520783	15.6415004654
H125	10.4337450423	12.8538867023	19.1089484094
H126	12.0854575940	14.6828191672	18.8537854661
H127	12.4143014574	15.7720572149	16.6451052366
H128	11.1082826801	15.0471033450	14.6759416792
C129	3.4204495135	6.1289214001	15.5141271865
C130	4.1126701132	4.9060821919	15.2835989392
C131	3.3930066103	3.7814827115	14.8223924546
C132	2.0346808984	3.8582709714	14.5707582352
C133	1.3574783257	5.0718162537	14.7615993841
C134	2.0434286750	6.1875910914	15.2221719636
H137	3.9303046581	2.8504906095	14.6610533533
H138	1.4969098429	2.9831372457	14.2145847411
H139	0.2952506818	5.1444356058	14.5452878407
H140	1.5071651970	7.1189171383	15.3447417868

$4^Y-(iqn)_2$

Y1	6.7885483668	9.3046716573	16.2991856522
Si2	9.5427768767	8.0600491235	14.1616717276
Si3	5.1206847585	11.1661220406	19.1422598205
N4	8.5716486528	8.0352100884	15.6224042247
N5	6.2455641998	10.0463034347	18.3827047653
N6	5.2586412287	7.1489348264	15.9811956521
N7	5.4375634571	10.1265608673	14.6394290249
C8	4.7805004328	9.3176124543	13.5953238777
H9	5.2094589018	8.3114968638	13.5827517836
C10	4.7326044043	12.0815427751	13.3703227255
H11	4.5734047465	13.1555150157	13.3568594212
C12	5.1716048175	11.4670299045	14.5110873571
H13	5.3980214576	12.0774920302	15.3855606553
C14	3.9343241705	7.0817918780	16.1211483107
C17	5.2430411391	5.1848348801	14.5810119067
H18	5.8023389296	4.4596627932	13.9980918321
C19	5.8975729984	6.2054706300	15.2154329917
H20	6.9700606207	6.3410253964	15.1373996632
C21	3.2825915380	8.1096168376	17.0187370660
H22	4.0749637350	8.7523953052	17.4177803219
H23	2.6267126983	8.7550627196	16.4212396927
C24	2.4970804820	7.5301498137	18.1845782786
C25	1.2963231390	8.1260563350	18.5905636610
H26	0.9171968114	8.9885073248	18.0462672830
C27	0.5842861587	7.6291037992	19.6834291225
H28	-0.3448518109	8.1064769219	19.9832393477
C29	1.0637177319	6.5250250342	20.3873154877
H30	0.5103150618	6.1354890359	21.2372639636
C31	2.2582170853	5.9218706363	19.9905378850
H32	2.6396269870	5.0603087491	20.5321191851
C33	10.9811401135	9.3102249895	14.2407453982
H34	10.6052321807	10.3349246195	14.3275352233
H35	11.5951988881	9.2668863454	13.3328481765
H36	11.6467136127	9.1257540541	15.0908249768
C37	8.4039311222	8.5804390014	12.7402082218
H38	7.7940029460	9.4533083725	12.9966246561
H39	7.7103820301	7.7825034759	12.4512677111
H40	8.9857827505	8.8433896342	11.8493662475
C41	10.3323955068	6.3367615867	13.7221198027
C42	3.9180252337	11.8182444651	17.8236945601
H43	3.6446998126	11.0561223617	17.0888367242
H44	4.3230023201	12.6719399738	17.2704927995
H45	2.9948640880	12.1606510015	18.3057208397
C46	4.1145678177	10.2764621350	20.4879352008
H47	3.4667935884	9.5032256852	20.0620243359
H48	3.4714060285	10.9780906513	21.0331563946
H49	4.7660291838	9.7889663536	21.2210360931
C50	5.9234651681	12.7313935963	19.9816116945
C51	9.1302631885	7.5050236435	16.7950354347
C52	8.7327662715	6.2916160653	17.4721147483
H53	7.9109913614	5.6552077123	17.1758326779
C54	9.6123370443	6.0563789533	18.5681346054
H55	9.5608092857	5.2252050029	19.2588403911
C56	10.5419237015	7.1368592229	18.6249949016
H57	11.3215936894	7.2661479344	19.3640378542
C58	10.2301835433	8.0365139326	17.5656931469
H59	10.7586211667	8.9499012419	17.3354472577
C60	6.6852969829	7.9247807775	19.7068630928
H61	5.8160768811	7.3704074419	19.3834355769
C62	7.6413927758	7.5038956109	20.6731118288
H63	7.6556313688	6.5513378323	21.1848660379
C64	8.6094660953	8.5421532761	20.8128045088
H65	9.4824401406	8.5156425437	21.4516493272
C66	8.2494302450	9.5974617279	19.9248536407
H67	8.7781445706	10.5333259556	19.8124152738
C68	7.0151504015	9.2537038617	19.2563101292
C69	2.9682269300	6.4202312113	18.8988462192
H70	3.8914006962	5.9338512053	18.5927724362
Fe71	8.6112950036	7.8293087008	18.8787737243
X74	7.8115906248#	8.7810945849#	18.8848746782#
X75	7.7817786471#	8.2137630082#	19.9975806928#
X76	9.8552562872#	6.9873509723#	17.6051997227#
C77	4.7159531813	11.3311560369	12.1275029119
C78	4.8569395186	9.9264369439	12.2114936055
C79	4.9736806782	9.1632592171	11.0537793671
C80	4.9189782376	9.7668060354	9.7930843531
C81	4.7565847928	11.1508973858	9.7018817226

C82	4.6633040410	11.9272201412	10.8557766770
H83	5.0900672616	8.0834940016	11.1350447090
H84	4.9961132145	9.1620953811	8.8934200640
H85	4.7098802831	11.6286519031	8.7260072730
H86	4.5597828420	13.0077566377	10.7790930116
C87	9.2817171491	5.2097851865	13.7961439851
H88	8.4187591971	5.4097737047	13.1481205404
H89	9.7159625622	4.2530176861	13.4694573505
H90	8.9151408225	5.0683420251	14.8183176668
C91	10.8859039340	6.3926756507	12.2794353630
H92	10.0965665719	6.5694126372	11.5406271651
H93	11.6400439098	7.1786218795	12.1549535608
H94	11.3693246560	5.4394650651	12.0193841219
C95	11.4984689502	5.9870502312	14.6736055499
H96	11.9430263242	5.0200251631	14.3940776114
H97	12.2992280194	6.7339108506	14.6281615584
H98	11.1745294088	5.9092985851	15.7160153516
C99	4.8211570025	13.7917686801	20.2118505779
H100	4.3898953763	14.1537015066	19.2726977989
H101	4.0002395316	13.4076021605	20.8292821359
H102	5.2371911718	14.6639583536	20.7372110496
C103	7.0096529048	13.3472450911	19.0771985104
H104	6.6201627518	13.6129080645	18.0862778240
H105	7.4136335900	14.2675740836	19.5248026401
H106	7.8476486117	12.6605008635	18.9238298623
C107	6.5427035169	12.3963349697	21.3563446892
H108	6.9832092902	13.2983952434	21.8067586059
H109	5.7914650166	12.0191297958	22.0589558521
H110	7.3338378522	11.6441760459	21.2884440271
C111	9.3156671048	11.4076977875	16.8815131228
N112	8.3587441119	11.3185384163	15.9696697675
C113	8.3991745823	12.1761707066	14.9024926364
C114	9.3851770906	13.1204386658	14.7477307524
H115	9.2653548654	10.7068394933	17.7100749503
H116	7.5935272333	12.0745028791	14.1834744245
H117	9.3720560192	13.7773957313	13.8836879673
C118	10.4230226182	13.2308925957	15.7092973888
C119	10.3826626258	12.3346990946	16.8201578031
C120	11.3974023120	12.3916438578	17.8115879347
C121	12.4169250534	13.3077558877	17.6985098597
C122	12.4587278363	14.1992287826	16.5966344931
C123	11.4863225163	14.1665190934	15.6225900154
H124	11.3571978378	11.7043268645	18.6526877424
H125	13.1963587287	13.3532546279	18.4534638491
H126	13.2720893692	14.9159258622	16.5236868259
H127	11.5228194799	14.8499744163	14.7786820726
H128	3.7092546708	9.2021394734	13.8637515807
C129	3.1534308326	6.0783800526	15.4560649537
C130	3.8317832958	5.0975255983	14.6707272654
C131	3.0868877136	4.0909958274	14.0040823012
C132	1.7146234820	4.0656863335	14.0971541360
C133	1.0331463093	5.0467405450	14.8575925927
C134	1.7329314807	6.0269011489	15.5279471398
H137	3.6193457037	3.3489126077	13.4150091052
H138	1.1474567115	3.2955105326	13.5817136561
H139	-0.0512356682	5.0218092237	14.9164131140
H140	1.1954466571	6.7592232505	16.1182498093

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