

Electronic Supplementary Information for:

Aryl C–H bond functionalization with diphenyldiazomethane induced by rare-earth metal alkyl complexes

*Dianjun Guo,^a Thayalan Rajeshkumar,^c Shan Zhu,^a Qingbing Yuan,^a Dongjing Hong,^a Shuangliu Zhou,^a Xiancui Zhu,^{*a} Laurent Maron^{*c} and Shaowu Wang^{*a,b}*

[†]Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu, Anhui 241002 (China).

[‡]Anhui Laboratory of Clean Catalytic Engineering, Anhui Laboratory of Functional Complexes for Materials Chemistry and Application, College of Biological and Chemical Engineering, Anhui Polytechnic University, Wuhu, Anhui 241000 (China).

[§]LPCNO, CNRS & INSA, Université Paul Sabatier, 135 Avenue de Rangueil, 31077 Toulouse, France

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1. Crystallographic data

Table S1. Crystallographic data of 1a'-2b

	1a' (Lu)	2a (Y)	2a' (Lu)	2b (Y)
CCDC	2192982	2192984	2192983	2192986
Empirical formula	C ₅₁ H ₅₈ LuN ₃ O ₂ Si	C ₆₉ H ₅₉ N ₆ OY	C ₆₉ H ₅₉ LuN ₆ O	C ₇₂ H ₅₉ N ₆ Y
Formula weight	948.06	1077.13	1162.18	1097.16
Crystal system	monoclinic	triclinic	triclinic	triclinic
Space group	<i>C2/c</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> (Å)	27.50(6)	14.43(7)	14.08(5)	11.9372(7)
<i>b</i> (Å)	12.35(3)	16.35(7)	16.13(6)	15.1671(8)
<i>c</i> (Å)	17.13(4)	17.84(8)	17.56(6)	16.1955(9)
α (°)	90	98.03(5)	77.87(4)	92.2250(10)
β (°)	120.84(3)	94.36(5)	86.86(9)	91.3580(10)
γ (°)	90	116.15(5)	64.85(4)	94.6340(10)
<i>V</i> (Å ³)	4993(20)	3698(28)	3528(22)	2919.4(3)
<i>Z</i>	4	2	2	2
<i>D</i> _{calcd} (mg m ⁻³)	1.261	0.967	1.094	1.248
μ (mm ⁻¹)	2.039	0.826	1.439	1.047
<i>F</i> (000)	1944.0	1124.0	1186.0	1144.0
θ range (°)	3.45 to 55.142	2.828 to 55.26	2.85 to 55.168	2.518 to 55.13
Reflections collected	28265	41043	39132	34612
Data/restraints/parameters	5690/1883/490	16609/12/695	15852/1248/729	13267/393/754
Goodness-of-fit on <i>F</i> ²	1.163	0.883	0.913	1.011
R(int)	0.0421	0.1406	0.1498	0.0521
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0685, 0.20299	0.0690, 0.1323	0.0733, 0.1492	0.0547, 0.1185

$\Delta\rho_{\max,\min}, \text{e}\text{\AA}^{-3}$	1.34, -2.25	0.39, -0.62	2.80, -1.74	0.51, -0.35
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Table S2. Crystallographic data of 2b'-2d

	2b' (Lu)	2c (Y)	2c' (Lu)	2d (Y)
CCDC	2192985	2192988	2192987	2192990
Empirical formula	C ₆₅ H ₅₁ LuN ₆	C ₆₆ H ₅₃ N ₆ OY	C ₆₆ H ₅₃ LuN ₆ O	C ₆₆ H ₅₃ N ₆ OY
Formula weight	1091.08	1035.05	1121.11	1035.05
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P</i> $\bar{1}$
<i>a</i> (Å)	13.6742(10)	12.84(2)	12.8580(6)	11.5090(10)
<i>b</i> (Å)	25.8835(18)	19.50(3)	19.4811(9)	14.3067(13)
<i>c</i> (Å)	20.5125(14)	24.86(4)	24.8098(11)	21.0746(19)
α (°)	90	90	90	75.5750(10)
β (°)	106.9660(10)	98.696(19)	98.7720(10)	85.9730(10)
γ (°)	90	90	90	69.0990(10)
<i>V</i> (Å ³)	6944.1(8)	6156(18)	6141.9(5)	3138.9(5)
<i>Z</i>	4	4	4	2
<i>D</i> _{calcd} (mg m ⁻³)	1.044	1.117	1.212	1.095
μ (mm ⁻¹)	1.457	0.990	1.650	0.971
<i>F</i> (000)	2216.0	2152.0	2280.0	1076.0
θ range (°)	2.604 to 54.976	2.666 to 55.038	2.67 to 54.986	3.14 to 55.054
Reflections collected	80822	71644	71263	37086
Data/restraints/parameters	15837/0/650	14096/0/669	14042/6/669	14255/0/669
Goodness-of-fit on <i>F</i> ²	0.952	0.958	1.007	0.926
R(int)	0.0996	0.1202	0.0631	0.0836
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0489, 0.1148	0.0564, 0.1127	0.0360, 0.0762	0.0572, 0.1081

$\Delta\rho_{\max,\min}$, eÅ⁻³ 0.88, -0.91 0.27, -0.32 1.24, -0.66 0.27, -0.27

Table S3. Crystallographic data of 2d'-2g

	2d' (Lu)	2e (Y)	2f (Y)	2g (Y)
CCDC	2192989	2192991	2192992	2192993
Empirical formula	C ₁₃₂ H ₁₀₆ Lu ₂ N ₁₂ O ₂	C ₆₅ H ₅₀ FN ₆ Y	C ₆₅ H ₅₇ N ₆ Y	C ₆₆ H ₅₃ N ₆ Y
Formula weight	2242.22	1023.02	1011.07	1019.05
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P</i> $\bar{1}$	<i>P2₁/c</i>
<i>a</i> (Å)	14.0687(10)	17.2922(10)	15.1303(12)	12.6440(9)
<i>b</i> (Å)	43.818(3)	20.3976(11)	15.1348(11)	19.4671(14)
<i>c</i> (Å)	20.2354(14)	17.3327(10)	15.3810(12)	24.5847(18)
α (°)	90	90	91.8130(10)	90
β (°)	108.3480(10)	91.7460(10)	100.9800(10)	99.3820(10)
γ (°)	90	90	110.0370(10)	90
<i>V</i> (Å ³)	11840.2(14)	6110.7(6)	3230.4(4)	5970.4(7)
<i>Z</i>	4	4	2	4
<i>D</i> _{calcd} (mg m ⁻³)	1.258	1.112	1.039	1.134
μ (mm ⁻¹)	1.712	0.998	0.941	1.019
<i>F</i> (000)	4560.0	2120.0	1056.0	2120.0
θ range (°)	2.316 to 54.918	3.084 to 54.938	2.712 to 55.038	2.682 to 54.958
Reflections collected	137606	71142	38210	69175
Data/restraints/parameters	26877/984/1337	13945/0/659	14656/0/650	13546/0/660
Goodness-of-fit on <i>F</i> ²	1.020	0.916	0.939	0.967
R(int)	0.1278	0.1547	0.0991	0.1208
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0722, 0.1415	0.0603, 0.1205	0.0699, 0.1363	0.0565, 0.1067

$\Delta\rho_{\max,\min}, \text{e}\text{\AA}^{-3}$ 1.33, -1.45 1.33, -0.33 0.65, -0.40 0.30, -0.27

Table S4. Crystallographic data of 2h-3a'

	2h (Y)	2i (Y)	2j (Y)	3a' (Lu)
CCDC	2192994	2192995	2192996	2192997
Empirical formula	C ₇₁ H ₅₅ N ₆ Y	C ₇₀ H ₅₇ N ₆ SY	C ₇₀ H ₅₇ N ₆ Y	C ₅₆ H ₅₂ LuN ₅ Si
Formula weight	1081.12	1103.18	1071.12	998.08
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> (Å)	13.339(19)	11.948(14)	11.494(9)	10.8724(6)
<i>b</i> (Å)	14.75(2)	14.873(16)	15.028(11)	13.1419(7)
<i>c</i> (Å)	18.38(3)	16.154(17)	15.994(13)	18.0651(10)
α (°)	81.977(15)	92.578(16)	90.881(10)	97.7980(10)
β (°)	76.954(14)	90.58(2)	95.81(2)	96.3490(10)
γ (°)	65.660(14)	93.366(12)	93.429(13)	111.5590(10)
<i>V</i> (Å ³)	3206(8)	2863(5)	2743(4)	2342.1(2)
<i>Z</i>	2	2	2	2
<i>D</i> _{calcd} (mg m ⁻³)	1.120	1.280	1.297	1.415
μ (mm ⁻¹)	0.953	1.103	1.113	2.176
<i>F</i> (000)	1124.0	1148.0	1116.0	1016.0
θ range (°)	3.034 to 55.29	2.524 to 55.044	2.56 to 55.04	2.31 to 54.936
Reflections collected	37959	33951	32614	27571
Data/restraints/parameters	14610/0/704	13018/42/705	12469/42/684	10573/0/572
Goodness-of-fit on <i>F</i> ²	0.909	0.951	0.970	1.031
R(int)	0.1056	0.0839	0.0902	0.0492
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0621, 0.1098	0.0588, 0.1012	0.0661, 0.1147	0.0455, 0.0840

$\Delta\rho_{\max,\min}$, eÅ⁻³ 0.25, -0.37 0.37, -0.36 0.43, -0.36 0.43, -0.71

Table S5. Crystallographic data of 4a'-7j

	4a'(Lu)	5c (Y)	6 (Y)	7j (Y)
CCDC	2192998	2192999	2193000	2193001
Empirical formula	C _{59.5} H ₅₃ LuN ₄ O	C ₅₇ H ₅₁ N ₄ O ₂ Y	C ₅₇ H ₅₅ N ₄ SiY	C ₅₄ H ₄₇ N ₄ OY
Formula weight	1015.03	912.92	913.05	856.86
Crystal system	triclinic	monoclinic	monoclinic	triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> $\bar{1}$
<i>a</i> (Å)	13.8291(7)	10.3399(9)	14.37(2)	10.74(3)
<i>b</i> (Å)	14.0855(7)	24.627(2)	10.679(18)	13.66(3)
<i>c</i> (Å)	14.6541(7)	20.7916(19)	36.16(6)	17.96(5)
α (°)	90.7390(10)	90	90	85.25(4)
β (°)	107.4760(10)	98.4700(10)	100.46(3)	76.64(3)
γ (°)	117.4340(10)	90	90	74.83(7)
<i>V</i> (Å ³)	2377.6(2)	5236.6(8)	5458(16)	2473(11)
<i>Z</i>	2	4	4	2
<i>D</i> _{calcd} (mg m ⁻³)	1.418	1.158	1.111	1.151
μ (mm ⁻¹)	2.122	1.156	1.127	1.218
<i>F</i> (000)	1034.0	1904.0	1912.0	892.0
θ range (°)	2.962 to 57.16	2.58 to 55.058	2.29 to 55.178	3.09 to 55.148
Reflections collected	28725	61104	62836	28928
Data/restraints/parameters	11329/87/612	11966/24/579	12492/422/654	11192/249/588
Goodness-of-fit on <i>F</i> ²	1.021	0.968	1.023	0.980
R(int)	0.0341	0.1292	0.1223	0.0665
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2 σ (<i>I</i>))	0.0350, 0.0768	0.0600, 0.1213	0.0691, 0.1497	0.0630, 0.1430

$\Delta\rho_{\max,\min}, \text{e}\text{\AA}^{-3}$ 1.13, -0.59 0.36, -0.29 0.57, -0.37 0.62, -0.35

Table S6. Crystallographic data of 8a-8d

	8a	8a'	8c	8d
CCDC	2193002	2193003	2193004	2193005
Empirical formula	C ₂₆ H ₂₁ N ₃	C ₂₆ H ₂₀ N ₂ O	C ₂₇ H ₂₃ N ₃ O	C ₂₇ H ₂₃ N ₃ O
Formula weight	375.46	376.44	405.48	405.48
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	9.90(3)	11.2744(10)	22.752(6)	14.63(2)
<i>b</i> (Å)	10.39(3)	10.6960(10)	9.525(2)	5.784(8)
<i>c</i> (Å)	10.65(3)	17.0182(16)	10.485(3)	25.69(4)
α (°)	76.10(3)	90	90	90
β (°)	74.76(3)	97.3680(10)	101.731(4)	104.741(17)
γ (°)	89.66(3)	90	90	90
<i>V</i> (Å ³)	1025(5)	2035.3(3)	2224.9(9)	2102(5)
<i>Z</i>	2	4	4	4
<i>D</i> _{calcd} (mg m ⁻³)	1.217	1.229	1.211	1.281
μ (mm ⁻¹)	0.072	0.075	0.075	0.079
<i>F</i> (000)	396.0	792.0	856.0	856.0
θ range (°)	4.046 to 55.08	4.104 to 55.05	3.656 to 55.074	2.928 to 49.996
Reflections collected	12167	21793	11429	8446
Data/restraints/parameters	4648/0/263	4600/7/263	4893/271/313	3673/0/235
Goodness-of-fit on <i>F</i> ²	0.969	0.999	1.060	1.135
R(int)	0.0424	0.0526	0.0332	0.1020
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2 σ (<i>I</i>))	0.0541, 0.1223	0.0488, 0.1219	0.0582, 0.1527	0.1432, 0.3662

$\Delta\rho_{\max,\min}, \text{e}\text{\AA}^{-3}$

0.15, -0.20

0.17, -0.24

0.25, -0.16

0.39, -0.42

Table S7. Crystallographic data of 8i and 8j

	8i	8j
CCDC	2193006	2193007
Empirical formula	C ₂₄ H ₁₉ N ₃ S	C ₂₄ H ₁₉ N ₃
Formula weight	381.48	349.42
Crystal system	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> (Å)	5.89(2)	9.0659(7)
<i>b</i> (Å)	15.53(6)	11.4910(8)
<i>c</i> (Å)	10.89(4)	17.7791(13)
α (°)	90	90
β (°)	95.96(3)	96.5740(10)
γ (°)	90	90
<i>V</i> (Å ³)	990(6)	1840.0(2)
<i>Z</i>	2	4
<i>D</i> _{calcd} (mg m ⁻³)	1.279	1.261
μ (mm ⁻¹)	0.177	0.075
<i>F</i> (000)	400.0	736.0
θ range (°)	3.76 to 55.146	4.228 to 54.948
Reflections collected	9829	20458
Data/restraints/parameters	3964/1/241	4201/0/244
Goodness-of-fit on <i>F</i> ²	1.028	0.998
R(int)	0.0356	0.0330
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0644, 0.1285	0.0495, 0.1378
$\Delta\rho_{\max,\min}, \text{e}\text{\AA}^{-3}$	0.16, -0.19	0.16, -0.25

2. Molecular structures of complexes 1a'-2h.

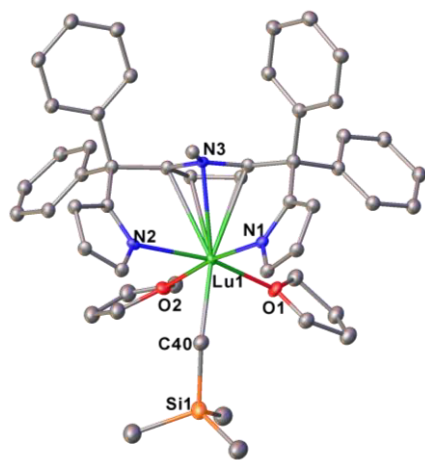


Figure S1. Molecular structure of **1a'**. All the hydrogen atoms are omitted. Selected bond lengths (Å) and angles (°): Lu(1)-N(1) 2.228(17), Lu(1)-N(2) 2.435(17), Lu(1)-N(3) 2.776(13), Lu(1)-C(40) 2.43(2), C(40)-Si(1) 1.951(19), C(40)-Lu(1)-N(1) 93.4(7), C(40)-Lu(1)-N(2) 86.2(7), N(1)-Lu(1)-N(2) 101.2(6), N(1)-Lu(1)-O(1) 89.9(5), N(2)-Lu(1)-O(2) 85.0(5), N(1)-Lu(1)-N(3) 71.2(5), N(2)-Lu(1)-N(3) 69.9(5).

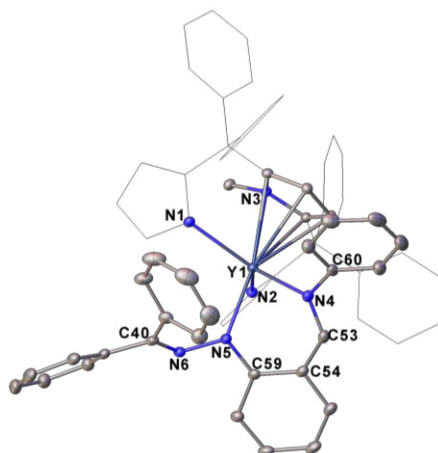


Figure S2. Molecular structure of **2b**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y-N(4) 2.398(2), Y-N(5) 2.316(2), N(5)-N(6) 1.414(3), C(59)-N(5) 1.373(3), C(40)-N(6) 1.283(4), C(53)-N(4) 1.304(4), N(5)-Y-N(4) 74.54(9), N(6)-N(5)-C(59) 110.8(2), C(40)-N(6)-N(5) 117.7(3), N(6)-N(5)-Y 123.03(17), Y-N(5)-C(59) 113.56(18), C(54)-C(53)-N(4) 127.6(3), Y-N(4)-C(53) 114.1(2).

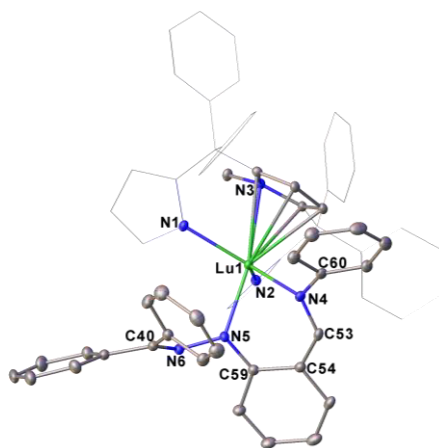


Figure S3. Molecular structure of **2b'**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu–N(4) 2.332(4), Lu–N(5) 2.267(4), N(5)–N(6) 1.411(5), C(59)–N(5) 1.360(6), C(40)–N(6) 1.274(6), C(53)–N(4) 1.310(6), N(5)–Lu–N(4) 75.81(13), N(6)–N(5)–C(59) 112.2(4), C(40)–N(6)–N(5) 117.0(4), N(6)–N(5)–Lu 122.4(3), Lu–N(5)–C(59) 117.0(3), C(54)–C(53)–N(4) 127.6(4), Lu–N(4)–C(53) 116.0(3).

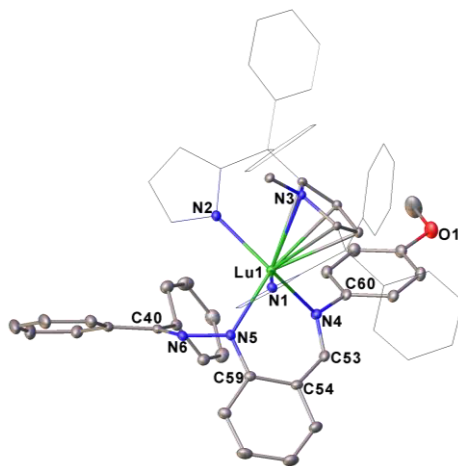


Figure S4. Molecular structure of **2c'**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu–N(4) 2.340(3), Lu–N(5) 2.263(3), N(5)–N(6) 1.428(4), C(59)–N(5) 1.364(4), C(40)–N(6) 1.285(4), C(53)–N(4) 1.293(4), N(5)–Lu–N(4) 75.42(9), N(6)–N(5)–C(59) 111.6(3), C(40)–N(6)–N(5) 116.0(3), N(6)–N(5)–Lu 120.55(19), Lu–N(5)–C(59) 119.3(2), C(54)–C(53)–N(4) 127.7(3), Lu–N(4)–C(53) 117.3(2).

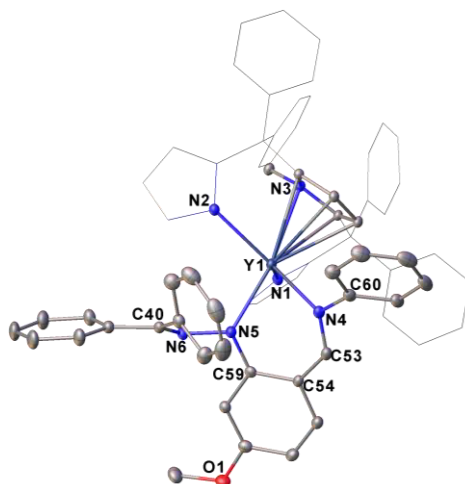


Figure S5. Molecular structure of **2d**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y–N(4) 2.392(3), Y–N(5) 2.315(3), N(5)–N(6) 1.424(3), C(59)–N(5) 1.367(4), C(40)–N(6) 1.279(4), C(53)–N(4) 1.305(4), N(5)–Y–N(4) 74.58(9), N(6)–N(5)–C(59) 110.4(3), C(40)–N(6)–N(5) 117.7(3), N(6)–N(5)–Y 123.03(17), Y–N(5)–C(59) 113.56(18), C(54)–C(53)–N(4) 127.6(3), Y–N(4)–C(53) 114.1(2).

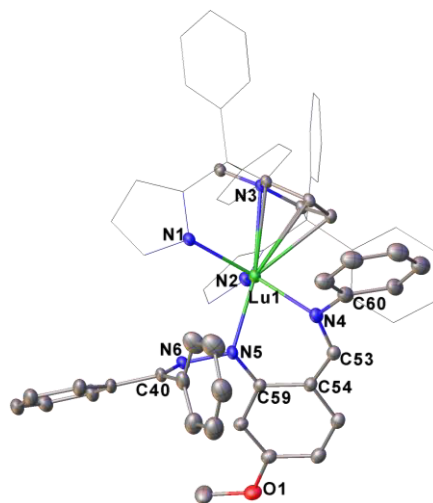


Figure S6. Molecular structure of **2d'**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu–N(4) 2.344(7), Lu–N(5) 2.255(7), N(5)–N(6) 1.438(9), C(59)–N(5) 1.351(10), C(40)–N(6) 1.254(10), C(53)–N(4) 1.288(10), N(5)–Lu–N(4) 74.4(3), N(6)–N(5)–C(59) 111.6(7), C(40)–N(6)–N(5) 115.8(7), N(6)–N(5)–Lu 117.6(5), Lu–N(5)–C(59) 118.4(5), C(54)–C(53)–N(4) 126.9(9), Lu–N(4)–C(53) 118.6(6).

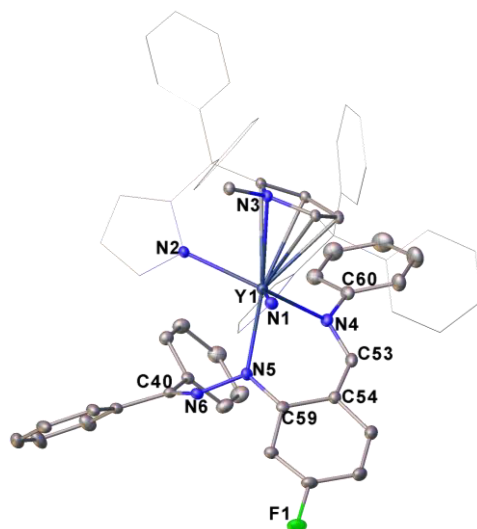


Figure S7. Molecular structure of **2e**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y–N(4) 2.400(3), Y–N(5) 2.310(3), N(5)–N(6) 1.429(4), C(59)–N(5) 1.360(4), C(40)–N(6) 1.280(4), C(53)–N(4) 1.311(5), N(5)–Y–N(4) 73.98(11), N(6)–N(5)–C(59) 73.98(11), C(40)–N(6)–N(5) 113.8(3), N(6)–N(5)–Y 120.6(2), Y–N(5)–C(59) 117.8(2), C(54)–C(53)–N(4) 127.7(4), Y–N(4)–C(53) 116.2(3).

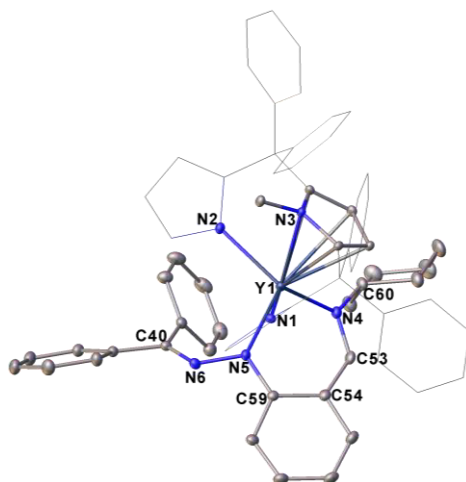


Figure S8. Molecular structure of **2f**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y–N(4) 2.389(3), Y–N(5)–Y–N5 2.300(3), N(5)–N(6) 1.413(4), C(59)–N(5) 1.372(4), C(40)–N(6) 1.286(4), C(53)–N(4) 1.294(5), N(5)–Y–N(4) 74.67(11), N(6)–N(5)–C(59) 111.8(3), C(40)–N(6)–N(5) 117.8(3), N(6)–N(5)–Y 120.0(2), Y–N(5)–C(59) 109.9(2), C(54)–C(53)–N(4) 127.1(4), Y–N(4)–C(53) 112.3(3).

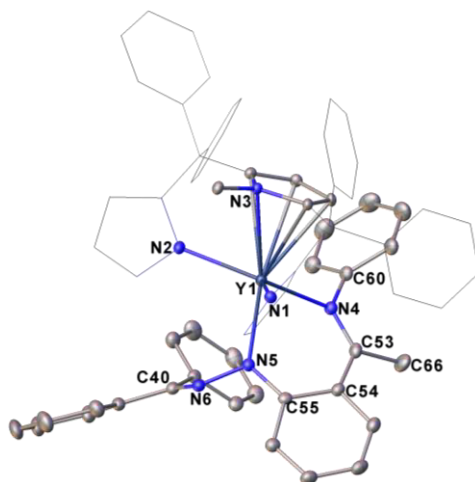


Figure S9. Molecular structure of **2g**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y–N(4) 2.388(2), Y–N(5) 2.290(3), N(5)–N(6) 1.429(3), C(59)–N(5) 1.371(4), C(40)–N(6) 1.292(4), C(53)–N(4) 1.302(4), N(5)–Y–N(4) 73.13(9), N(6)–N(5)–C(59) 73.13(9), C(40)–N(6)–N(5) 114.6(3), N(6)–N(5)–Y 119.02(17), Y–N(5)–C(59) 117.83(19), C(54)–C(53)–N(4) 122.2(3), Y–N(4)–C(53) 124.8(2).

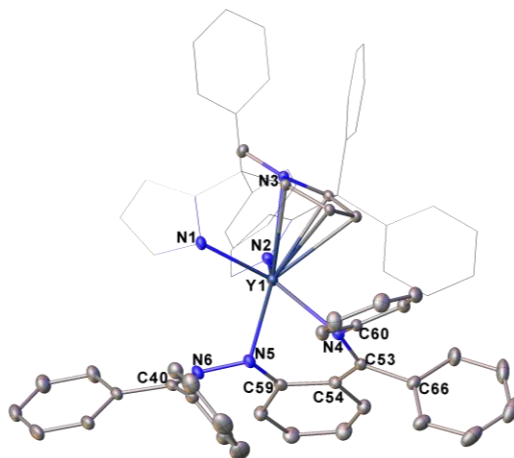


Figure S10. Molecular structure of **2h**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y–N(4) 2.368(4), Y–N(5) 2.287(4), N(5)–N(6) 1.412(4), C(59)–N(5) 1.378(4), C(40)–N(6) 1.278(4), C(53)–N(4) 1.310(4), N(5)–Y–N(4) 72.18(11), N(6)–N(5)–C(59) 111.3(3), C(40)–N(6)–N(5) 115.9(3), N(6)–N(5)–Y 119.2(2), Y–N(5)–C(59) 114.0(2), C(54)–C(53)–N(4) 121.2(3), Y–N(4)–C(53) 120.1(2).

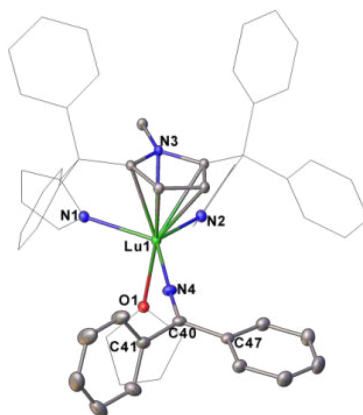


Figure S11. Molecular structure of **4a'**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand and the carbon atoms of THF were depicted in wireframe style for clarity. Selected bond lengths (Å): Lu1–N1 2.262(3), Lu1–N2 2.272(3), Lu1–N3 2.617(2), Lu1–N4 2.127(3), N4–C40 1.265(4).

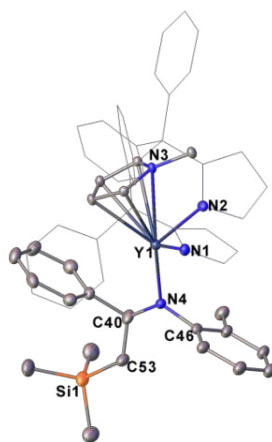


Figure S12. Molecular structure of **6**. All the hydrogen atoms are omitted. The rings of benzene and pyrrole on the ligand were depicted in wireframe style for clarity. Selected bond lengths (Å): Y1–N1 2.267(5), Y1–N2 2.267(4), Y1–N3 2.742(5), Y1–N4 2.164(5), N4–C40 1.454(6), N4–C46 1.431(5), C40–C53 1.438(7).

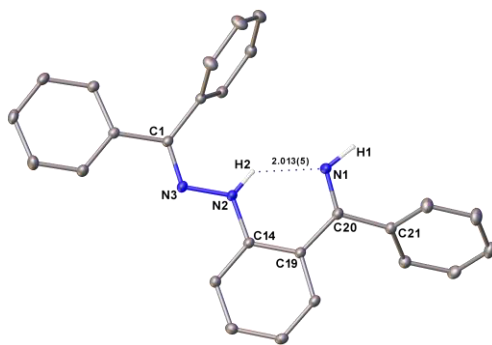


Figure S13. Molecular structure of **8a**. All the hydrogen atoms (except for H1 and H2) are omitted. Selected bond lengths (Å) and angles (°): N(3)-N(2) 1.370(4), C(1)-N(3) 1.288(4), C(20)-N(1) 1.262(4), C(14)-N(2) 1.377(4); C(1)-N(3)-N(2) 117.54(17), N(3)-N(2)-C(14) 118.56(16), N(2)-C(14)-C(19) 120.30(17), C(19)-C(20)-N(1) 120.53(19), N(1)-C(20)-C(21) 120.07(19).

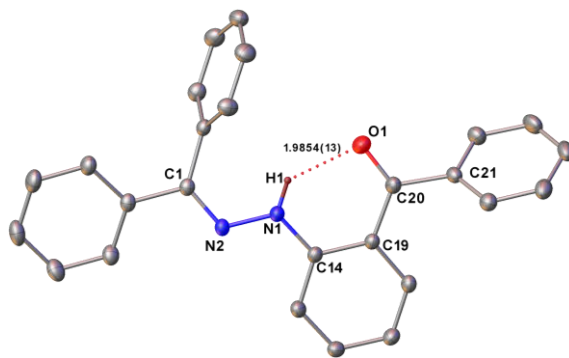


Figure S14. Molecular structure of **8a'**. All the hydrogen atoms (except for H1) are omitted. Selected bond lengths (Å) and angles (°): N(2)-N(1) 1.3660(18), C(1)-N(2) 1.292(2), C(20)-O(1) 1.271(4), C(14)-N(1) 1.391(4); C(1)-N(2)-N(1) 117.1(3), N(2)-N(1)-C(14) 119.0(3), N(1)-C(14)-C(19) 120.0(3), C(19)-C(20)-O(1) 120.8(3), O(1)-C(20)-C(21) 118.3(3).

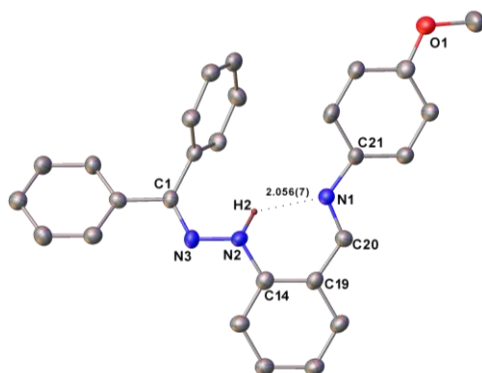


Figure S15. Molecular structure of **8c**. All the hydrogen atoms (except for H2) are omitted. Selected bond lengths (Å) and angles (°): N(3)-N(2) 1.332(9), C(1)-N(3) 1.278(10), C(20)-N(1) 1.266(10), C(14)-N(2) 1.364(8), C(21)-N(1) 1.391(8), C(1)-N(3)-N(2) 117.8(7), N(3)-N(2)-C(14) 120.6(7), N(2)-C(14)-C(19) 121.4(5), C(14)-C(19)-C(20) 124.1(4), C(19)-C(20)-N(1) 123.2(8), C(21)-N(1)-C(20) 121.7(7).

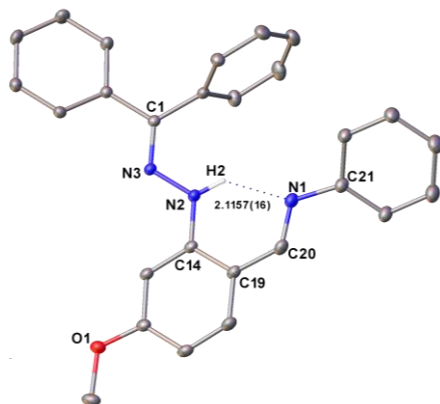


Figure S16. Molecular structure of **8d**. All the hydrogen atoms (except for H2) are omitted. Selected bond lengths (Å) and angles (°): N(3)-N(2) 1.371(2), C(1)-N(3) 1.290(2), C(20)-N(1) 1.276(3), C(14)-N(2) 1.377(2), C(21)-N(1) 1.398(3), C(1)-N(3)-N(2) 117.58(15), N(3)-N(2)-C(14) 118.78(15), N(2)-C(14)-C(19) 119.30(17), C(14)-C(19)-C(20) 123.96(18), C(19)-C(20)-N(1) 125.69(19), C(21)-N(1)-C(20) 116.8(2).

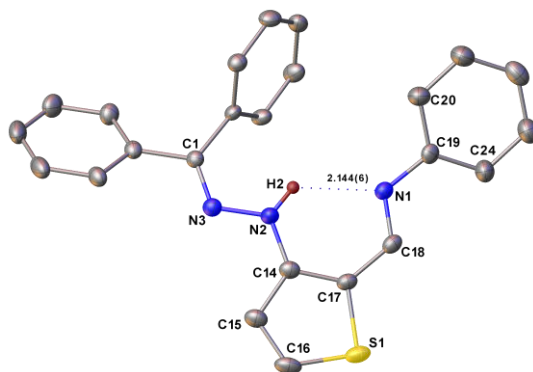


Figure S17. Molecular structure of **8i**. All the hydrogen atoms (except for H2) are omitted. Selected bond lengths (Å) and angles (°): N(3)-N(2) 1.363(4), C(1)-N(3) 1.271(4), C(18)-N(1) 1.266(4), C(14)-N(2) 1.353(4), C(19)-N(1) 1.395(3), C(1)-N(3)-N(2) 117.32(10), N(3)-N(2)-C(14) 118.75(12), N(2)-C(14)-C(17) 121.29(13), C(14)-C(17)-C(18) 128.35(12), C(17)-C(18)-N(1) 121.63(18), C(18)-N(1)-C(19) 120.36(18).

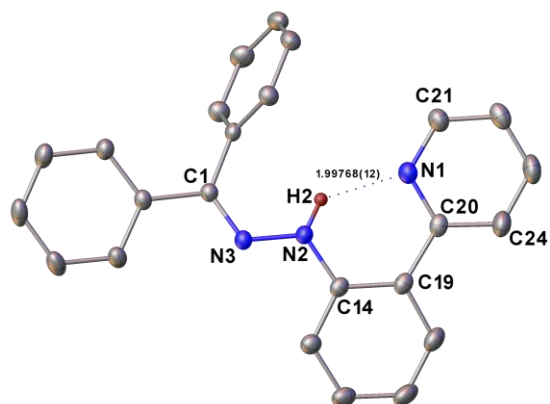


Figure S18. Molecular structure of **8j**. All the hydrogen atoms (except for H2) are omitted. Selected bond lengths (Å) and angles (°): N(3)-N(2) 1.35733(7), C(1)-N(3) 1.29097(7), C(20)-N(1) 1.33259(7), C(14)-N(2) 1.38069(7), C(21)-N(1) 1.33699(7), C(1)-N(3)-N(2) 118.8005(18), N(3)-N(2)-C(14) 119.115(2), N(2)-C(14)-C(19) 120.877(2), C(14)-C(19)-C(20) 124.226(3), C(19)-C(20)-N(1) 118.314(4), C(21)-N(1)-C(20) 119.211(4).

3. Characterization data for the rare-earth metal complexes and hydrazone-imines

General procedures.

All manipulations of oxygen- or moisture-sensitive materials were carried out under an atmosphere of argon in BRAUN glovebox or using standard Schlenk techniques. All glassware was rigorously dried one hour at 110 °C and cooled under vacuum before use. Toluene, *n*-hexane, and THF were dried and distilled at atmospheric pressure from sodium benzophenone ketyl; sodium was used to dry these solvents. Diphenyldiazomethane¹, $\text{LY}(\text{CH}_2\text{SiMe}_3)(\text{THF})_2$,² and substituted imines³ were prepared according to literature methods. All other reagents were purchased from commercial sources and used as received. Elemental analyses data were obtained on a PerkinElmer 2400 Series II elemental analyzer. The NMR spectra were collected on a Bruker AV-500 NMR spectrometer (500 MHz for ¹H; 126 MHz for ¹³C; 471 MHz for ¹⁹F). Chemical shifts (δ) and *J* values were reported in ppm and Hz respectively. Under argon protection, suitable crystals of rare-earth metal complexes were sealed in a thin-walled capillary. X-ray crystallographic diffraction was performed on a Bruker SMART CCD area detector diffractometer using graphite-monochromated Mo-K α radiation ($\lambda = 0.71073$ Å). An empirical absorption correction was applied using the SADABS program.⁴ All structures were solved by direct methods, completed by subsequent difference Fourier syntheses, and refined

anisotropically for all non-hydrogen atoms by full-matrix least-squares calculations on F^2 using the SHELXTL program package. The solvents of some structures were moved by Platon Squeeze.⁵

Preparation of 1a'. To a clear colorless solution of the ligand H₂L (1.00 g, 1.84 mmol) in 7.0 mL of THF was added a clear colorless solution of Lu(CH₂SiMe₃)₃(THF)₂ (0.91 g, 1.84 mmol) in 7.0 mL of THF at room temperature. Then 4.0 mL of *n*-hexane was added, and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still for 12 h. During this course, crystals precipitated and were collected by filtration, washed with 3 mL of *n*-hexane, and dried in *vacuo*. Yield: 155 mg (89%). ¹H NMR (C₆D₆): δ 7.47 (d, *J* = 7.8 Hz, 3H, Ph), 7.30–7.26 (m, 1H), 7.22 (d, *J* = 1.5 Hz, 1H), 7.20 (s, 2H), 7.18 (d, *J* = 1.5 Hz, 1H Ph), 6.97 (t, *J* = 1.0 Hz, 1H), 6.76–6.65 (m, 1H, Py), 6.72–6.67 (m, 1H, Py), 6.61 (dd, *J* = 3.0, 1.5 Hz, 2H, Py), 6.58 (t, *J* = 2.5 Hz, 2H, Py), 6.15 (s, 2H, Py), 3.64 (s, 8H, THF), 2.42 (s, 3H, NMe), 1.336 (s, 8H, THF), -0.07 (s, 9H, SiMe₃), -1.09 (s, 2H, CH₂SiMe₃) ppm. ¹³C{¹H} NMR (C₆D₆): δ 149.8 (Ph), 148.9, 145.4, 144.2, 130.2, 129.6, 128.4, 127.5, 127.1 (Ph), 127.2 (Ph), 113.6 (Py), 110.6 (Py), 108.4 (Py), 68.9 (THF), 58.2 (CPh₂), 35.9 (Lu-CH₂SiMe₃), 35.5 (NMe), 25.6 (THF), 4.5 (SiMe₃) ppm. Anal. Calcd for C₅₁H₅₈N₃O₂SiLu: C, 64.61; H, 6.17; N, 4.43. Found: C, 64.36; H, 6.51; N, 4.03.

Preparation of 2a' from 3a' and Ph₂CN₂

To a clear colorless solution of 3a' (100 mg, 0.100 mmol) in 1.5 mL of toluene was added a brown solution of Ph₂CN₂ (19 mg, 0.174 mmol) in 1.5 mL of toluene at room temperature. Then 100 μL of THF was added. During the process, the color of the solution changed to deep red slowly. After 5 h, 4.5 mL of *n*-hexane was added and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still. Red crystals appeared and dried in *vacuum*. Yield: 104 mg (90%).

Preparation of 2a' from 4a' and Ph₂CN₂:

To a clear colorless solution of 4a' (91 mg, 0.100 mmol) in 1.5 mL of toluene was added a brown solution of Ph₂CN₂ (19 mg, 0.100 mmol) in 1.5 mL of toluene at room temperature. During the process, the color of the solution changed to deep red slowly. After 3 h, 4.5 mL of *n*-hexane was added and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still. Red crystals appeared and dried in *vacuum*. Yield: 105 mg (91%).

Preparation of 2b-2j

Under an argon atmosphere, to a clear colorless solution of the complex **1** (0.174 mmol) in 1.5 mL of toluene was added a clear solution of imine (0.174 mmol) in 1.5 mL of toluene and the mixture was stirred at room temperature for 3 h. During this course, the color of the solution changed to green slowly. Then Ph₂CN₂ (33 mg, 0.174 mmol) and a suitable amount of *n*-hexane were added, the color of the solution changes from green to red and finally to dark red. Red crystals were obtained by standing the solution at room temperature for several hours.

Preparation of 2b. The complex **2b** was isolated as red crystals by treatment of **1a** (150 mg, 0.174 mmol) with PhCH=NPh (31 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 187 mg (90%). ¹H NMR (THF-*d*₈): δ 7.86 (s, 1H, imine *H*), 7.73 (d, *J* = 7.0 Hz, 2H, Ph), 7.34 (s, 2H), 7.28–7.24 (m, 6H), 7.21 (d, *J* = 7.5 Hz, 3H), 7.15–7.09 (m, 8H), 7.08–7.04 (m, 7H), 7.01 (d, *J* = 7.0 Hz, 2H), 6.98 (d, *J* = 7.5 Hz, 3H), 6.81 (d, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.5 Hz, 2H), 6.58 (s, 2H), 6.44 (d, *J* = 7.0 Hz, 1H, Ph), 5.93 (s, 2H, Py), 5.82 (d, *J* = 7.5 Hz, 2H, Py), 5.66 (s, 2H, Py), 4.94 (s, 2H, Py), 2.16 (s, 3H, *NMe*) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 163.9 (CH=N), 162.0 (NN-*C*_{aryl}), 152.1 (Ph), 151.2, 150.1, 149.0, 143.7, 138.6, 137.1, 133.7, 133.5, 131.6, 129.4, 129.2, 128.7, 128.3, 128.1, 127.9, 127.6, 127.4, 127.0, 126.3, 126.1, 125.9, 125.6, 124.9, 121.5, 120.7 (Ph), 117.4 (Py), 115.2, 114.4, 112.4, 110.9, 107.7, 106.2 (Py), 57.2 (CPh₂), 34.9 (*NMe*) ppm. Anal. Calcd for C₆₅H₅₁N₆Y·C₇H₈: C, 78.82; H, 5.42; N, 7.66. Found: C, 78.85; H, 5.37; N, 7.34.

Preparation of 2b'. The complex **2b'** was isolated as red crystals by treatment of **1a'** (168 mg, 0.174 mmol) with PhCH=NPh (31 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 173 mg (91%). ¹H NMR (THF-*d*₈): δ 7.84 (s, 1H, imine *H*), 7.79 (d, *J* = 3.5 Hz, 2H, Ph), 7.46 (s, 1H), 7.44 (s, 1H), 7.36–7.32 (m, 3H), 7.24–7.18 (m, 8H), 7.14–7.09 (m, 15H), 7.02 (s, 1H), 7.00 (s, 1H), 6.96 (d, *J* = 7.0 Hz, 1H), 6.91 (d, *J* = 7.0 Hz, 2H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.69 (t, *J* = 7.5 Hz, 2H, Ph), 6.47–6.44 (m, 1H), 5.97 (s, 2H, Py), 5.67 (s, 4H, Py), 5.05 (s, 1H, Py), 4.61 (s, 1H, Py), 2.14 (s, 3H, *NMe*) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 164.1 (CH=N), 163.2 (NN-*C*_{aryl}), 153.0 (Ph), 151.2, 149.7, 149.1, 143.6, 138.2, 135.9, 135.5, 134.1, 129.4, 129.1, 128.8, 128.3, 128.2, 127.9, 127.6, 127.4, 127.3, 127.0, 126.3, 126.1, 126.0, 124.6 (Ph), 115.1 (Py), 114.0, 113.0, 107.9, 106.2 (Py), 57.0 (CPh₂), 34.4 (*NMe*) ppm. Anal. Calcd for C₆₅H₅₁N₆Lu: C, 71.55; H, 4.71; N, 7.70. Found: C, 71.93; H, 5.19; N, 7.54.

Preparation of 2c. To a clear colorless solution of **5c** (150 mg, 0.164 mmol) in 3.0 mL of toluene was added a clear colorless solution of Ph₂CN₂ (35 mg, 0.164 mmol) in 1.5 mL of toluene at room temperature. The mixture was stirred for 1 h and the color of the solution changed to dark red slowly. Then 2.0 mL of *n*-hexane was added and red crystals appeared after standing the

solution at room temperature for 24 h. Yield: 165 mg (92%). ^1H NMR (THF- d_8): δ 7.83 (s, 1H, imine *H*), 7.74 (d, $J = 7.5$ Hz, 2H, Ph), 7.36–7.25 (m, 8H), 7.24–7.19 (m, 4H), 7.14–7.07 (m, 13H), 7.03–6.96 (m, 5H), 6.58 (s, 3H), 6.42 (t, $J = 7.3$ Hz, 1H), 6.28 (d, $J = 8.5$ Hz, 2H, Ph), 5.92 (s, 2H, Py), 5.72 (d, $J = 8.0$ Hz, 2H, Py), 5.65 (s, 2H, Py), 4.92 (s, 2H, Py), 3.56 (s, 3H, *OMe*), 2.15 (s, 3H, *NMe*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (THF- d_8): δ 163.3 (CH=N), 160.0, 157.2 (NN- C_{aryl}), 151.9 (Ph), 150.0, 149.1, 143.8, 143.7, 143.0, 138.6, 135.3, 133.5, 129.5, 129.2, 128.8, 128.7, 128.3, 128.1, 127.6, 127.5, 127.4, 127.0, 126.7, 126.1, 125.9, 125.6, 124.7, 122.2 (Ph), 114.9 (Py), 114.1, 113.8, 113.1, 107.6, 106.1 (Py), 57.2 ($C\text{Ph}_2$), 54.3 (*OMe*), 34.3 (*NMe*) ppm. Anal. Calcd for $\text{C}_{66}\text{H}_{53}\text{N}_6\text{OY}\cdot 0.5\text{C}_6\text{H}_{11}$: C, 76.87; H, 5.61; N, 7.79. Found: C, 76.72; H, 6.07; N, 7.32.

Preparation of 2c'. The complex **2c'** was isolated as pale red crystals by treatment of **1a'** (168 mg, 0.174 mmol) with *p*-MeOC₆H₄N=CHPh (37 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 177 mg (91%). ^1H NMR (THF- d_8): δ 7.82 (s, 1H, imine *H*), 7.79 (d, $J = 3.5$ Hz, 2H, Ph), 7.46 (d, $J = 8.5$ Hz, 2H), 7.36–7.32 (m, 4H, Ph), 7.23–7.20 (m, 7H, Ph), 7.15 (d, $J = 7.5$ Hz, 5H), 7.13–7.09 (m, 8H), 7.01 (m, 3H), 6.91 (d, $J = 7.5$ Hz, 2H), 6.71–6.66 (m, 1H), 6.51–6.43 (m, 2H), 6.23 (d, $J = 8.5$ Hz, 2H, Ph), 5.96 (s, 2H, Py), 5.67 (s, 2H, Py), 5.58 (d, $J = 7.6$ Hz, 2H, Py), 5.02 (s, 1H, Py), 4.65 (s, 1H, Py), 3.56 (s, 3H, *OMe*), 2.13 (s, 3H, *NMe*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (THF- d_8): δ 163.6 (CH=N), 160.6, 157.1 (NN- C_{aryl}), 152.9, 149.6, 149.1, 143.8, 138.3, 137.1, 136.0, 135.4, 133.8, 129.5, 129.2, 129.1, 128.9, 128.3, 128.2, 127.4, 126.7, 126.2, 126.1, 126.0, 122.6, 121.7, 117.3, 115.2, 113.9, 113.7, 113.1 (Py), 113.0 (Py), 108.6 (Py), 106.2 (Py), 57.0 ($C\text{Ph}_2$), 54.2 (*OMe*), 34.4 (*NMe*) ppm. Anal. Calcd for $\text{C}_{66}\text{H}_{53}\text{N}_6\text{OLu}\cdot 0.5\text{C}_7\text{H}_8$: C, 71.52; H, 4.92; N, 7.20. Found: C, 71.66; H, 5.41; N, 6.81.

Preparation of 2d. The complex **2d** was isolated as deep red crystals by treatment of **1a** (150 mg, 0.174 mmol) with *p*-MeOC₆H₄CH=NPh (37 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 167 mg (93%). ^1H NMR (THF- d_8): δ 7.80 (dd, $J = 6.5, 2.7$ Hz, 2H), 7.68 (s, 1H, imine *H*), 7.37 (s, 2H, Ph), 7.34–7.32 (m, 3H, Ph), 7.20–7.17 (m, 5H), 7.13–7.05 (m, 14H), 7.03–7.00 (m, 5H), 6.96 (t, $J = 7.0$ Hz, 1H), 6.78–6.74 (m, 2H), 6.70 (d, $J = 7.7$ Hz, 2H), 6.57 (s, 2H, Ph), 6.11 (dd, $J = 9.0, 2.5$ Hz, 1H, Py), 5.92 (s, 1H, Py), 5.73 (d, $J = 7.5$ Hz, 2H, Py), 5.65 (s, 2H, Py), 4.94 (s, 2H, Py), 3.67 (s, 3H, *OMe*), 2.14 (s, 3H, *NMe*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (THF- d_8): δ 165.0 (CH=N), 162.7, 162.0 (NN- C_{aryl}), 154.1 (Ph), 151.3 (Ph), 149.9, 149.0, 143.6, 138.3, 137.8, 135.7, 129.4, 129.1, 129.0, 128.5, 128.1, 127.8, 127.6, 127.3, 126.9, 126.9, 126.7, 126.3, 125.9, 125.6, 124.6, 124.2, 121.4 (Ph), 120.6 (Ph), 108.5 (Py), 106.1 (Py), 106.0 (Py), 94.0, 57.1 ($C\text{Ph}_2$), 53.9 (*OMe*), 34.3 (*NMe*) ppm. Anal. Calcd for $\text{C}_{66}\text{H}_{53}\text{N}_6\text{OY}\cdot 1.5\text{C}_7\text{H}_8$: C, 78.31; H, 5.58; N, 7.16. Found: C, 77.80; H, 5.79; N, 6.94.

Preparation of 2d'. The complex **2d'** was isolated as deep red crystals by treatment of **1a'** (168 mg, 0.174 mmol) with *p*-MeOC₆H₄CH=NPh (37 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 175 mg (90%). ¹H NMR (THF-*d*₈): δ 7.82 (s, 2H), 7.71 (s, 1H, imine *H*), 7.56 (s, 1H), 7.47 (s, 1H), 7.35 (d, *J* = 3.5 Hz, 1H), 7.27–7.16 (m, 11H), 7.14–7.06 (m, 8H), 7.00–6.98 (m, 6H), 6.94 (d, *J* = 7.0 Hz, 3H), 6.72 (d, *J* = 6.5 Hz, 1H), 6.64 (s, 2H), 6.49 (d, *J* = 7.0 Hz, 1H), 6.27 (s, 1H), 6.16–6.12 (m, 1H, Py), 6.03 (s, 1H, Py), 5.88 (s, 1H, Py), 5.74 (s, 1H, Py), 5.58 (s, 2H, Py), 5.03 (s, 1H, Py), 4.44 (s, 1H, Pyr*H*), 3.69 (s, 3H, OMe), 2.12 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 165.0 (CH=N), 163.4, 162.7 (NN-C_{aryl}), 155.0 (Ph), 149.5 (Ph), 143.3, 138.1, 137.6, 135.8, 129.4, 129.2, 128.7, 128.1, 127.6, 127.4, 127.3, 127.1, 126.7, 126.1, 125.9, 124.1, 121.8 (Ph), 120.5 (Ph), 108.1 (Py), 106.2 (Py), 94.5 (Py), 56.9 (CPh₂), 53.9 (OMe), 34.3 (NMe) ppm. Anal. Calcd for C₆₆H₅₃N₆OLu·1.5C₇H₈: C, 72.96; H, 5.20; N, 6.67. Found: C, 72.68; H, 5.10; N, 6.30.

Preparation of 2e. The complex **2e** was isolated as red crystals by treatment of **1a** (150 mg, 0.174 mmol) with *p*-FC₆H₄CH=NPh (35 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 148 mg (83%). ¹H NMR (THF-*d*₈): δ 7.82 (s, 1H, imine *H*), 7.80–7.76 (m, 2H, Ph), 7.35 (d, *J* = 5.5 Hz, 5H, Ph), 7.23–7.17 (m, 8H), 7.15–7.08 (m, 12H), 7.03–6.98 (m, 4H), 6.82–6.80 (m, 1H), 6.73 (t, *J* = 7.5 Hz, 2H), 6.60–6.51 (m, 3H), 6.25–6.21 (m, 1H, Ph), 5.94 (s, 2H, Py), 5.74 (d, *J* = 7.5 Hz, 2H, Py), 5.67 (s, 2H, Py), 4.87 (s, 2H, Py), 2.16 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 167.1 (d, *J*_{F-C} = 253.3 Hz), 163.9 (CH=N), 162.7 (NN-C_{aryl}), 161.0 (Ph), 154.1 (d, *J*_{F-C} = 11.4 Hz), 150.8 (Ph), 150.2, 149.9, 145.6, 143.5, 143.1, 138.9 (d, *J*_{F-C} = 12.6 Hz), 138.1, 135.6, 130.0, 129.4, 129.3, 129.1, 129.0, 128.4, 128.2, 127.9, 127.8, 127.7, 127.4, 127.0, 127.6, 126.5, 126.1, 126.0, 125.4, 125.1, 124.9, 124.8, 121.5 (Ph), 120.6 (Ph), 111.2, 107.8, 106.3 (Py), 105.1 (Py), 103.5 (Py), 103.3, 98.7, 98.6, 57.2 (CPh₂), 34.5 (NMe) ppm. ¹⁹F NMR (471 MHz, THF-*d*₈): δ -103.97 (s). Anal. Calcd for C₆₅H₅₀N₆FY·1.5C₇H₈: C, 77.55; H, 5.24; N, 7.54. Found: C, 77.88; H, 5.54; N, 7.82.

Preparation of 2f. The complex **2f** was isolated as red crystals by treatment of **1a** (150 mg, 0.174 mmol) with PhCH=NC₆H₁₁ (33 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 158 mg (90%). ¹H NMR (THF-*d*₈): δ 7.90 (s, 1H, imine *H*), 7.41 (d, *J* = 7.0 Hz, 2H, Ph), 7.24 (s, 4H, Ph), 7.13 (d, *J* = 8.0 Hz, 3H, Ph), 7.11–7.06 (m, 5H), 7.02–6.07 (m, 10H), 6.94 (d, *J* = 7.0 Hz, 3H), 6.83–6.75 (m, 7H, Ph), 6.28 (t, *J* = 7.5 Hz, 1H, Py), 5.98 (s, 5H, Py), 5.68 (t, *J* = 2.5 Hz, 2H, Py), 2.82 (s, 1H, Cy), 2.22 (s, 3H, NMe), 1.53 (s, 2H, Cy), 1.45 (s, 1H, Cy), 1.13 (s, 1H, Cy), 1.11 (s, 1H, Cy), 0.99 (s, 5H, Cy) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 160.8 (CH=N), 160.5 (NN-C_{aryl}), 150.0 (Ph), 149.6 (Ph), 148.9, 144.3, 142.5, 139.6, 136.4, 132.2, 131.2, 130.3, 129.5, 129.3, 128.8, 128.3, 127.9, 127.3, 127.0, 126.9, 126.1, 125.9, 125.8 (Ph), 117.1, 116.4, 115.2, 112.2 (Py), 109.3 (Py), 107.5 (Py), 105.7

(Cy), 70.0 (Cy), 63.7 (Cy), 57.4 (CPh₂), 34.9 (NMe), 33.1 (Cy) ppm. Anal. Calcd for C₆₅H₅₇N₆Y·2C₇H₈: C, 79.38; H, 6.16; N, 7.03. Found: C, 79.35; H, 6.35; N, 7.48.

Preparation of 2g. The complex **2g** was isolated as deep red crystals by treatment of **1a** (150 mg, 0.174 mmol) with PhMeC=NPh (34 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 158 mg (90%). ¹H NMR (THF-*d*₈): δ 8.25 (s, 1H, Ph), 8.09 (d, *J* = 7.0 Hz, 1H, Ph), 7.98 (d, *J* = 7.5 Hz, 1H, Ph), 7.90 (s, 1H), 7.49 (s, 1H), 7.33 (d, *J* = 7.5 Hz, 1H), 7.26–7.18 (m, 3H), 7.15–7.12 (m, 6H), 7.02 (s, 8H), 6.90 (s, 2H), 6.67 (s, 3H), 6.62 (m, 6H), 6.55 (t, *J* = 7.3 Hz, 3H), 6.50–6.47 (m, 2H, Ph), 6.17 (d, *J* = 7.5 Hz, 2H, Py), 5.49 (s, 2H, Py), 5.32 (s, 2H, Py), 4.46 (s, 2H, Py), 2.68 (s, 3H, NMe), 2.32 (s, 3H, N=CMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 170.9 (CH=N), 160.8 (NN-C_{aryl}), 151.6 (Ph), 151.1 (Ph), 150.8, 147.4, 139.6, 138.1, 137.9, 133.9, 131.6, 130.5, 130.4, 130.1, 129.5, 129.4, 129.3, 129.1, 128.6, 127.2, 127.0, 126.9, 126.4, 125.7, 125.3 (Ph), 123.4 (Ph), 118.0, 117.9, 115.2 (Py), 107.8 (Py), 58.1 (Ph₂C), 35.6 (NMe), 32.0 (N=CMe) ppm. Anal. Calcd for C₆₆H₅₃N₆Y: C, 77.79; H, 5.24; N, 8.25. Found: C, 77.72; H, 5.55; N, 7.88.

Preparation of 2h. The complex **2h** was isolated as deep red crystals by treatment of **1a** (150 mg, 0.174 mmol) with Ph₂C=NPh (45 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 175 mg (93%). ¹H NMR (THF-*d*₈): δ 7.76–7.73 (m, 2H, Ph), 7.50 (s, 1H, Ph), 7.34–7.28 (m, 7H), 7.23–7.00 (m, 6H), 7.13–7.02 (m, 12H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.54 (s, 6H), 6.43–6.38 (m, 3H), 6.23 (d, *J* = 7.0 Hz, 1H), 6.06–6.03 (m, 1H, Ph), 5.92 (s, 3H, Ph), 5.67 (s, 2H, Py), 5.32 (d, *J* = 6.5 Hz, 3H, Py), 4.39 (s, 2H, Py), 4.11 (m, 1H, Py), 2.17 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 171.3 (CH=N), 160.3 (NN-C_{aryl}), 151.8 (Ph), 149.9 (Ph), 146.3, 138.8, 136.8, 134.4, 132.7, 130.0, 129.3, 129.1, 128.7, 128.4, 128.3, 127.9, 127.6, 127.5, 127.3, 127.2, 127.1, 126.8, 126.5, 126.1, 126.0, 125.7 (Ph), 123.9 (Ph), 116.1, 115.6, 113.3 (Py), 106.0 (Py), 105.0 (Py), 57.1 (CPh₂), 34.6 (NMe) ppm. Anal. Calcd for C₇₁H₅₅N₆Y: C, 78.88; H, 5.13; N, 7.77. Found: C, 78.72; H, 5.35; N, 7.31.

Preparation of 2i. The complex **2i** was isolated as red crystals by treatment of **1a** (150 mg, 0.174 mmol) with C₄H₃SCH=NPh (33 mg, 0.174 mmol) and Ph₂CN₂ (33 mg, 0.174 mmol) following the same procedure as that described above. Yield: 171 mg (89%). ¹H NMR (THF-*d*₈): δ 7.74 (dd, *J* = 7.0, 2.5 Hz, 2H, Ph), 7.67 (s, 1H, imine *H*), 7.66 (s, 1H, Ph), 7.35–7.31 (m, 3H), 7.20 (m, 8H), 7.14 (s, 4H), 7.11–7.06 (m, 6H), 7.05 (d, *J* = 4.0 Hz, 2H), 7.03–6.99 (m, 3H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.65 (m, 4H, Ph), 6.58 (s, 3H, Ph), 5.93 (s, 2H, Py), 5.72–5.61 (m, 4H, Py), 4.97 (s, 1H, Py), 4.66 (s, 1H, Pyr*H*), 2.13 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (C₆D₆): δ 162.5 (CH=N), 158.3 (NN-C_{aryl}), 151.5 (Ph), 150.5 (Ph), 143.5, 138.3, 138.0, 135.1, 129.7, 129.4, 128.6, 127.9, 127.6, 127.9, 127.3, 126.9, 126.1, 126.0, 123.4 (Ph), 120.9 (Ph), 118.0 (Py), 106.1 (Py), 104.1

(Py), 57.1(CPh₂), 34.3 (NMe) ppm. Anal. Calcd for C₆₃H₄₉N₆SY·C₇H₈: C, 76.21; H, 5.21; N, 7.62. Found: C, 76.11; H, 5.37; N, 7.44.

Preparation of 2j. To a clear yellow solution of **7j** (149 mg, 0.174 mmol) in 2.0 mL of toluene was added a clear brown solution of Ph₂CN₂ (33 mg, 0.174 mmol) in 2.0 mL of toluene at room temperature. Then 3.0 mL of *n*-hexane was added and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still for 24 h. Red crystals were appeared and dried in *vacuum*. Yield: 164 mg (88%). ¹H NMR (THF-*d*₈): δ 8.40 (d, *J* = 1.5 Hz, 1H, Ph), 7.59 (dd, *J* = 7.5, 6.5 Hz, 1H, Ph), 7.36 (s, 2H), 7.30 (dd, *J* = 7.0, 2.0 Hz, 3H), 7.24–7.17 (m, 6H), 7.10–7.06 (m, 9H), 7.01–6.99 (m, 4H), 6.97 (s, 1H), 6.82 (t, *J* = 7.0 Hz, 2H), 6.79–6.75 (m, 2H), 6.74–6.70 (m, 2H), 6.67 (d, *J* = 7.0 Hz, 1H), 6.61–6.56 (m, 2H), 6.52 (t, *J* = 7.5 Hz, 2H), 6.28 (t, *J* = 7.0 Hz, 2H), 6.15 (d, *J* = 2.0 Hz, 1H), 6.09 (d, *J* = 2.5 Hz, 1H), 6.05–6.02 (m, 1H), 5.45 (d, *J* = 3.5 Hz, 1H), 5.26 (d, *J* = 3.0 Hz, 1H), 5.10 (d, *J* = 8.0 Hz, 1H), 2.14 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 157.9 (NN-C_{aryl}), 149.6 (Ph), 149.0 (Ph), 148.4, 147.8, 147.2, 146.4, 145.6, 145.1, 142.7, 142.2, 141.6, 141.3, 138.9, 130.6, 130.1, 129.8, 129.2, 128.0, 127.0, 126.9, 126.8, 126.2, 126.1, 126.0, 125.9, 125.7, 125.5, 125.2, 124.9, 124.4, 124.1 (Ph), 120.2 (Ph), 115.9, 115.5, 111.6, 108.4, 108.3, 107.9 (Py), 106.6 (Py), 106.3 (Py), 105.0 (Py), 57.4 (CPh₂), 35.4 (NMe) ppm. Anal. Calcd for C₆₃H₄₉N₆Y: C, 77.29; H, 5.04; N, 8.58. Found: C, 77.20; H, 5.40; N, 8.05.

Preparation of 3a'. To a clear colorless solution of **1a'** (168 mg, 0.174 mmol) in 2.0 mL of toluene was added a clear brown solution of Ph₂CN₂ (33 mg, 0.174 mmol) in 1.0 mL of toluene at room temperature. The mixture was stirred for 3 h and the color of the solution gradually changed from red to colorless. Then 1.5 mL of *n*-hexane was added and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still for 24 h. White crystals were appeared and dried in *vacuo*. Yield: 108 mg (62%). ¹H NMR (C₆D₆): δ 7.33 (s, 2H, Ph), 7.27 (s, 3H, Ph), 7.05–7.00 (m, 10H, Ph), 6.95 (s, 6H), 6.91–6.87 (m, 5H, Ph), 6.82–6.80 (m, 4H), 6.78–6.74 (m, 2H, Py), 6.54 (d, *J* = 2.0 Hz, 2H, Py), 6.52–6.46 (m, 2H, Py), 5.35 (d, *J* = 3.0 Hz, 2H, Py), 3.22 (s, 2H, CH₂SiMe₃), 2.46 (s, 3H, NMe), -0.16 (s, 9H, CH₂SiMe₃) ppm. ¹³C{¹H} NMR (C₆D₆): δ 151.5 (imine C), 149.8 (Ph), 144.5 (Ph), 143.5, 143.2, 137.9, 136.2, 131.2, 129.8, 129.6, 128.8, 127.4, 127.3, 127.2, 127.1 (Ph), 126.2 (Ph), 111.8, 110.5, 109.0, 58.5 (CPh₂), 50.1 (CH₂SiMe₃), 36.7 (NMe), -1.5 (CH₂SiMe₃) ppm. Anal. Calcd for C₅₆H₅₂N₅SiLu: C, 67.39; H, 5.25; N, 7.02. Found: C, 67.01; H, 5.24; N, 7.03.

Preparation of 4a'. To a clear colorless solution of **1a'** (168 mg, 0.174 mmol) in 2.0 mL of toluene was added a clear colorless solution of Ph₂C=NH (30.3 μL, 0.174 mmol) in 1.0 mL of toluene at room temperature. The mixture was stirred for 3 h and the color of the solution

changed from colorless to red. Then 2.5 mL of *n*-hexane was added and the resulting mixture was stirred vigorously for 2 min before being allowed to stand still for 24 h. Yellow crystals were appeared and dried in *vacuo*. Yield: 39 mg (22%). ^1H NMR (C_6D_6): δ 7.45 (s, 3H, Ph), 7.27 (s, 5H, Ph), 7.20 (d, $J = 6.5$ Hz, 3H, Ph), 7.14–7.11 (m, 8H), 7.08–7.07 (m, 6H), 7.05–7.04 (m, 5H, Ph), 7.02 (s, 1H, Py), 7.01 (s, 1H, Py), 6.75–6.71 (m, 2H, Py), 6.65 (s, 2H, Py), 5.86 (s, 2H, Py), 3.74 (s, 4H, THF), 2.59 (s, 3H, *NMe*), 1.15 (s, 4H, THF) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 165.8 (imine C), 149.8 (Ph), 148.6 (Ph), 145.3, 144.7, 143.1, 130.4, 129.6, 128.3, 126.9 (Ph), 126.8 (Ph), 112.5 (Py), 110.3 (Py), 108.5 (Py), 70.7 (THF), 58.5 (CPh_2), 35.8 (*NMe*), 25.1 (THF) ppm. Anal. Calcd for $\text{C}_{56}\text{H}_{49}\text{N}_4\text{OLu}$: C, 69.41; H, 5.10; N, 5.78. Found: C, 69.28; H, 5.26; N, 5.52.

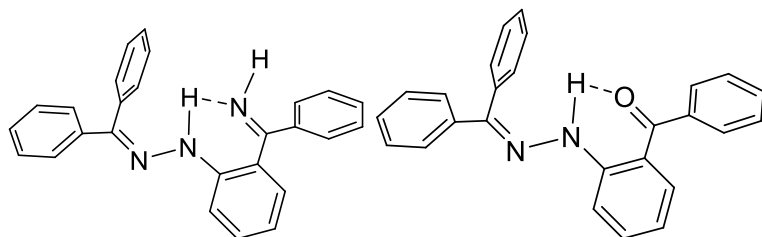
Preparation of 5c. To a clear colorless solution of **1a** (150 mg, 0.174 mmol) in 1.5 mL of toluene was added a clear colorless solution of *p*-MeOC₆H₄N=CHPh (37 mg, 0.174 mmol) in 1.5 mL of toluene at room temperature. The mixture was stirred for 5 h and the color of the solution changed to green slowly. Then 2.5 mL of *n*-hexane was added and green crystals appeared after standing the solution at room temperature for 12 h. The crystals were washed with 2.0 mL of cold *n*-hexane and dried in *vacuo*. Yield: 101 mg (63%). ^1H NMR (THF-*d*₈): δ 8.43 (d, $J = 6.5$ Hz, 1H, Ph), 7.98 (s, 1H, imine H), 7.89 (s, 2H, Ph), 7.45 (s, 4H), 7.33–7.26 (m, 2H, Ph), 7.13–7.12 (m, 7H), 7.06–7.016 (m, 4H), 6.91–6.85 (m, 6H), 6.66 (d, $J = 2.0$ Hz, 2H), 6.64 (dd, $J = 5.0, 3.0$ Hz, 2H, Py), 6.52 (dd, $J = 9.0, 2.5$ Hz, 2H, Py), 6.33–6.28 (m, 2H, Py), 5.76 (d, $J = 2.5$ Hz, 2H, Py), 3.33 (s, 4H, THF), 3.24 (s, 3H, *OMe*), 2.62 (s, 3H, *NMe*), 1.13 (s, 4H, THF) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (THF-*d*₈): δ 193.4 (d, $J_{\text{Y-C}} = 59.9$ Hz), 180.3 (Ph), 158.4 (Ph), 150.6, 150.5, 149.9, 145.2, 145.0, 144.0, 143.4, 139.2, 133.1, 131.7, 130.5, 129.3, 128.6, 126.8, 126.5, 125.9 (Ph), 123.8 (Ph), 114.5, 110.6 (Py), 110.4 (Py), 109.6 (Py), 107.8, 70.0 (THF), 58.4 (CPh_2), 55.1 (*OMe*), 36.7 (*NMe*), 25.2 (THF) ppm. Anal. Calcd for $\text{C}_{57}\text{H}_{51}\text{N}_4\text{O}_2\text{Y}\cdot 0.5\text{C}_7\text{H}_8$: C, 75.45; H, 6.18; N, 5.82. Found: C, 75.06; H, 5.79; N, 5.61.

Preparation of 6. The complex **6** was isolated as white crystals by treatment of **1a** (150 mg, 0.174 mmol) with 2-MeC₆H₄N=CHPh (34 mg, 0.174 mmol) following the same procedure as that described above for the preparation of **5c**. Yield: 157 mg (70%). ^1H NMR (C_6D_6): δ 7.34 (s, 2H, Ph), 7.33 (s, 2H, Ph), 7.23 (d, $J = 5.5$ Hz, 3H), 7.22–7.21 (m, 2H), 7.20–7.18 (m, 3H), 7.18–7.17 (m, 3H), 7.16 (t, $J = 1.5$ Hz, 2H), 7.15–7.12 (m, 5H), 7.11–7.10 (m, 2H), 7.10–7.07 (m, 2H), 7.06–7.05 (m, 1H), 7.04 (m, 1H), 7.02 (s, 1H, Ph), 7.00 (s, 1H, Py), 6.99 (s, 1H, Py), 6.57 (d, $J = 3.0$ Hz, 2H, Py), 6.53 (t, $J = 3.0$ Hz, 1H, Py), 6.49 (d, $J = 3.0$ Hz, 1H, Py), 5.28–5.14 (m, 2H, Py), 4.78 (dd, $J = 12.0, 3.5$ Hz, 1H, N-CHCH₂SiMe₃), 2.42 (s, 3H, *NMe*), 2.38 (s, 3H, *PhMe*), 1.37–1.34 (m, 1H, CH₂SiMe₃), 1.23–1.11 (m, 1H, CH₂SiMe₃), -0.25 (s, 9H, CH₂SiMe₃) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 151.3 (Ph), 150.8 (Ph), 149.8 (Ph), 148.5, 147.8, 144.2, 144.0, 143.7, 143.5, 133.6, 130.3, 129.9, 128.9, 128.4, 127.2, 127.1, 126.9, 125.1, 124.2 (Ph), 112.5 (Ph), 111.7,

110.1, 110.0 (Py), 108.4 (Py), 108.2 (Py), 58.5 (CPh₂), 58.4 (NCHCH₂SiMe₃), 36.1(NMe), 27.2 (Me), 20.0 (CH₂SiMe₃), -1.1 (CH₂SiMe₃) ppm. Anal. Calcd for C₅₇H₅₅N₄SiY·C₇H₈: C, 76.47; H, 6.32; N, 5.57. Found: C, 76.16; H, 6.81; N, 5.63.

Preparation of 7j. To a clear colorless solution of **1a** (150 mg, 0.174 mmol) in 2.0 mL of toluene was added a clear colorless solution of 2-phenylpyridine (24.5 μ L, 0.174 mmol) in 2.0 mL of *n*-hexane at room temperature. The mixture was stirred for 2 h and the color of the solution changed to yellow slowly. Yellow crystals appeared after standing the solution at room temperature for 12 h and dried in *vacuo*. Yield: 121 mg (65%). ¹H NMR (THF-*d*₈): δ 7.91 (d, *J* = 4.5 Hz, 1H, Ph), 7.71 (d, *J* = 8.5 Hz, 1H, Ph), 7.62–7.57 (m, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 4H), 7.23 (t, *J* = 7.5 Hz, 2H), 7.09–6.85 (m, 4H), 7.00 (m, 6H), 7.00–6.91 (m, 6H), 6.83 (s, 2H), 6.73–6.68 (m, 1H), 6.48 (t, *J* = 7.0 Hz, 1H), 6.26 (d, *J* = 6.5 Hz, 1H), 6.16 (d, *J* = 2.0 Hz, 2H), 6.12 (s, 1H), 5.90 (s, 2H), 2.21 (s, 3H, NMe) ppm. ¹³C{¹H} NMR (THF-*d*₈): δ 188.7 (d, *J*_{Y-C} = 42.8 Hz), 164.8 (Ph), 150.8 (Ph), 148.2 (Ph), 148.1, 145.1, 143.8, 138.3, 137.5, 129.8, 128.3, 127.8, 126.8, 126.0, 125.5, 125.2, 124.0, 122.3 (Ph), 120.4 (Ph), 118.2, 110.8 (Py), 107.8 (Py), 106.3 (Py), 57.7 (CPh₂), 34.9 (NMe) ppm. Anal. Calcd for C₅₄H₄₇N₄OY·0.5C₇H₈: C, 76.48; H, 5.69; N, 6.20. Found: C, 76.25; H, 5.69; N, 5.71.

Preparation of 8a-8j

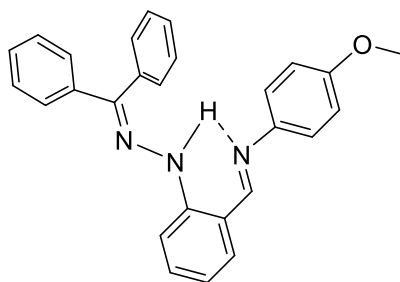


8a

8a'

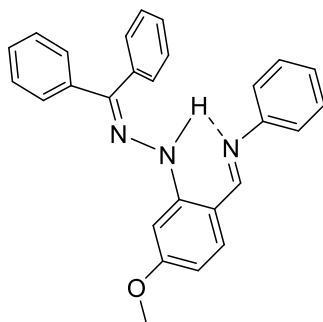
Preparation of 8a and 8a': Red crystals of **2a** (0.10 mmol) were stirred in methanol (5 mL) at room temperature for 10 min to give a yellow mixture. After filtration, a clear yellow solution was evaporated under reduced pressure. The crude product was purified by column chromatography with ethyl acetate/petroleum ether (v/v = 1:20) to give the desired product as a yellow oil. Yield: (90%). Recrystallization from methanol afforded two different yellow crystals **8a** and **8a'**. ¹H NMR (C₆D₆): δ 13.19 (s, 1H, NH), 12.01 (s, 2H, NH), 8.95 (s, 1H), 8.49 (dd, *J* = 8.5, 1.0 Hz, 1H, Ph), 8.37 (dd, *J* = 8.5, 1.0 Hz, 2H, Ph), 7.91–7.87 (m, 2H, Ph), 7.86–7.81 (m, 4H), 7.38 (dd, *J* = 8.0, 1.5 Hz, 2H, Ph), 7.35–7.31 (m, 6H, Ph), 7.29–7.25 (m, 5H, Ph), 7.24–7.21 (m, 4H, Ph), 7.19–7.16 (m, 10H, Ph), 7.14–7.11 (m, 4H,

Ph), 7.03–6.99 (m, 2H, Ph), 6.99–6.96 (m, 1H, Ph), 6.94–6.90 (m, 5H, Ph), 6.83 (t, $J = 1.5$ Hz, 1H, Ph), 6.81 (d, $J = 1.5$ Hz, 1H, Ph), 6.54 (ddd, $J = 8.0, 7.0, 1.0$ Hz, 1H, Ph), 6.48 (ddd, $J = 8.0, 7.0, 1.0$ Hz, 2H, Ph). $^{13}\text{C}\{^1\text{H}\}$ (C_6D_6): δ 198.6 (C=O), 179.9 (C=N), 148.7 (Ph), 148.6 (Ph), 148.1 (Ph), 147.1, 142.6, 140.5, 139.4, 139.0, 135.7, 134.9, 134.7, 134.0, 133.8, 132.5, 130.8, 129.9, 129.6, 129.5, 129.3, 129.1, 128.8, 128.7, 128.6, 128.5, 128.4 (Ph), 127.6 (Ph), 127.4 (Ph), 117.8, 117.3, 114.8, 114.2 ppm. ^1H NMR (CDCl_3): δ 12.63 (s, 1H, NNHN), 11.45 (s, 2H, NNHO), 9.06 (s, 1H, C=NH), 8.08 (d, $J = 1.0$ Hz, 1H), 8.06 (d, $J = 1.0$ Hz, 1H), 8.05 (s, 1H), 7.69–7.62 (m, 9H), 7.58–7.53 (m, 4H), 7.52–7.45 (m, 9H), 7.40–7.32 (m, 19H), 7.25–7.22 (m, 1H), 7.06 (dd, $J = 8.0, 1.5$ Hz, 1H), 6.72 (ddd, $J = 8.0, 7.0, 1.0$ Hz, 2H), 6.65 (t, $J = 7.5$ Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3): δ 199.2 (C=O), 180.1 (C=N), 148.4 (Ph), 148.3 (Ph), 147.4 (Ph), 147.1, 142.5, 140.4, 139.0, 138.8, 135.2, 134.9, 133.8, 132.4, 131.2, 130.1, 129.9, 129.8, 129.4, 129.3, 129.1, 128.9, 128.7, 128.6, 128.4, 127.6, 127.5 (Ph), 127.2 (Ph), 117.8, 117.4, 114.6, 113.8 ppm. HRMS (ESI):calcd for $\text{C}_{26}\text{H}_{21}\text{N}_3$ $[\text{M}+\text{H}]^+$: 376.1808, found 376.1806. HRMS (ESI):calcd for $\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}[\text{M}+\text{H}]^+$: 377.1648, found 377.1651



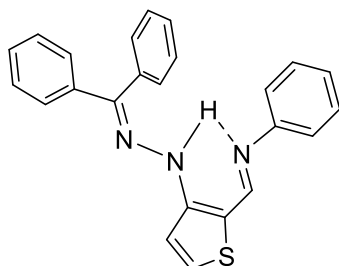
8c

Preparation of 8c. The compound of **8c** was isolated as red crystals by treatment of **2c** (0.10 mmol) with methanol (5 mL) following the same procedure as that described above for the preparation of **8a**. Yield: (92%). ^1H NMR (C_6D_6): δ 12.64 (s, 1H, NH), 8.39 (d, $J = 8.5$ Hz, 1H, CH=N), 8.09 (s, 1H, Ph), 7.81 (t, $J = 2.0$ Hz, 1H, Ph), 7.79 (d, $J = 1.0$ Hz, 1H, Ph), 7.34 (s, 2H, Ph), 7.15–7.14 (m, 1H, Ph), 7.14–7.12 (m, 2H, Ph), 7.11–7.06 (m, 5H, Ph r), 6.77 (dd, $J = 6.5, 1.5$ Hz, 2H, Ph), 6.75 (d, $J = 2.0$ Hz, 1H, Ph), 6.49 (d, $J = 2.0$ Hz, 1H, Ph), 6.47 (d, $J = 2.0$ Hz, 1H, Ph), 3.37 (s, 3H, OMe) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 193.3 (MeO- C_{aryl}), 161.0 (CH=N), 158.6 (NHN- C_{aryl}), 147.1 (Ph), 146.8 (Ph), 144.6 (Ph), 139.6, 135.2, 134.1, 132.4, 129.7, 129.6, 129.1, 128.9 (Ph), 127.5 (Ph), 112.7, 118.4, 118.1, 117.9, 114.1, 113.8, 55.0 (OMe) ppm. HRMS (ESI): calcd for $\text{C}_{27}\text{H}_{23}\text{ON}_3$ $[\text{M}+\text{H}]^+$: 406.1914, found 406.1920.



8d

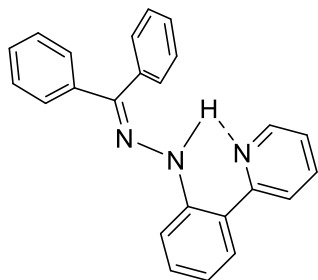
Preparation of 8d. The compound of **8d** was isolated as yellow crystals by treatment of **2d** (0.10 mmol) with methanol (5 mL) following the same procedure as that described above for the preparation of **8a**. Yield: (93%). ^1H NMR (C_6D_6): δ 12.76 (s, 1H, NH), 8.01 (s, 1H, CH=N), 7.95 (d, $J = 2.4$ Hz, 1H, Ph), 7.80 (s, 1H, Ph), 7.79 (s, 1H, Ph), 7.16–7.13 (m, 4H, Ph), 7.14–7.13 (m, 1H, Ph), 7.11–7.06 (m, 3H, Ph), 7.04 (dd, $J = 5.5, 4.0$ Hz, 2H, Ph), 6.96 (d, $J = 8.5$ Hz, 2H, Ph), 6.55 (s, 1H, Ph), 6.53 (s, 1H, Ph), 6.46 (dd, $J = 8.5, 2.5$ Hz, 1H, Ph), 3.45 (s, 3H, OMe) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 164.0 (MeO- C_{aryl}), 161.9 (CH=N), 151.9 (NHN- C_{aryl}), 148.8 (Ph), 147.7 (Ph), 139.4, 136.3, 135.1, 129.7, 129.4, 129.2, 128.5, 128.4, 127.5, 125.3 (Ph), 121.7 (Ph), 112.0, 106.5, 97.2, 54.9 (OMe) ppm. HRMS (ESI): calcd for $\text{C}_{27}\text{H}_{23}\text{ON}_3$ $[\text{M}+\text{H}]^+$: 406.1914, found 406.1911.



8i

Preparation of 8i. The compound of **8i** was isolated as red crystals by treatment of **2i** (0.10 mmol) with methanol (5 mL) following the same procedure as that described above for the preparation of **8a**. Yield: (91%). ^1H NMR (C_6D_6): δ 11.76 (s, 1H, NH), 8.02 (s, 1H, imine H), 7.81 (d, $J = 1.5$ Hz, 1H, Ph), 7.79 (t, $J = 1.5$ Hz, 1H, Ph), 7.69 (d, $J = 5.5$ Hz, 1H), 7.24–7.20 (m, 3H), 7.19–7.15 (m, 7H), 7.11–7.07 (m, 1H), 6.98 (d, $J = 5.5$ Hz, 1H), 6.59 (d, $J = 1.5$ Hz, 1H), 6.58 (t, $J = 1.5$ Hz, 1H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 181.7 (CH=N), 152.9 (Ph), 151.5 (Ph), 149.8, 147.0, 138.9, 134.4, 130.8, 129.8, 129.3, 129.2, 128.9, 128.5, 127.4 (Ph), 125.3 (Ph),

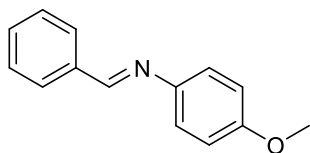
121.5 (Ph), 119.4, 111.1 ppm. HRMS (ESI): calcd for C₂₄H₁₉N₃S[M+H]⁺: 382.1372, found 382.1367.



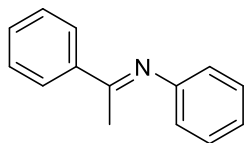
8j

Preparation of 8j. The compound of **8j** was isolated as yellow crystals by treatment of **2j** (0.10 mmol) with methanol (5 mL) following the same procedure as that described above for the preparation of **8a**. Yield: (92%). ¹H NMR (C₆D₆): δ 12.78 (s, 1H, NH), 8.49 (dd, *J* = 8.5, 1.5 Hz, 1H, Ph), 7.86–7.79 (m, 2H), 7.61 (ddd, *J* = 5.0, 2.0, 1.0 Hz, 1H, Ph), 7.47 (dd, *J* = 8.0, 1.5 Hz, 1H, Ph), 7.38 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H, Ph), 7.21 (d, *J* = 8.0 Hz, 1H, Ph), 7.20–7.15 (m, 5H, Ph), 7.14–7.12 (m, 2H), 7.11–7.07 (m, 1H), 6.95 (td, *J* = 8.0, 2.0 Hz, 1H), 6.81 (ddd, *J* = 8.0, 7.0, 1.5 Hz, 1H), 6.43 (ddd, *J* = 7.5, 5.0, 1.0 Hz, 1H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 158.8 (NHN-C_{aryl}), 146.8 (Ph), 145.6 (Ph), 145.5 (Ph), 139.5, 136.6, 136.1, 131.0, 129.9, 129.5, 128.6, 128.5, 128.4, 128.2, 127.1, 121.3 (Ph), 120.1, 120.0, 118.9, 114.8 ppm. HRMS (ESI): calcd for C₂₄H₁₉N₃ [M+H]⁺: 350.1652, found 350.1655.

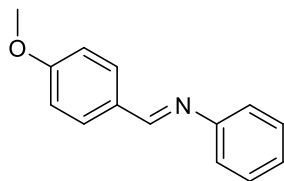
Synthesis of different imines



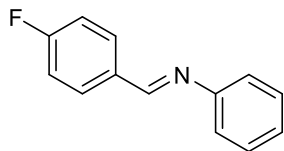
1. Methoxy-*N*-(phenylmethylene)benzenamine⁶: Yellow solid. ¹H NMR (C₆D₆): δ 8.22 (s, 1H), 7.88–7.82 (m, 2H), 7.21–7.16 (m, 2H), 7.15–7.09 (m, 3H), 6.80–6.74 (m, 2H), 3.29 (s, 3H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 158.9, 157.9, 145.5, 137.4, 131.0, 129.0, 129.1, 122.8, 114.8, 55.0 ppm.



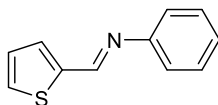
N-(1-phenylethylidene)benzenamine⁶: Yellow solid. ¹H NMR (C₆D₆): δ 7.95 (ddd, *J* = 4.0, 3.0, 1.5 Hz, 2H), 7.19–7.17 (m, 2H), 7.17–7.12 (m, 4H), 6.95–6.91 (m, 1H), 6.77–6.73 (m, 1H), 1.81 (s, 3H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 164.5, 152.6, 140.0, 131.0, 129.3, 128.4, 127.7, 123.5, 120.0, 16.8 ppm.



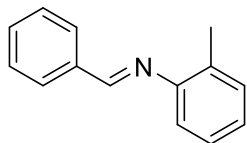
1. (*p*-Anisal)aniline⁷: Yellow solid. ¹H NMR (C₆D₆): δ 8.15 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 4.5 Hz, 3H), 7.05–6.99 (m, 1H), 6.93 (d, *J* = 8.0 Hz, 2H), 2.01 (s, 3H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 162.6, 159.4, 153.3, 130.9, 130.1, 129.4, 125.8, 121.5, 114.5, 54.9 ppm.



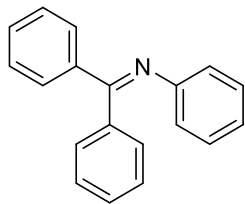
N-(4-fluorobenzylidene)Aniline⁷: White solid. ¹H NMR (C₆D₆): δ 7.95 (s, 1H), 7.58–7.52 (m, 2H), 7.18–7.15 (m, 2H), 7.14–7.10 (m, 2H), 7.04–7.00 (m, 1H), 6.74–6.68 (m, 2H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 164.9 (d, *J*_{C-F} = 252.0 Hz), 163.9, 158.5, 152.6, 131.1 (d, *J*_{C-F} = 8.8 Hz), 129.5, 126.2, 121.3, 116.0, 115.9 (d, *J*_{C-F} = 22.7 Hz) ppm.



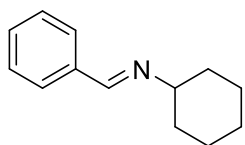
N-(2-thienylmethylene)benzenamine⁷: Yellow oil ¹H NMR (C₆D₆): δ 8.16 (s, 1H), 7.18 (s, 1H), 7.16–7.13 (m, 3H), 7.03 (dd, *J* = 5.5, 2.5 Hz, 1H), 6.99 (dd, *J* = 3.5, 1.0 Hz, 1H), 6.86 (d, *J* = 5.0 Hz, 1H), 6.67 (dd, *J* = 5.0, 3.5 Hz, 1H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 152.8, 152.1, 143.8, 132.1, 130.3, 129.4, 127.6, 126.2, 121.5 ppm.



1. Methyl-*N*-(phenylmethylene)benzenamine⁸: Yellow oil ¹H NMR (C₆D₆): δ 8.05 (s, 1H), 7.81 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.14–7.11 (m, 3H), 7.10–7.05 (m, 2H), 6.75 (d, *J* = 7.5 Hz, 1H), 2.42 (s, 3H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 159.3, 151.7, 137.2, 132.4, 131.2, 130.6, 129.1, 128.9, 128.3, 128.1, 127.9, 127.1, 126.1, 118.0, 18.2 ppm.



N-(diphenylmethylene)benzenamine⁹: Yellow solid. ¹H NMR (C₆D₆): δ 7.95–7.91 (m, 2H), 7.14–7.06 (m, 3H), 7.00–6.95 (m, 2H), 6.95–6.89 (m, 2H), 6.87–6.82 (m, 3H), 6.82–6.76 (m, 2H), 6.76–6.71 (m, 1H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 140.2, 136.8, 130.9, 129.8, 129.7, 128.8, 128.2, 123.4, 121.3 ppm.



N-(phenylmethylene)cyclohexanamine¹⁰: Yellow oil. ¹H NMR (C₆D₆): δ 8.01 (s, 1H), 7.77 (s, 1H), 7.75 (s, 1H), 7.10 (d, *J* = 7.4 Hz, 2H), 7.06 (dd, *J* = 8.5, 5.5 Hz, 1H), 3.01 (dt, *J* = 14.0, 7.0 Hz, 1H), 1.71 (dd, *J* = 12.5, 6.5 Hz, 5H), 1.56–1.48 (m, 1H), 1.29–1.15 (m, 3H) ppm. ¹³C{¹H} NMR (C₆D₆): δ 158.1, 137.5, 130.4, 128.6, 70.2, 34.9, 26.2, 25.0 ppm.

4. Copies of NMR spectra of the rare-earth metal complexes

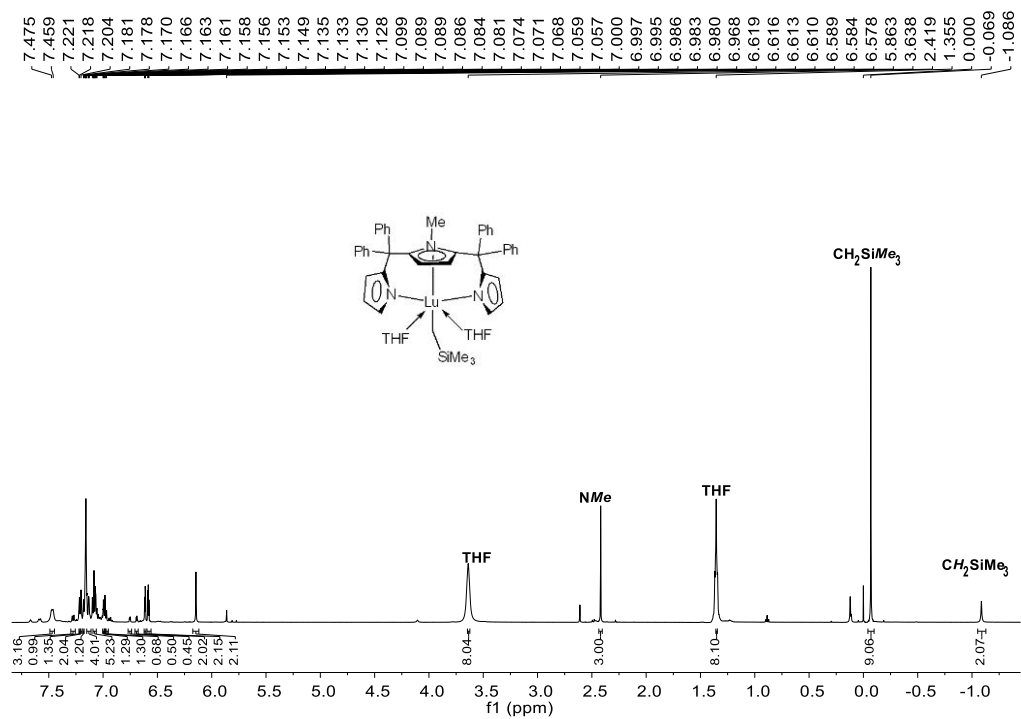


Figure S19. ¹H NMR (500 MHz, C₆D₆, 25 °C) spectrum of complex **1a'**.

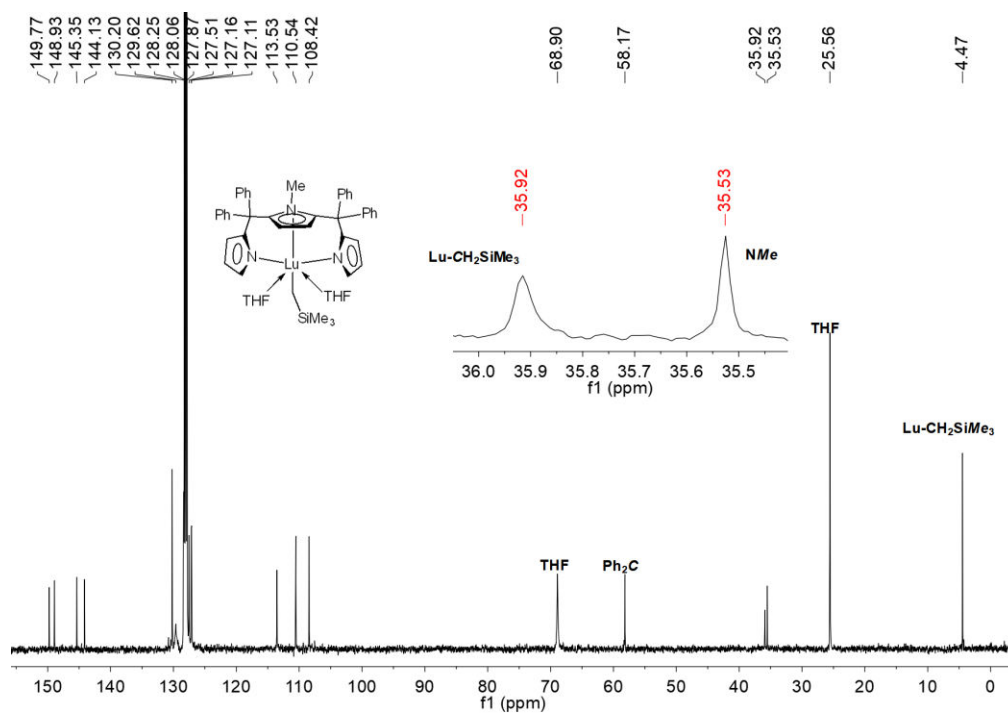


Figure S20. ¹³C{¹H} NMR (126 MHz, C₆D₆, 25 °C) spectrum of complex **1a'**.

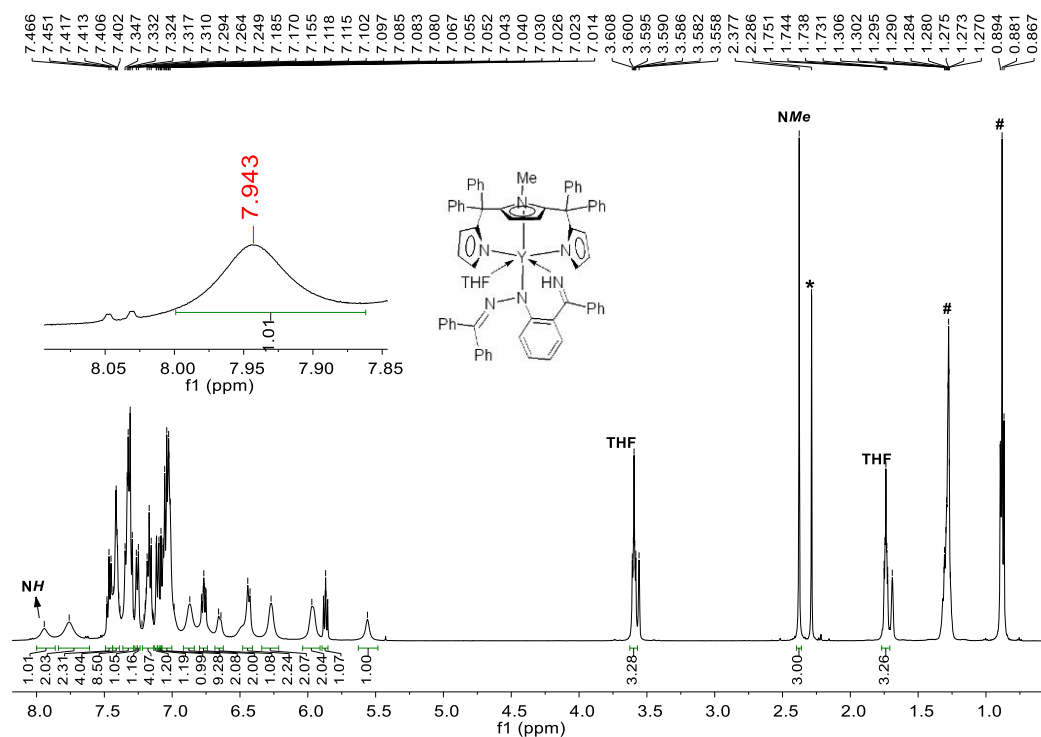


Figure S21. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25°C) spectrum of complex **2a**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

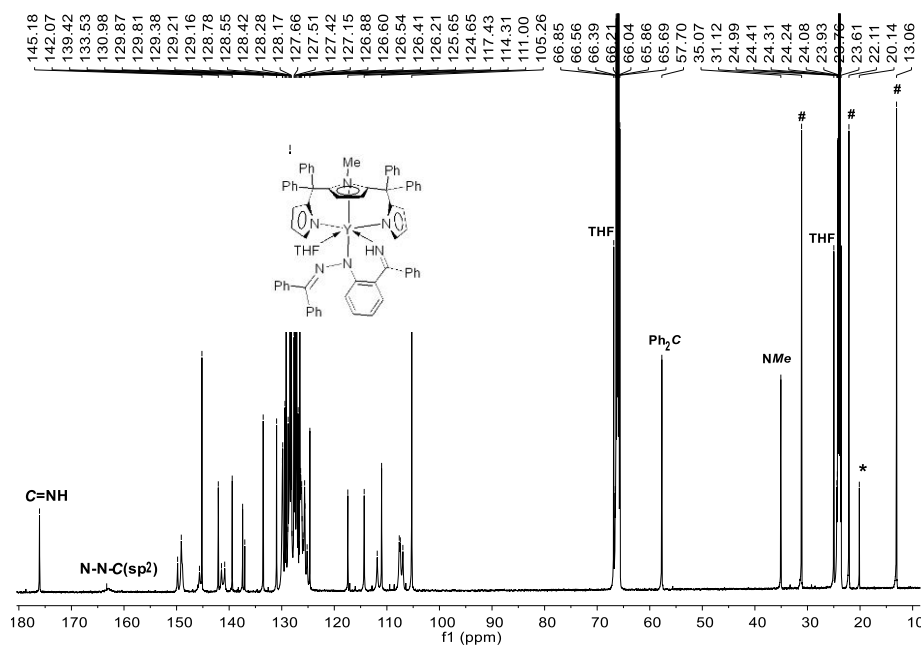


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{THF-}d_8$, 25°C) spectrum of complex **2a**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

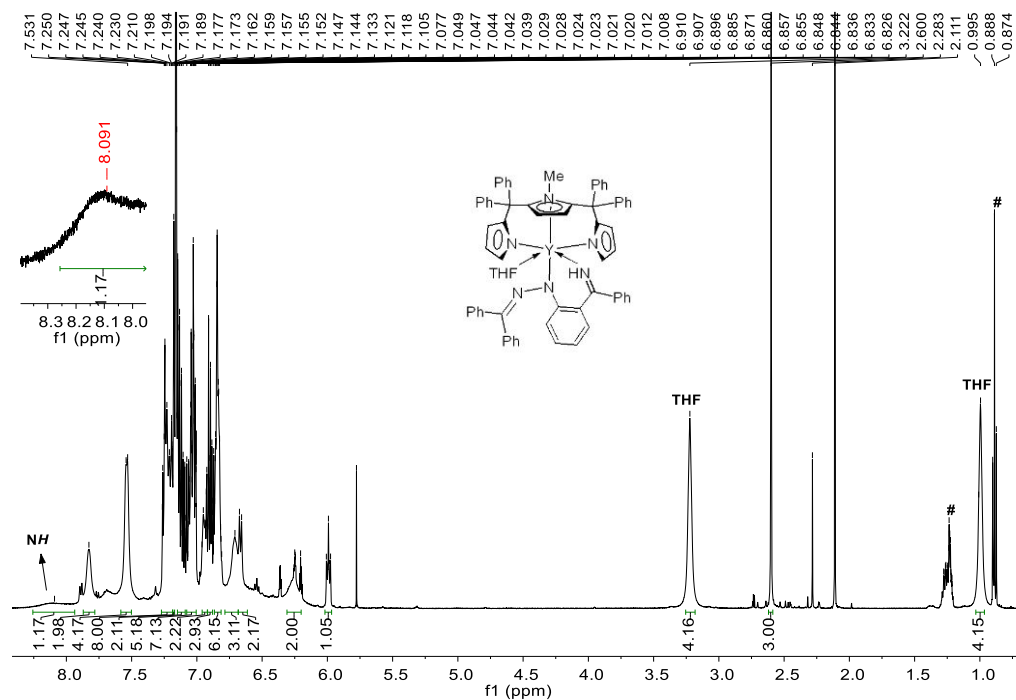


Figure S23. ^1H NMR (500 MHz, C_6D_6 , 25 $^\circ\text{C}$) spectrum of complex **2a**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

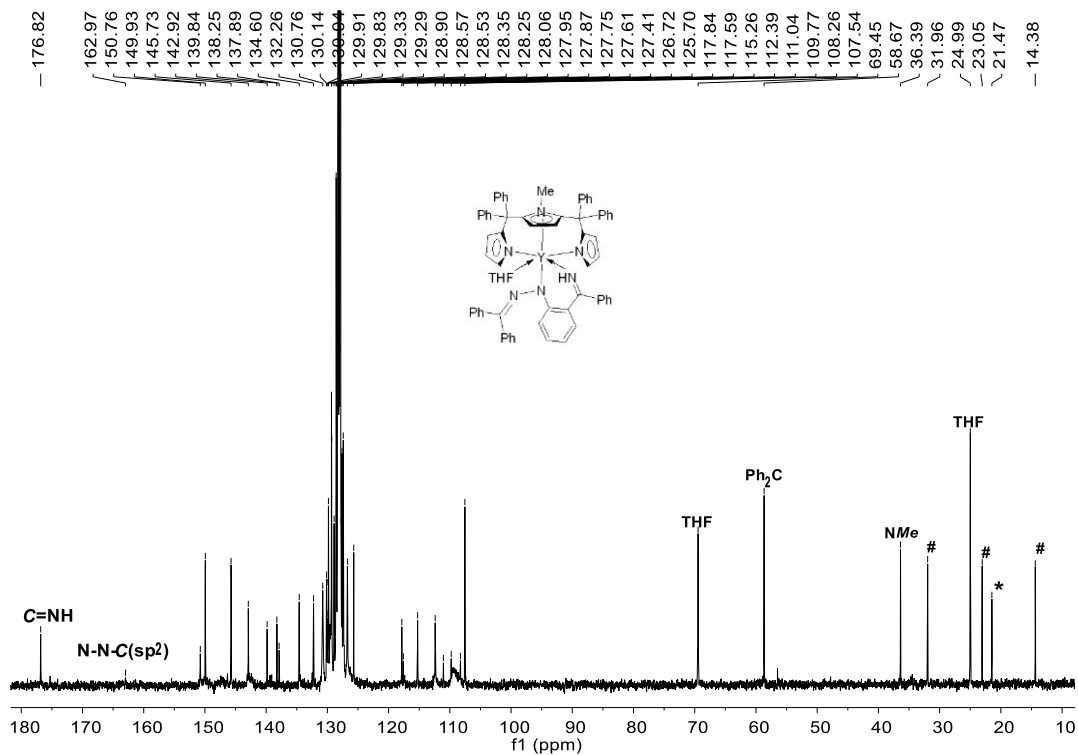


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of complex **2a**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

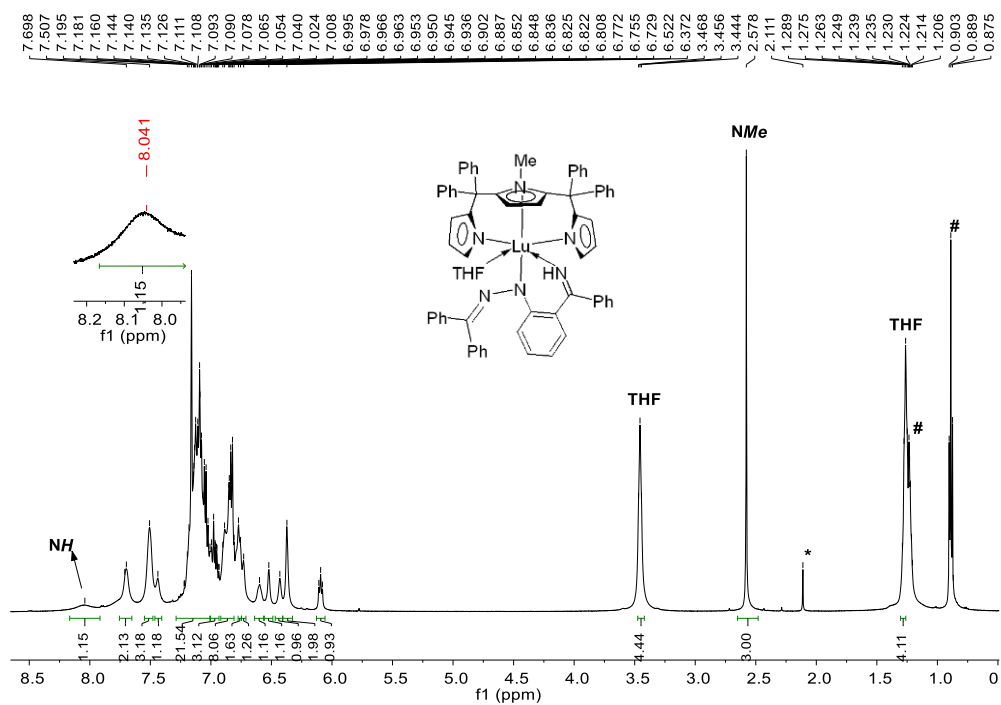


Figure S25. ^1H NMR (500 MHz, C_6D_6 , 25 °C) spectrum of complex **2a'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

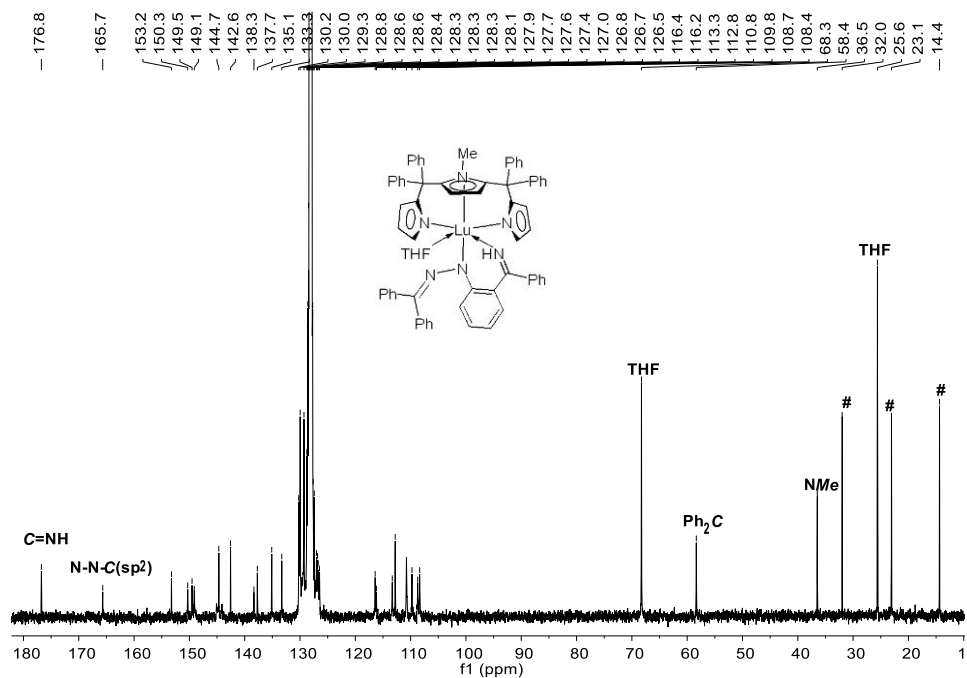


Figure S26. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of complex **2a'**. The peaks labelled with # represent residual *n*-hexane

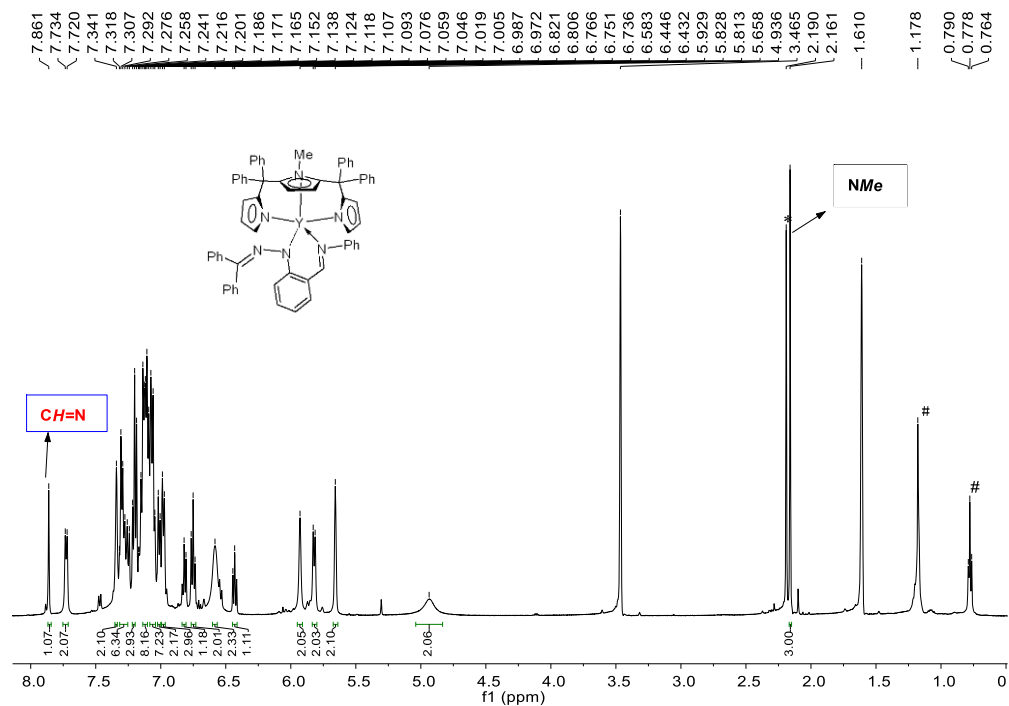


Figure S27. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2b**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

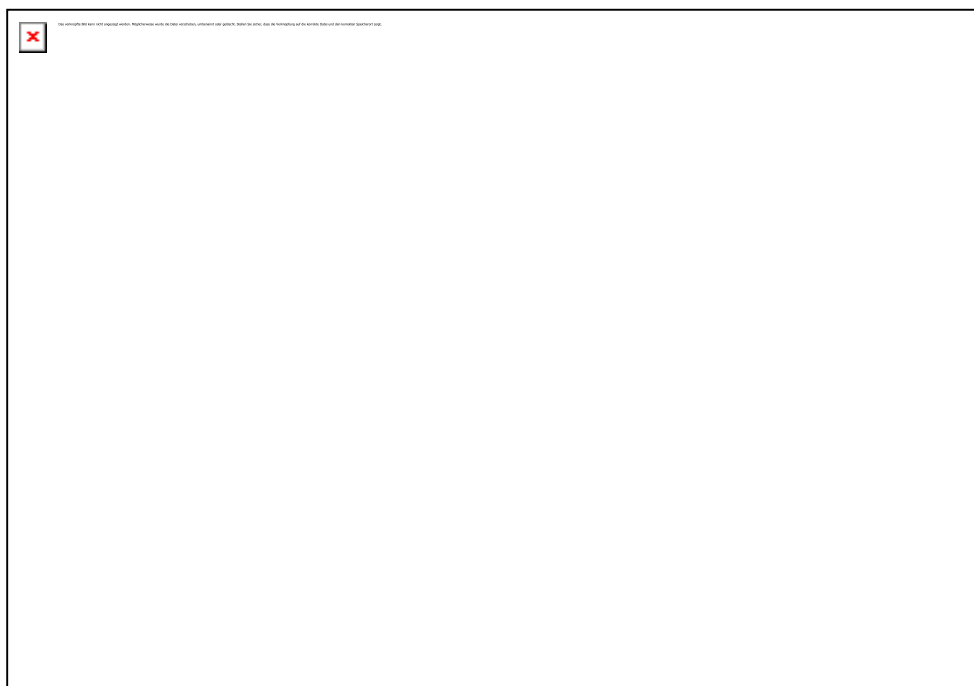


Figure S28. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2b**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

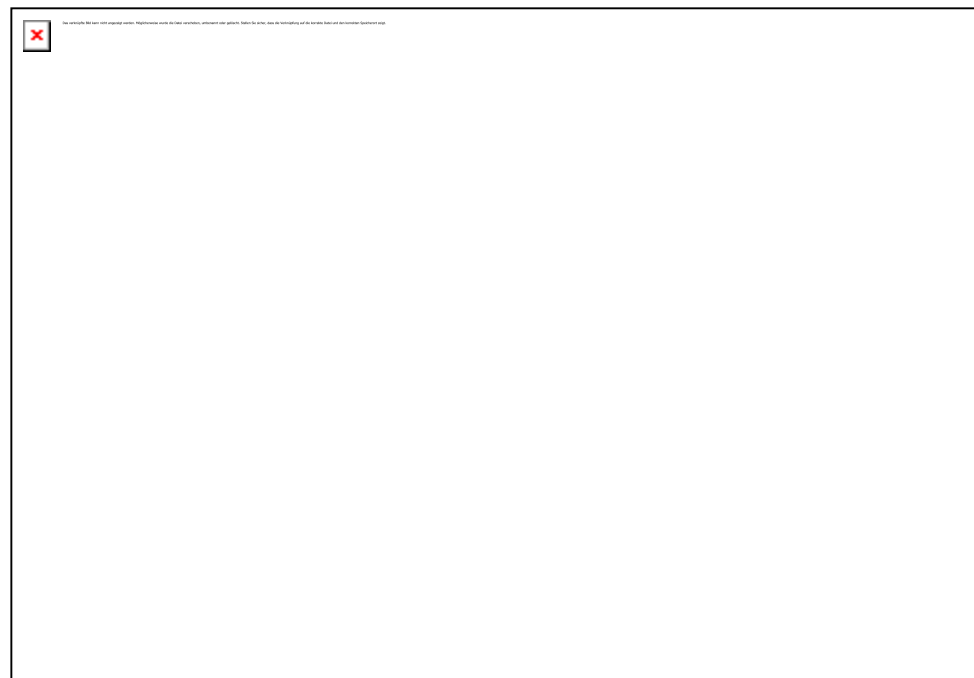


Figure S29. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2b'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.



Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2b'**. The peaks labelled with *, # and • represent residual toluene, *n*-hexane and impurities respectively.

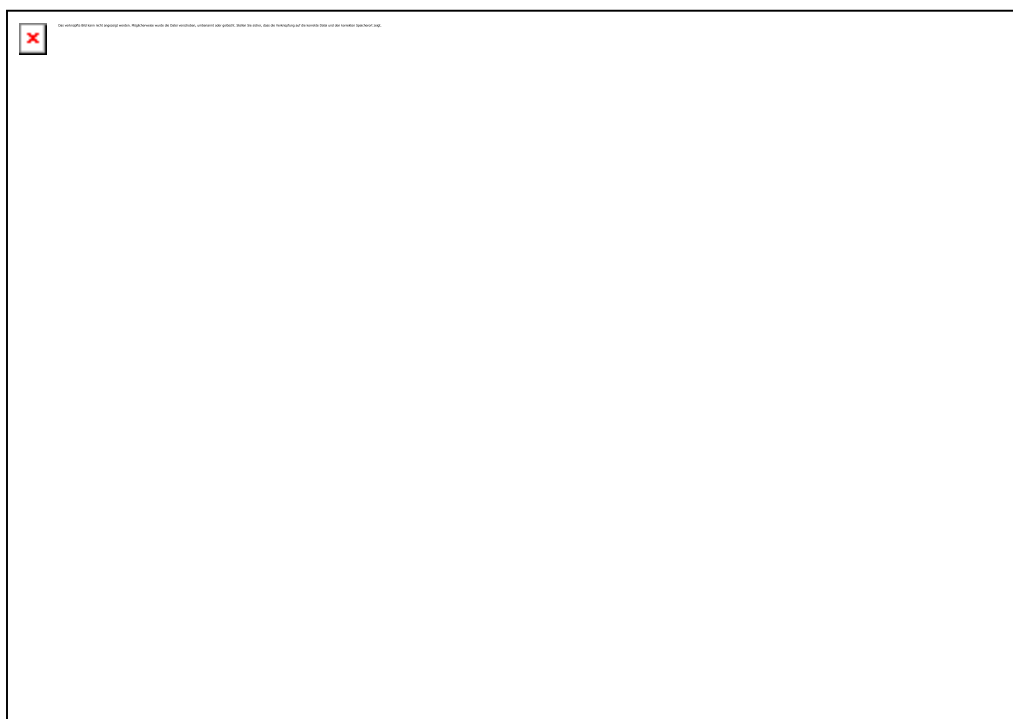


Figure S31. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2c**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

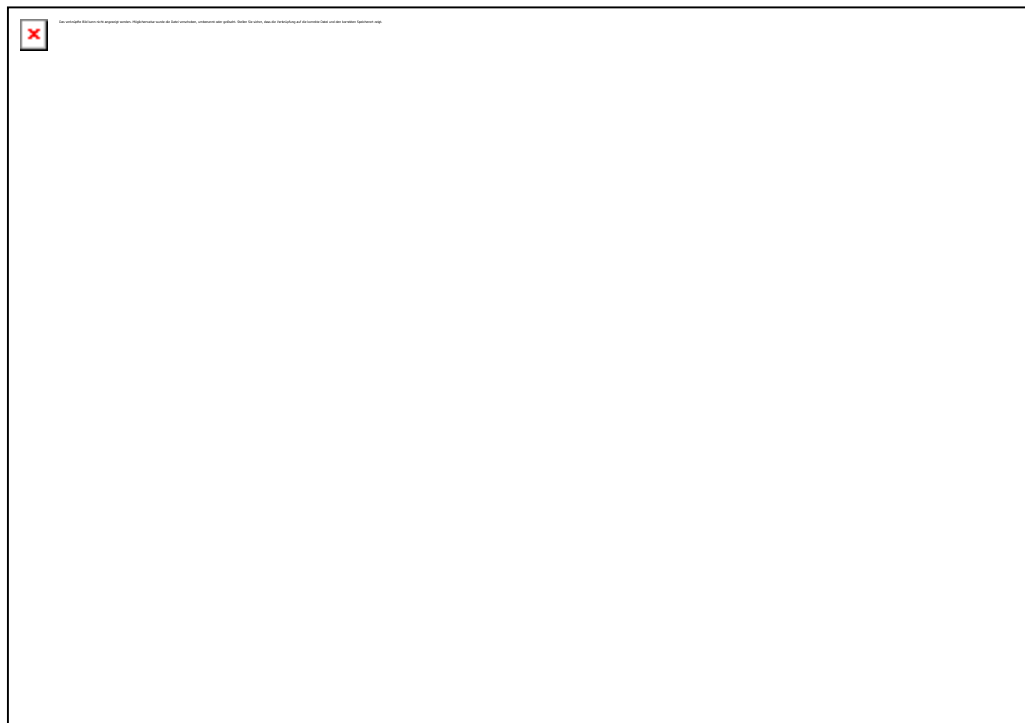


Figure S32. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2c**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

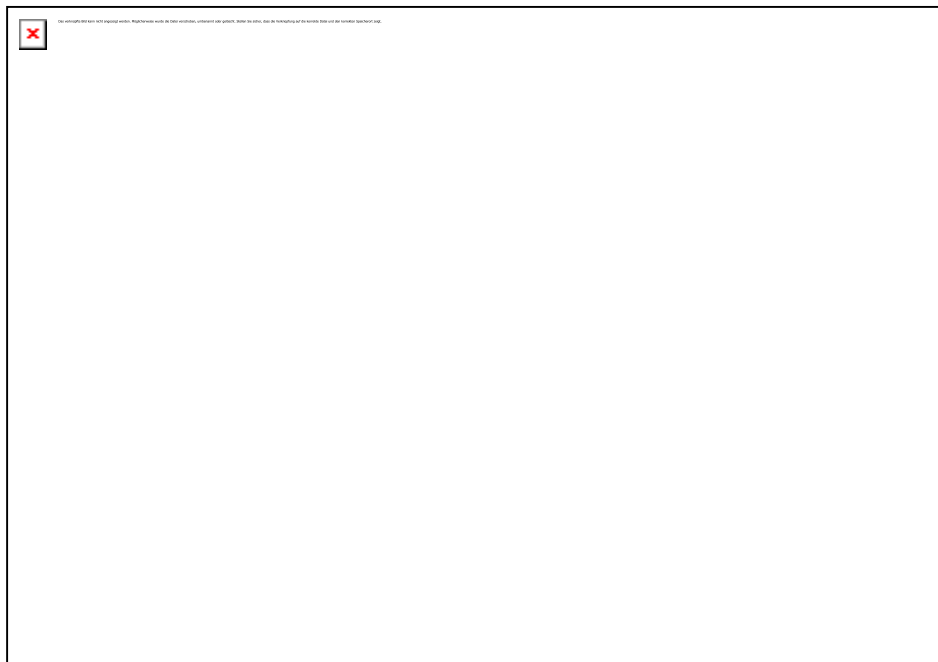


Figure S33. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2c'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

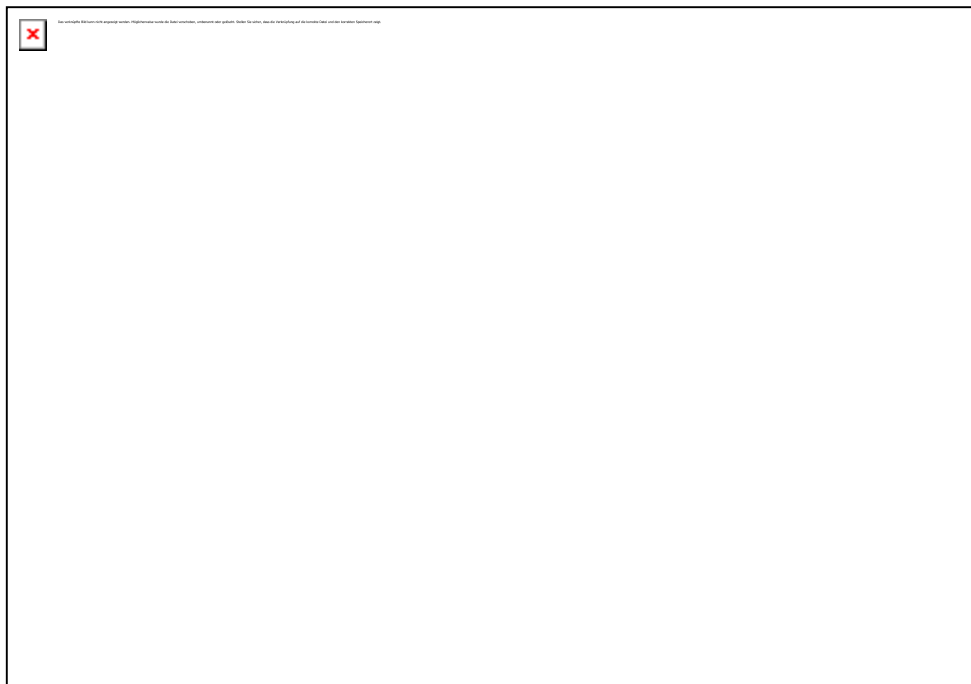


Figure S34. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2c'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.



Figure S35. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2d**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

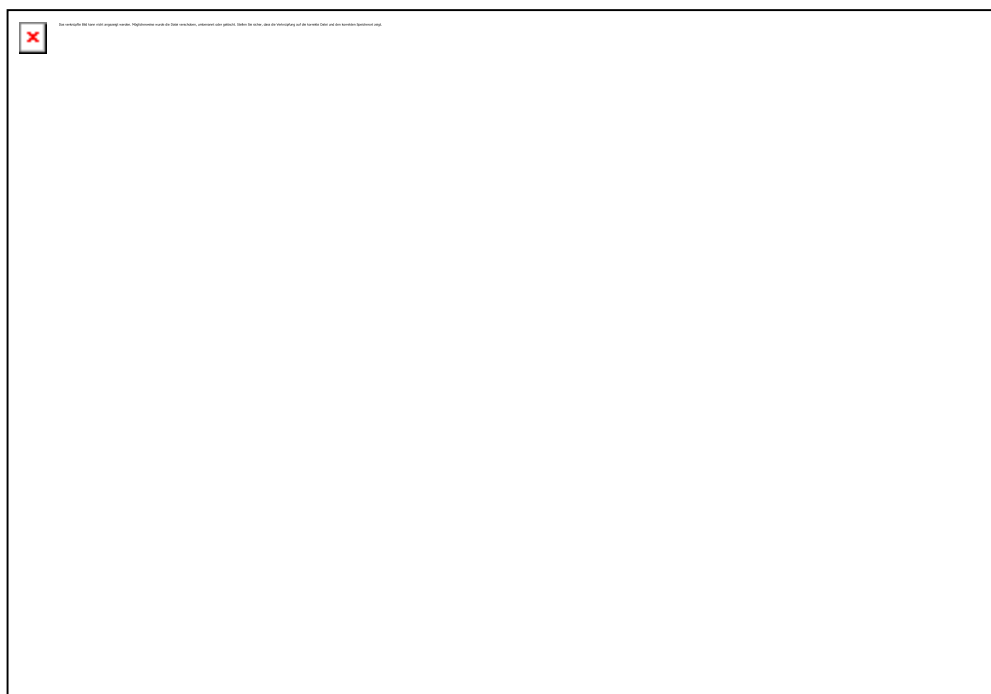


Figure S36. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2d**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

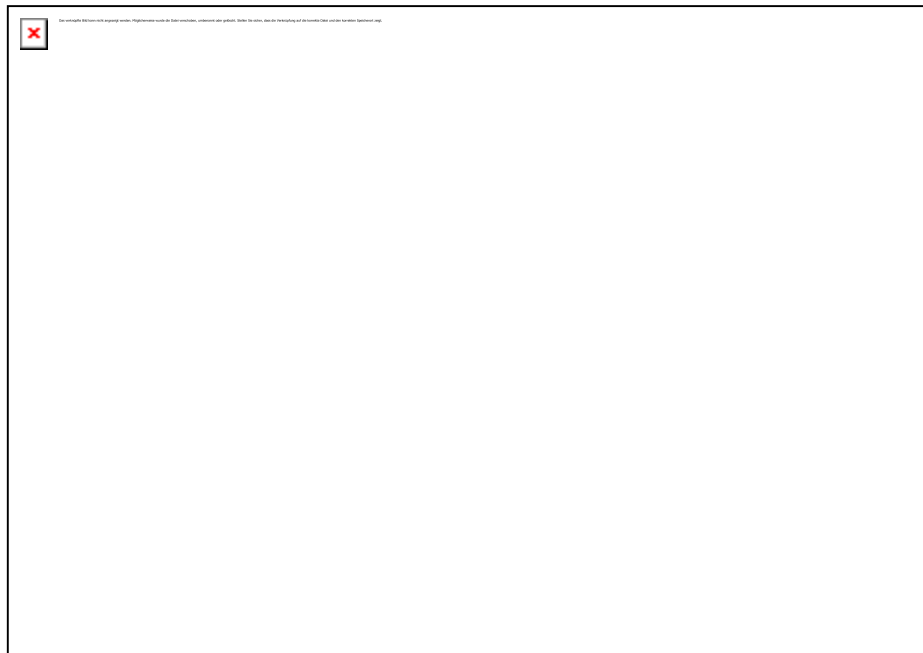


Figure S37. ^1H NMR (500 MHz, THF- d_8 , -20 °C) spectrum of complex **2d'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

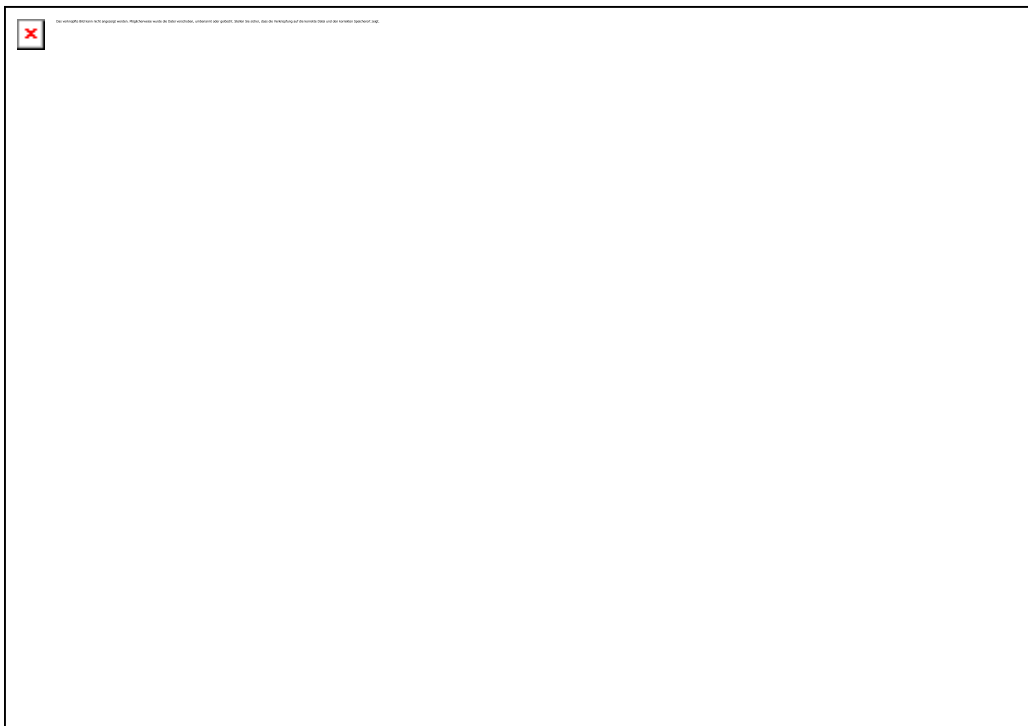


Figure S38. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2d'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

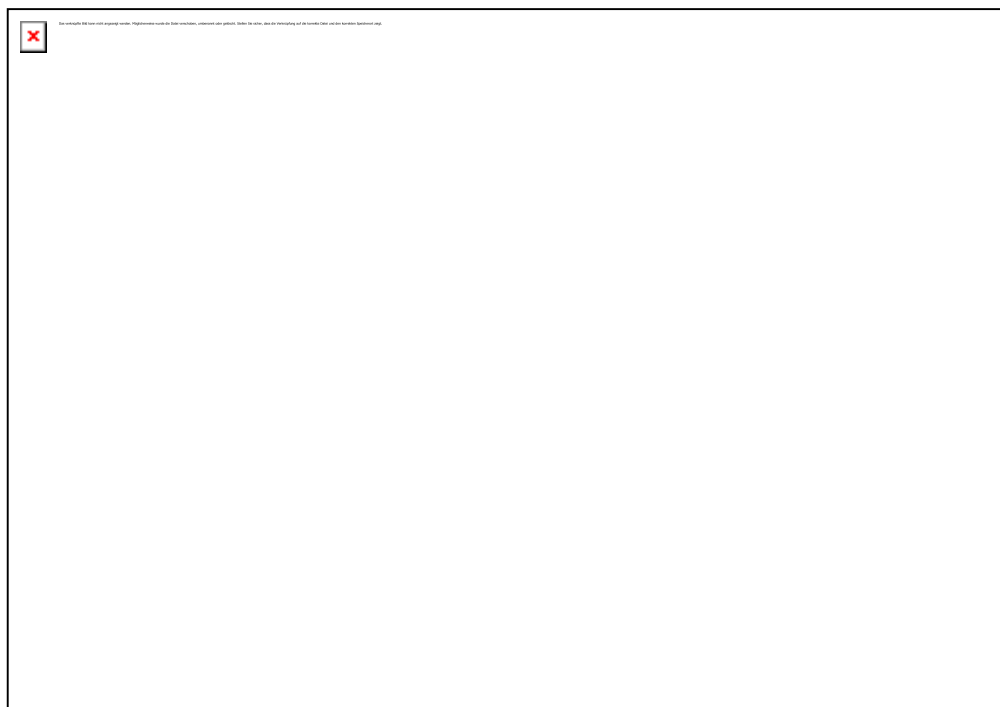


Figure S39. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2e**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

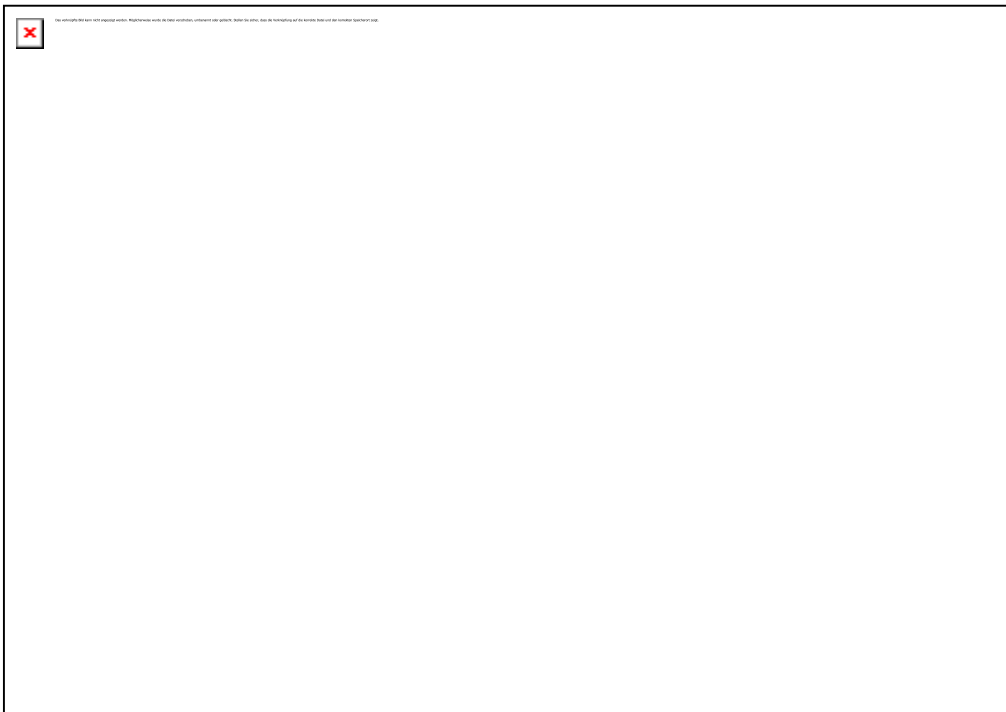


Figure S40. $^{13}\text{C}\{^1\text{H}\}$ NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2e**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

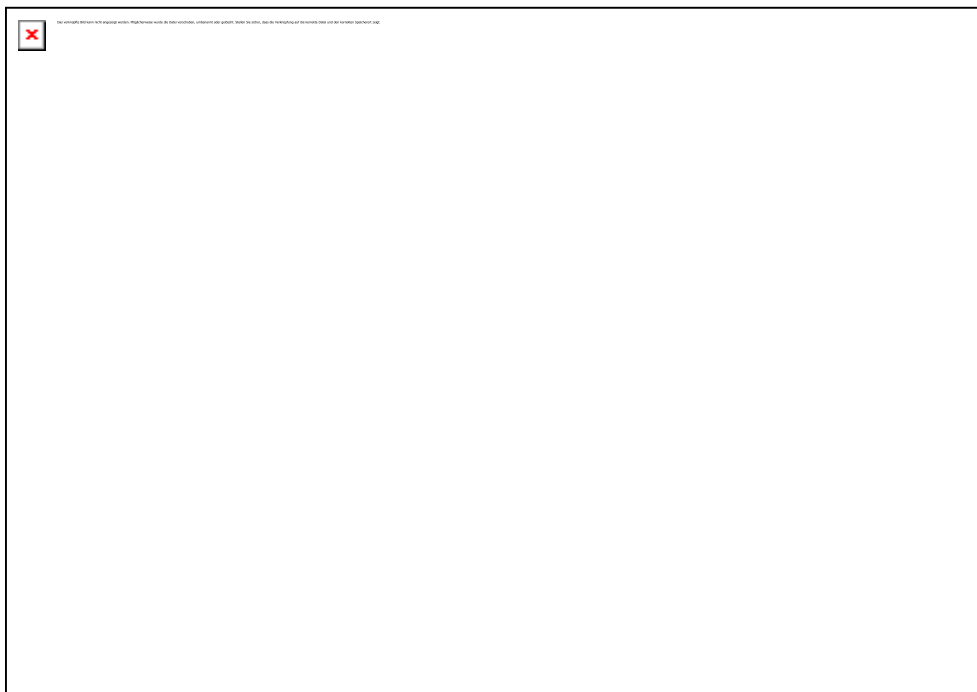


Figure S41. ^{19}F NMR (471 MHz, $\text{THF-}d_8$, 25 °C): δ -103.97 (s).



Figure S42. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2f**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

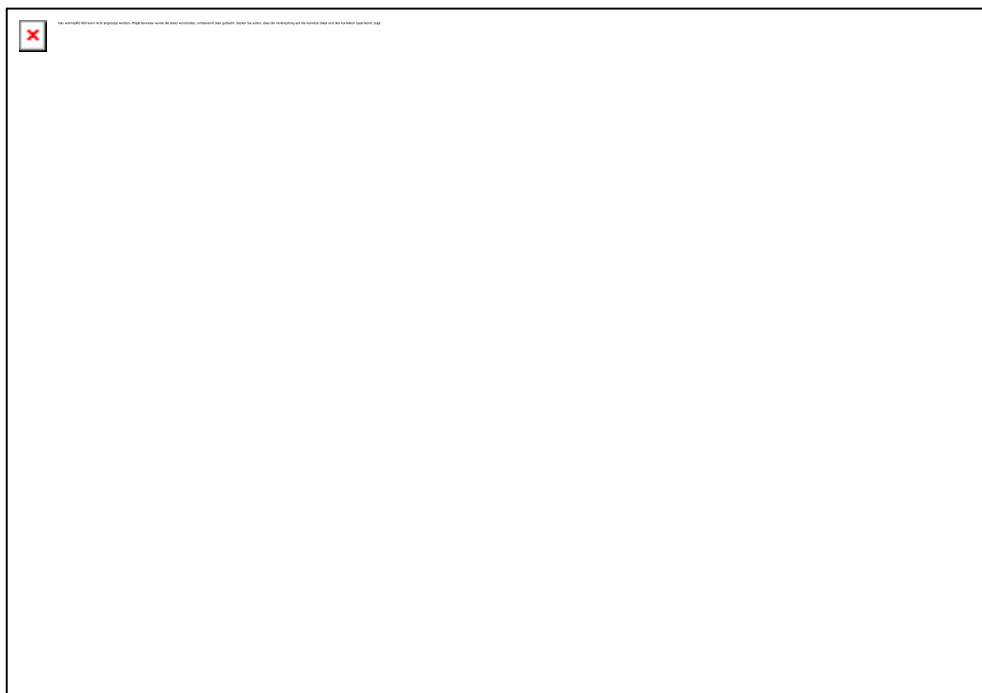


Figure S43. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2f**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

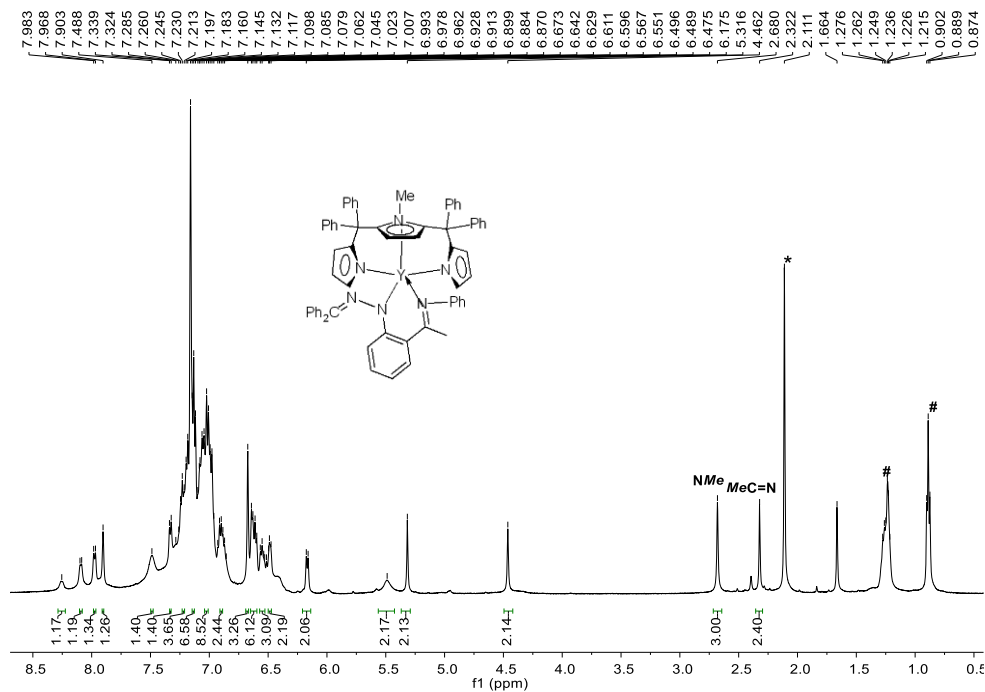


Figure S44. ^1H NMR (500 MHz, C_6D_6 , 25 °C) spectrum of complex **2g**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively

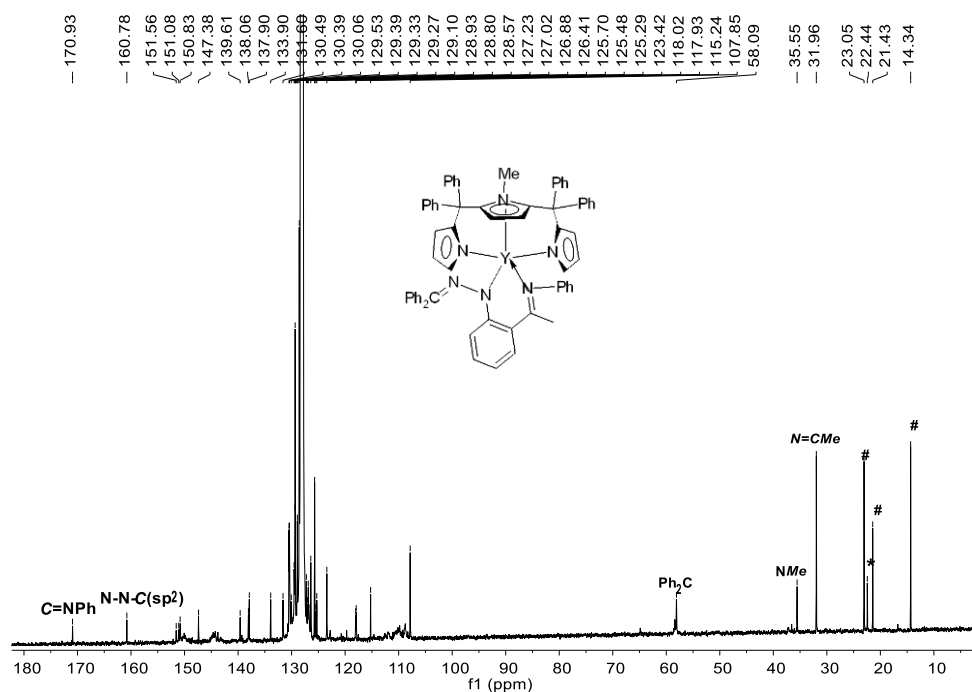


Figure S45. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2g**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

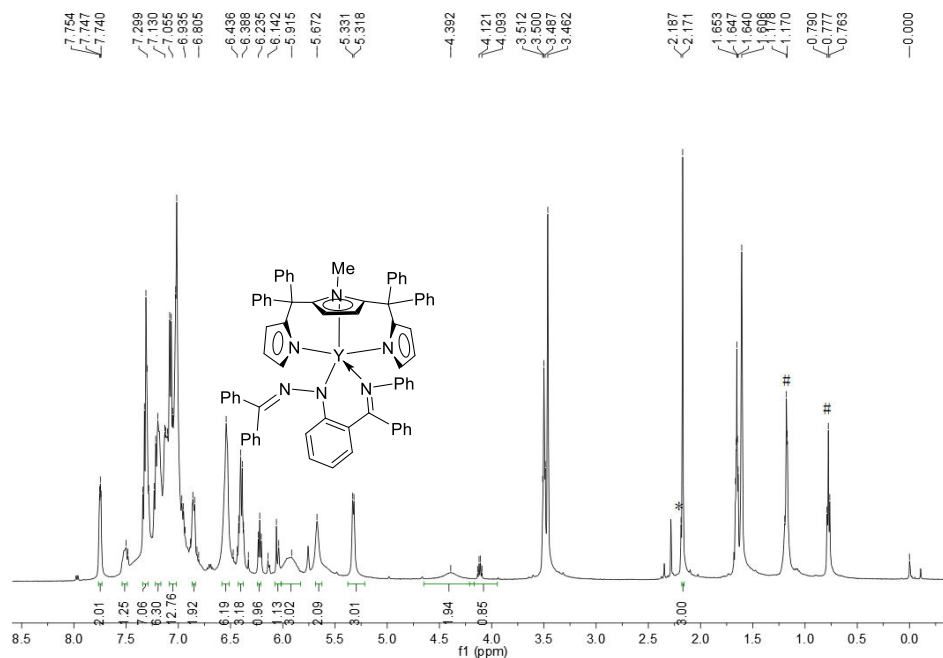


Figure S46. ^1H NMR (500 MHz, THF- d_8 , 25 °C) spectrum of complex **2h**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

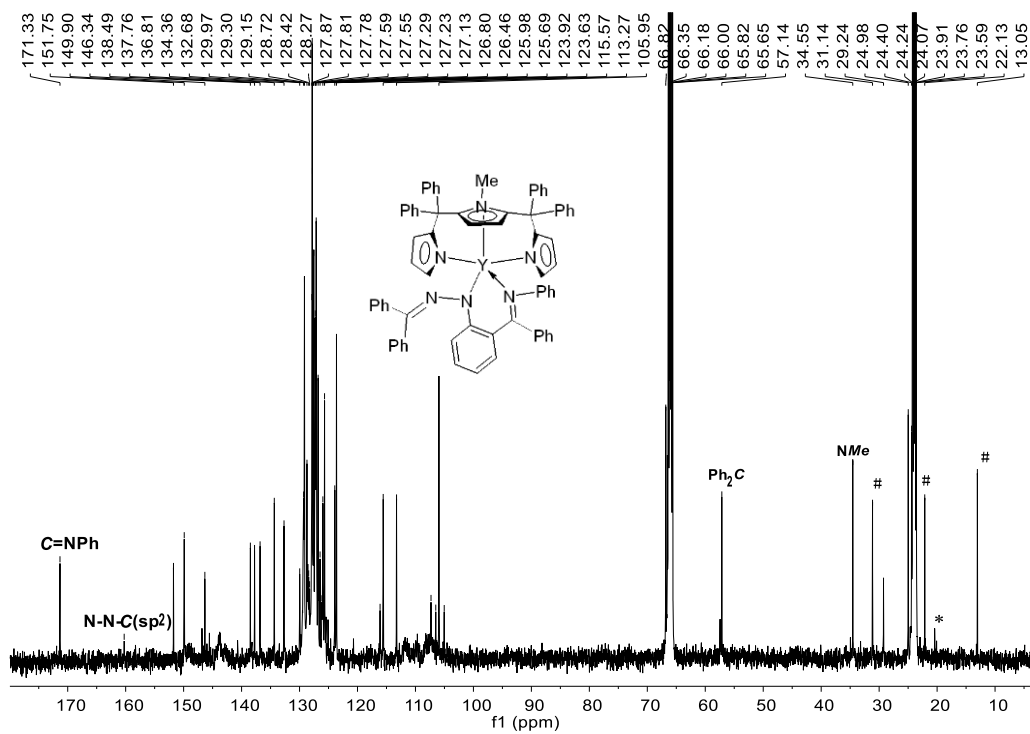


Figure S47. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, THF- d_8 , 25 °C) spectrum of complex **2h**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

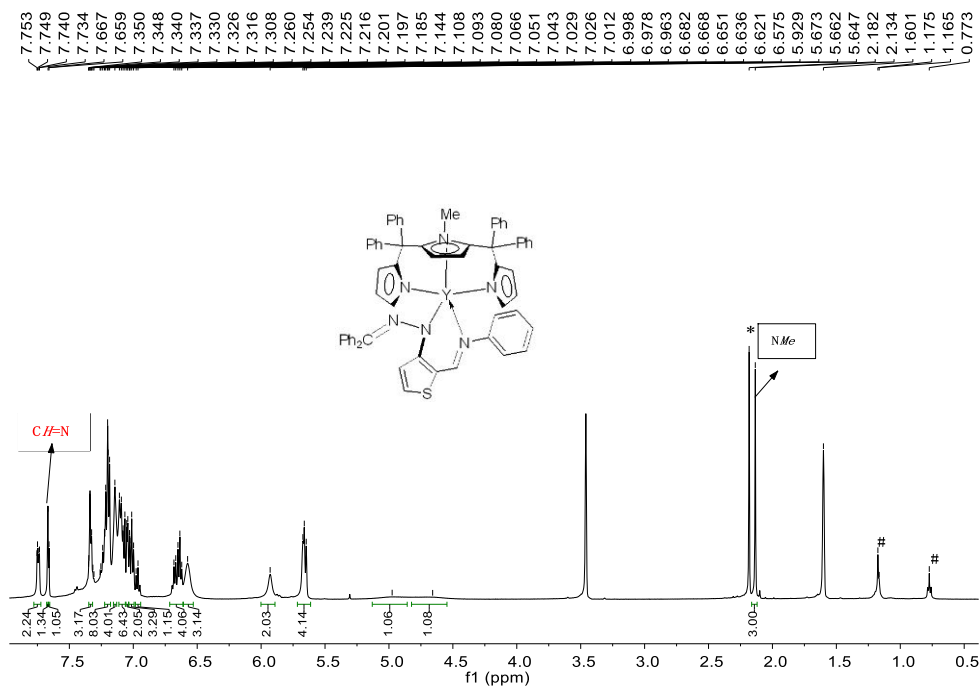


Figure S48. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2i**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively

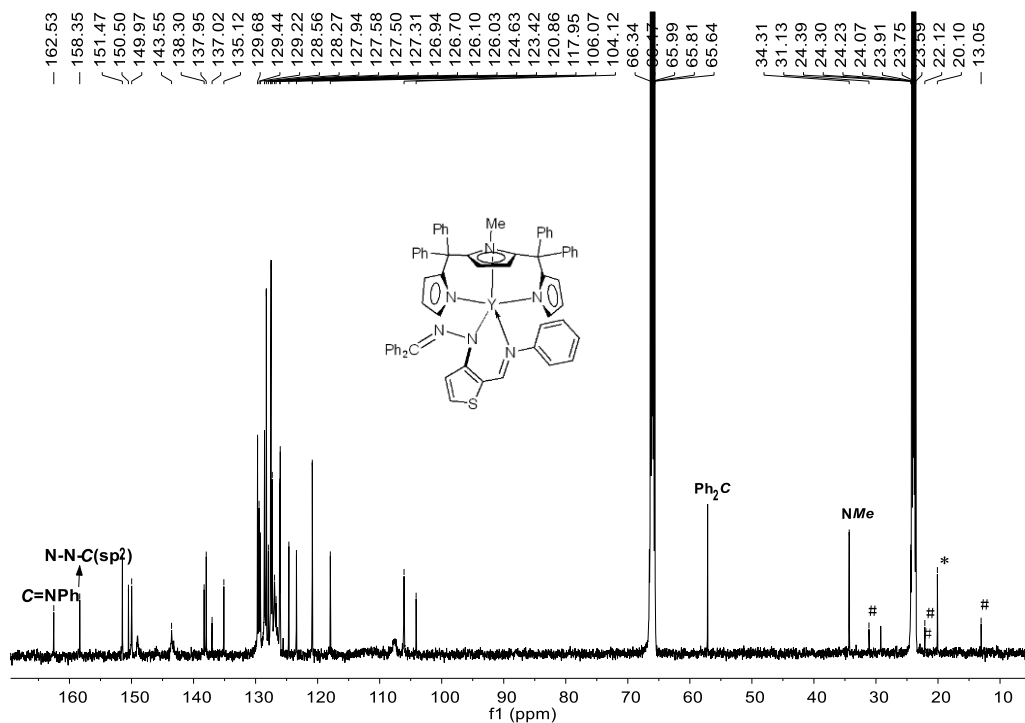


Figure S49. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2i**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

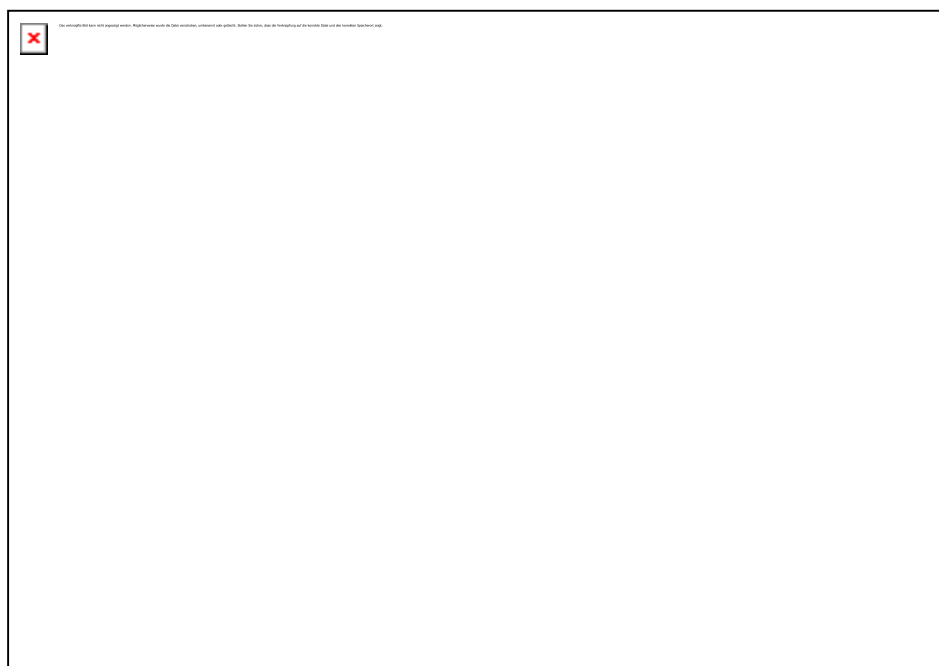


Figure S50. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2j**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively

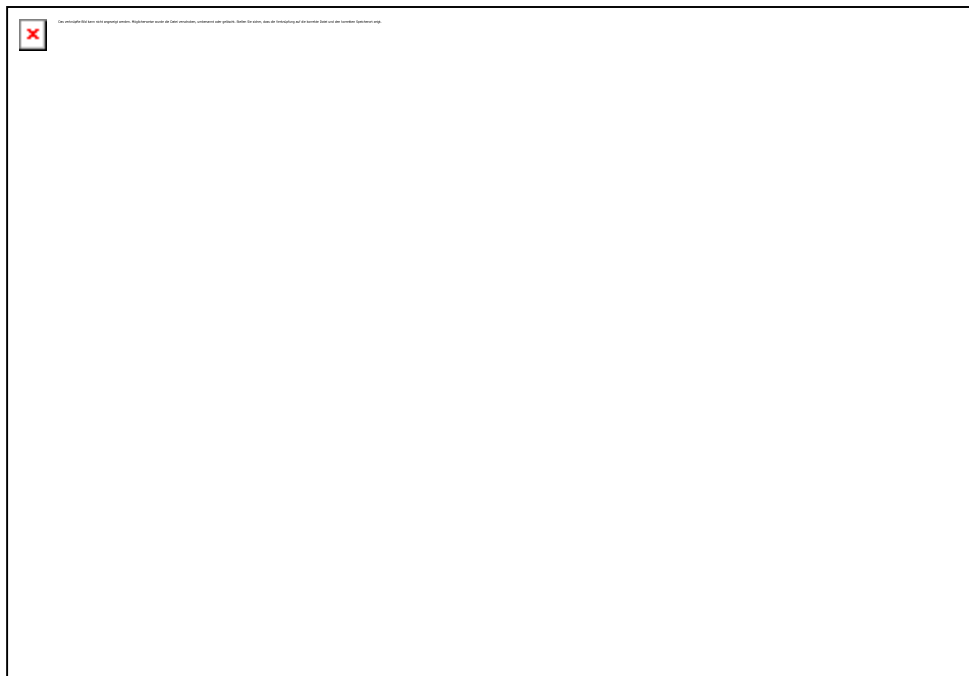


Figure S51. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **2j**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.



Figure S52. ^1H NMR (500 MHz, C_6D_6 , 25 °C) spectrum of complex **3a'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively



Figure S53. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of complex **3a'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

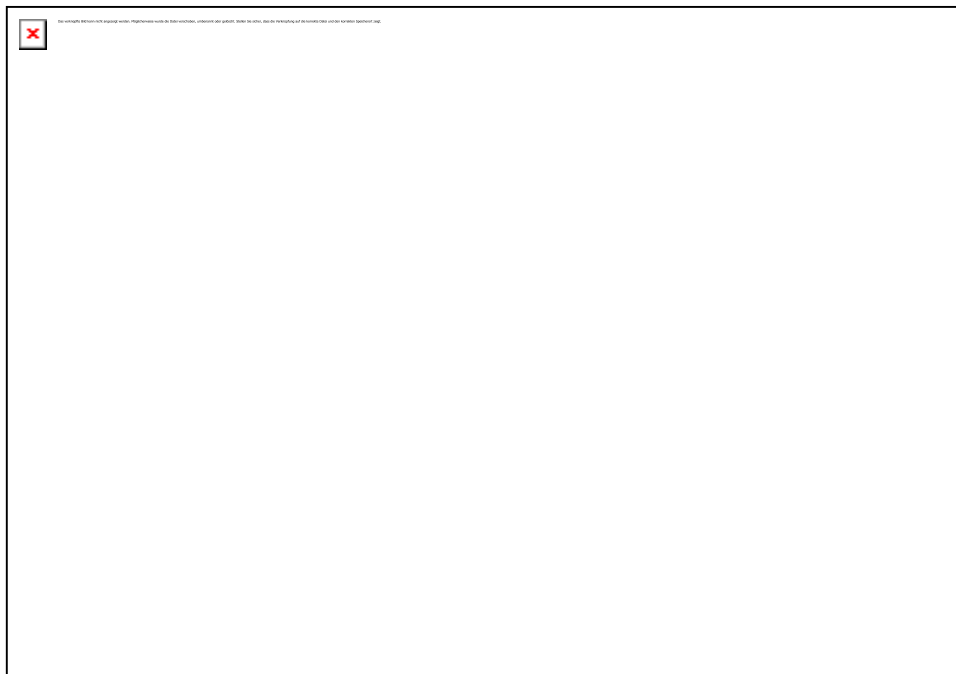


Figure S54. ^1H NMR (500 MHz, C_6D_6 , 25 °C) spectrum of complex **4a'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively

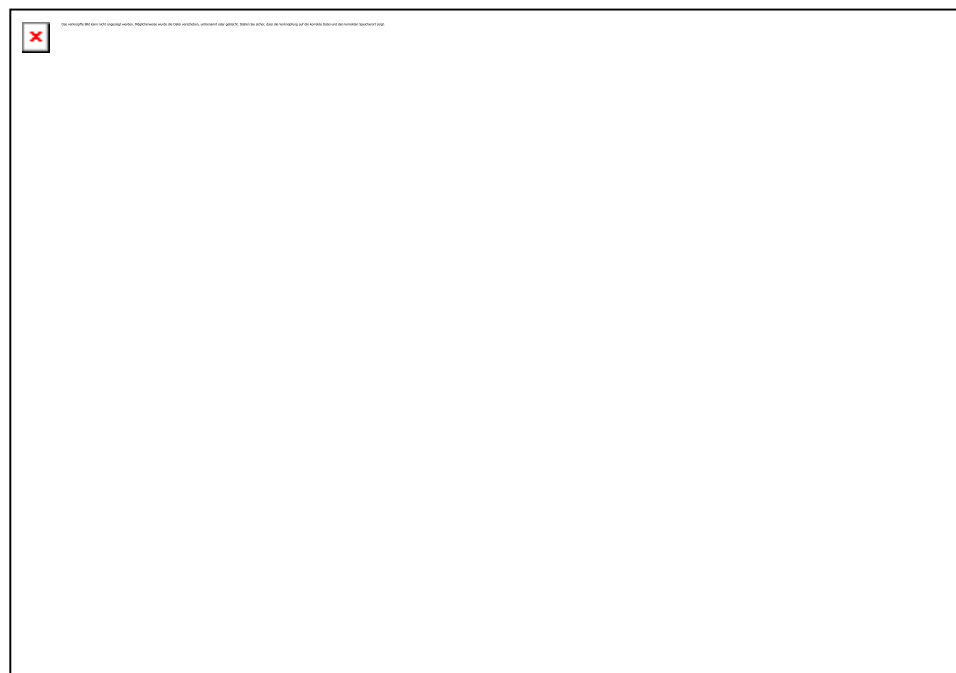


Figure S55. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of complex **4a'**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

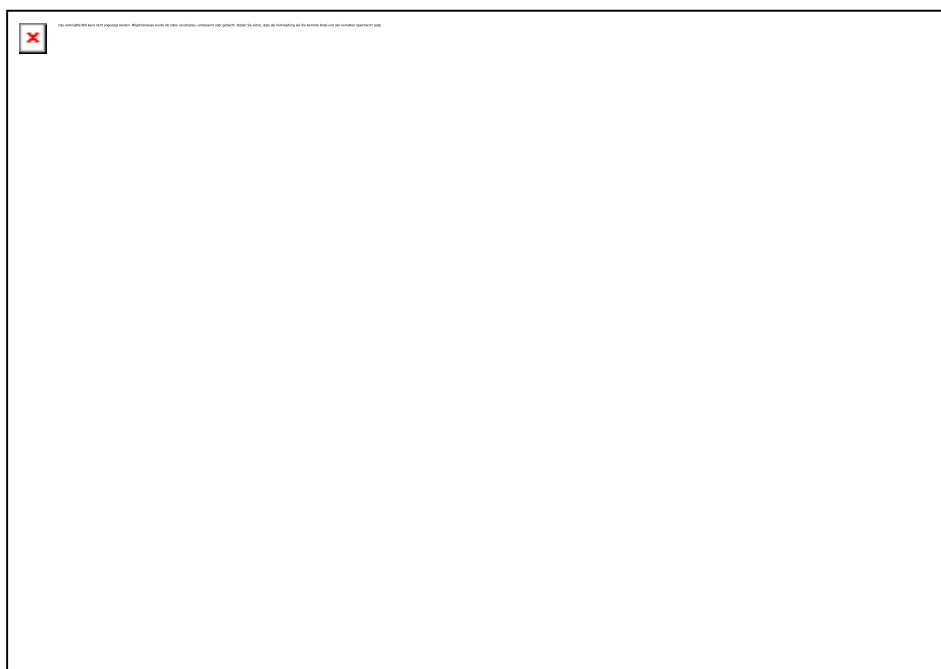


Figure S56. ^1H NMR (500 MHz, C_6D_6 , 25 °C) spectrum of complex **5c**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

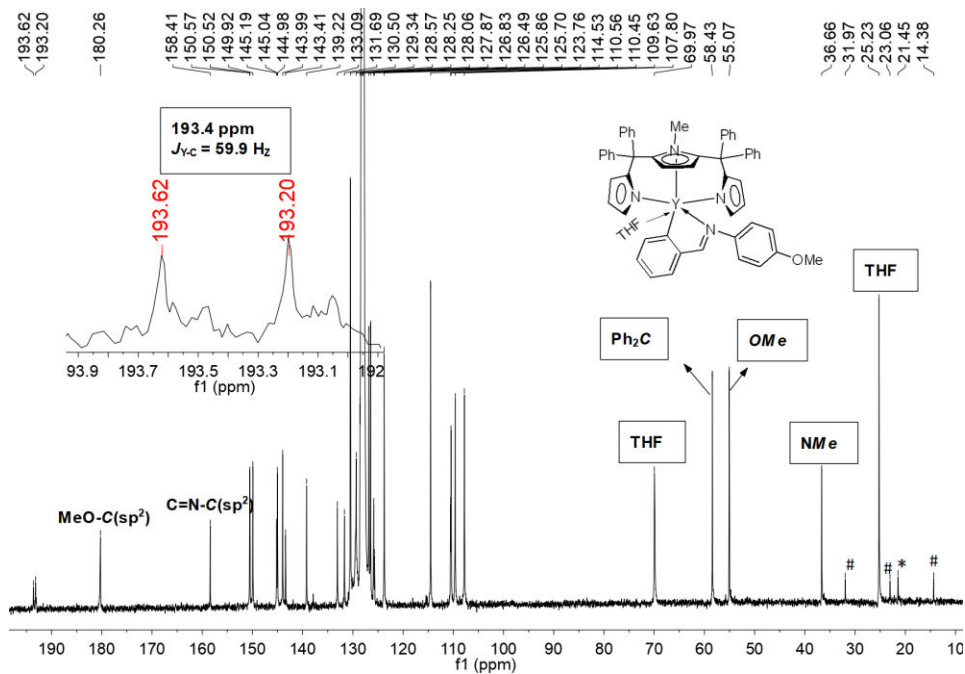


Figure S57. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of complex **5c**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

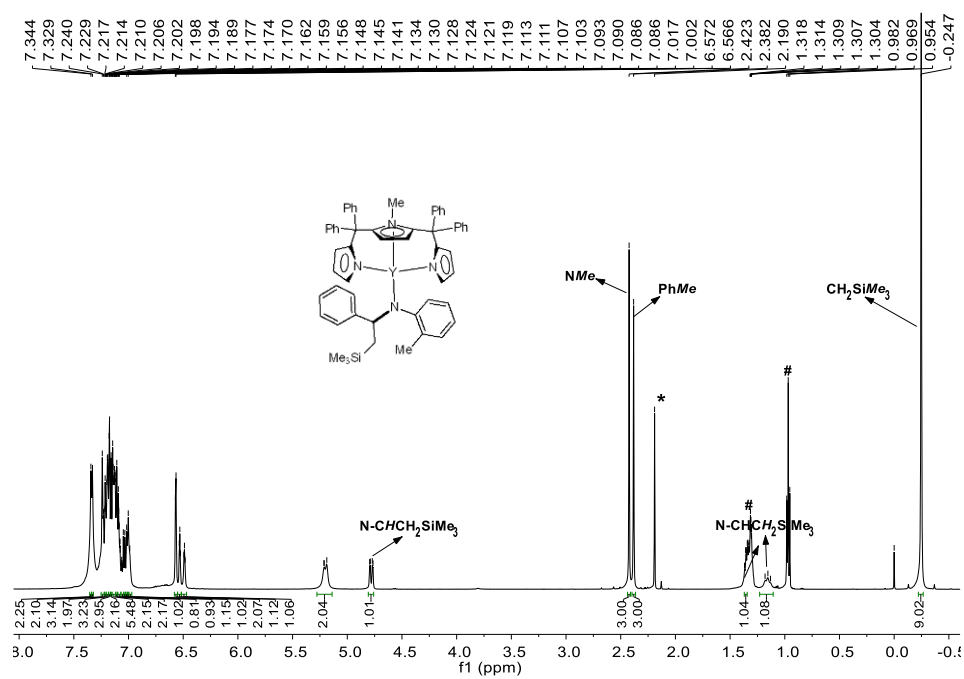


Figure S58. ^1H NMR (500 MHz, C_6D_6 , 25 $^\circ\text{C}$) spectrum of complex **6**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

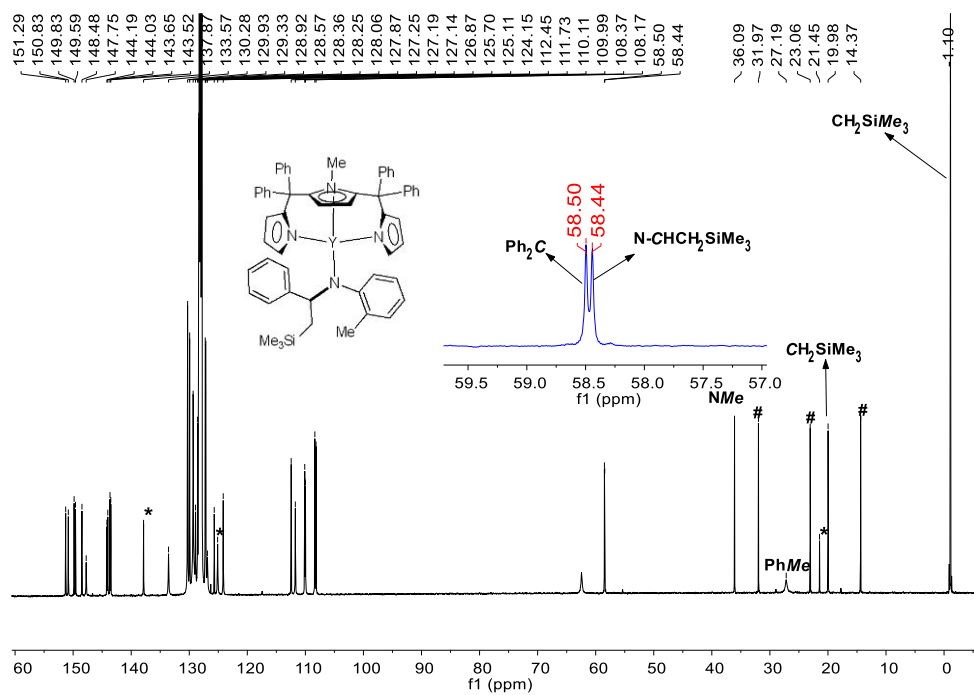


Figure S59. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 $^\circ\text{C}$) spectrum of complex **6**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

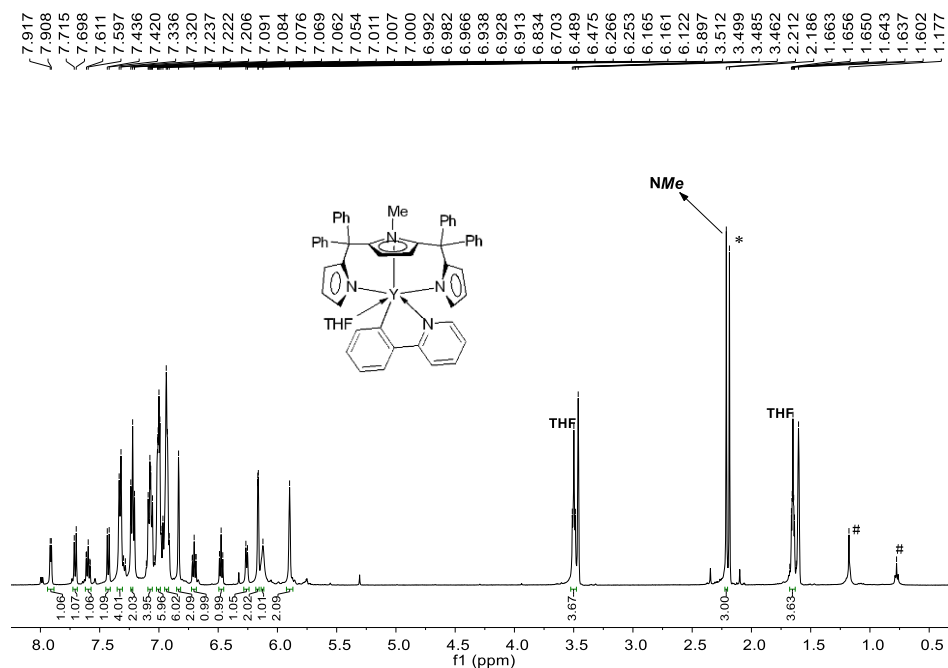


Figure S60. ^1H NMR (500 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **7j**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

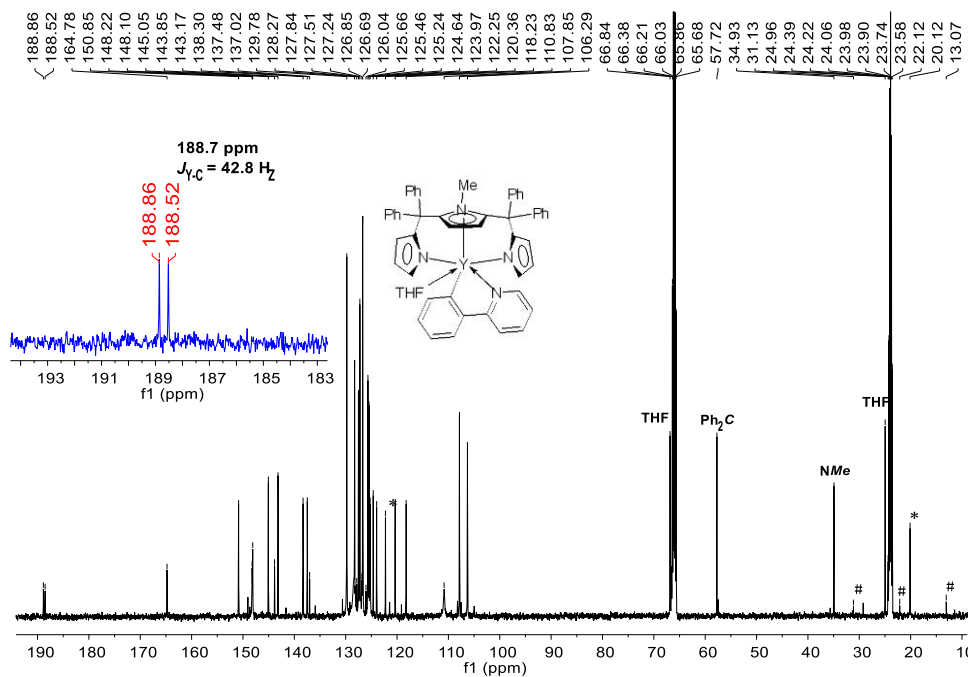


Figure S61. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{THF-}d_8$, 25 °C) spectrum of complex **7j**. The peaks labelled with * and # represent residual toluene and *n*-hexane, respectively.

1. NMR monitoring the transformation of **3a'** to **2a'**

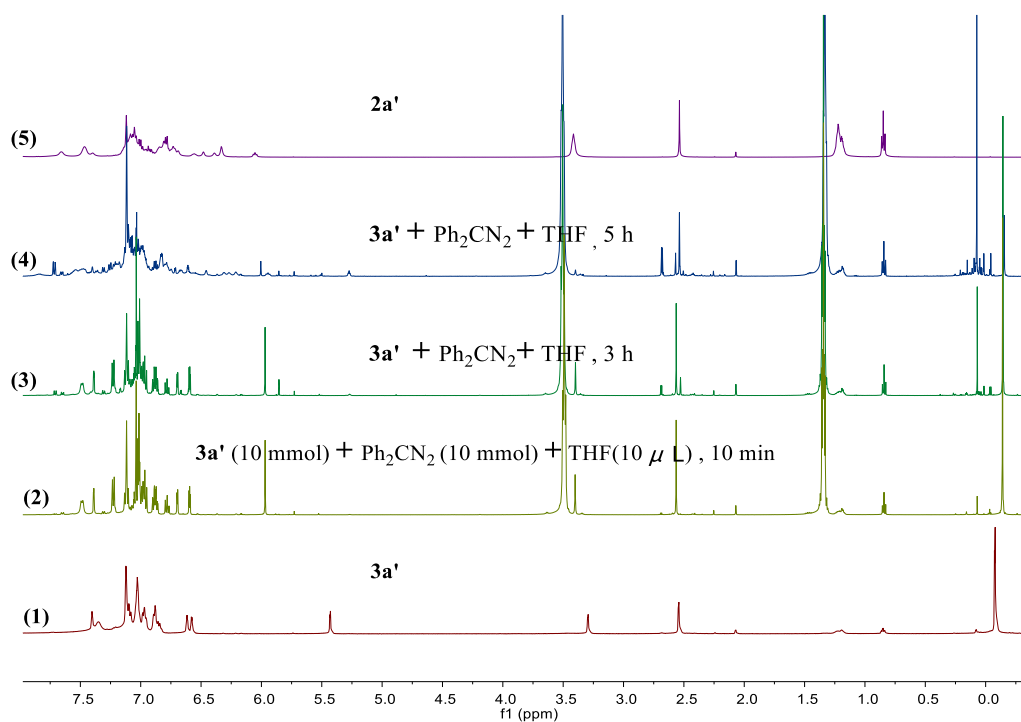


Figure S62. ^1H NMR (500 MHz, C_6D_6) monitoring the transformation of **3a'** to **2a'**.

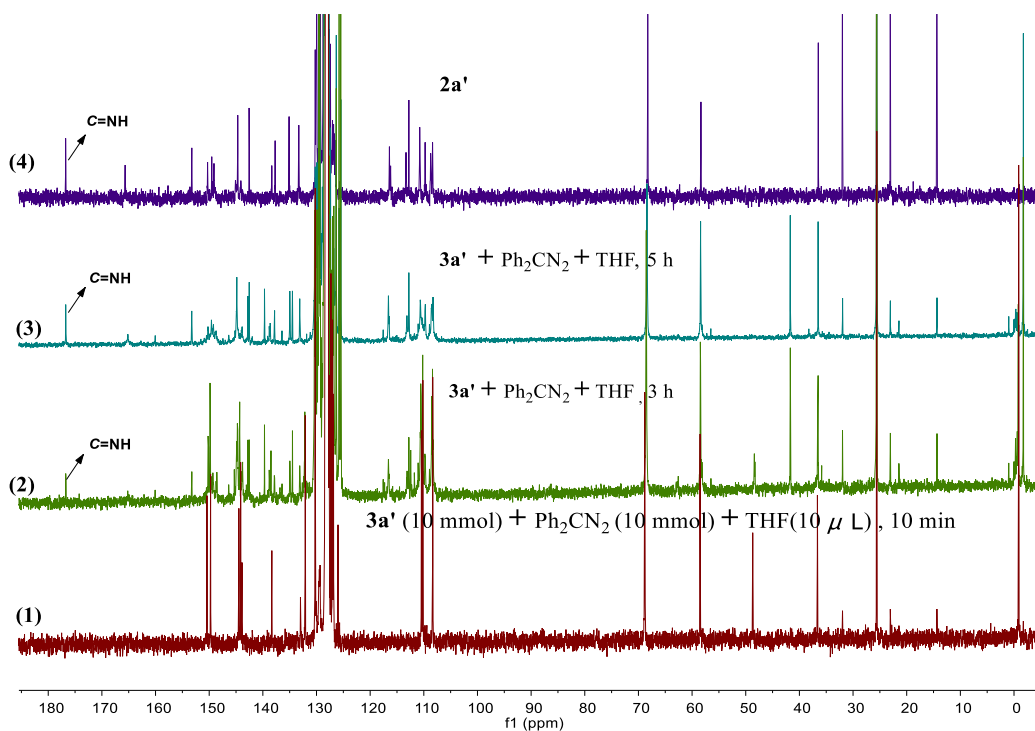


Figure S63. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6) monitoring the transformation of **3a'** to **2a'**.

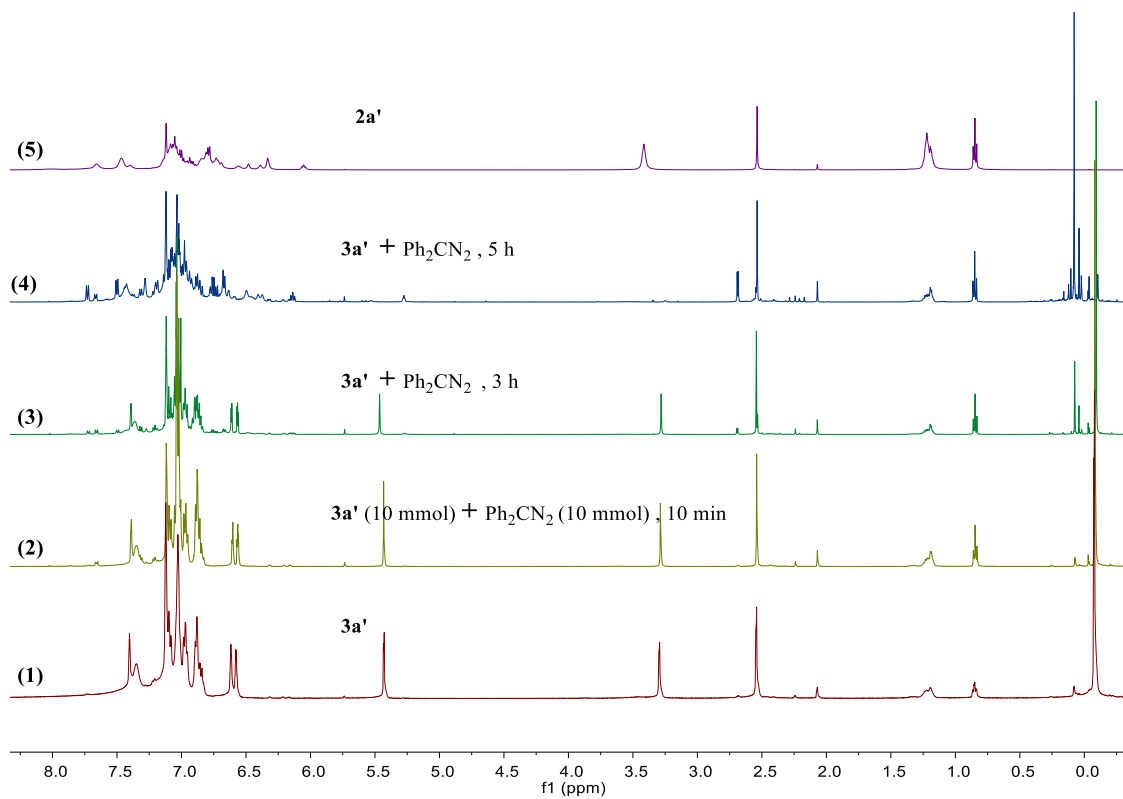


Figure S64. ^1H NMR (500 MHz, C_6D_6) monitoring the reaction of **3a'** with Ph_2CN_2 in C_6D_6 .

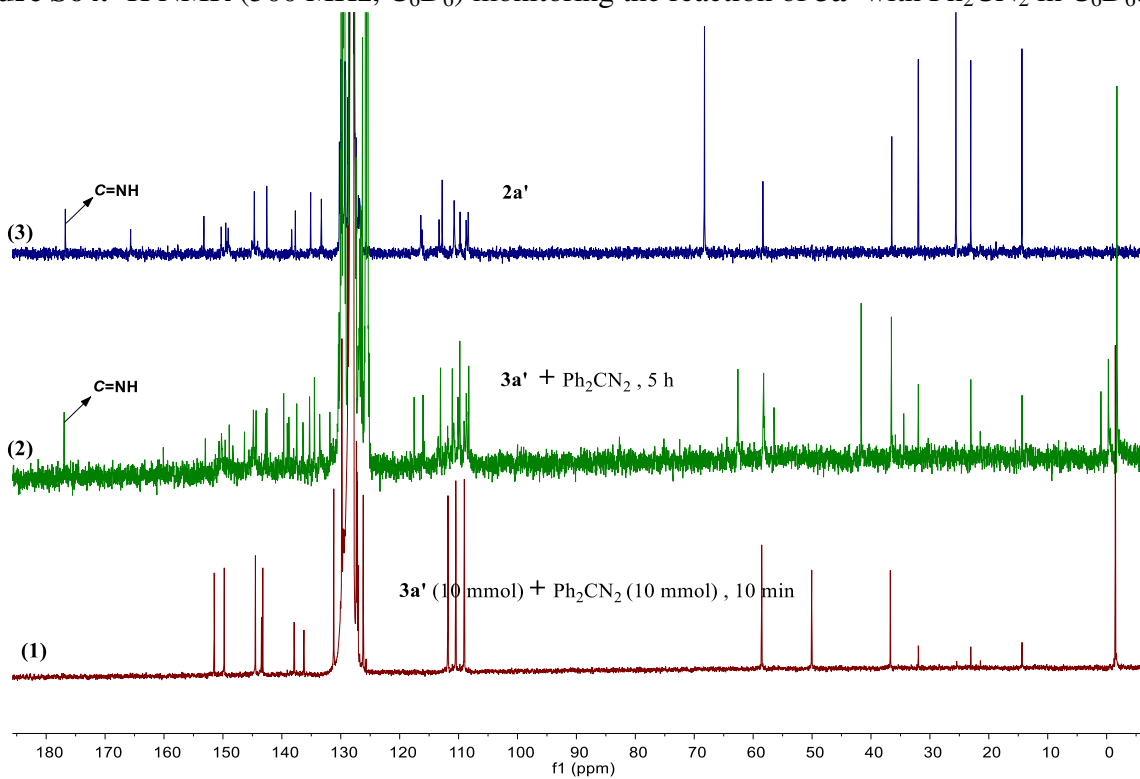


Figure S65. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz) monitoring the reaction of **3a'** with Ph_2CN_2 in C_6D_6 .

2. NMR monitoring the transformation of 4a' to 2a'

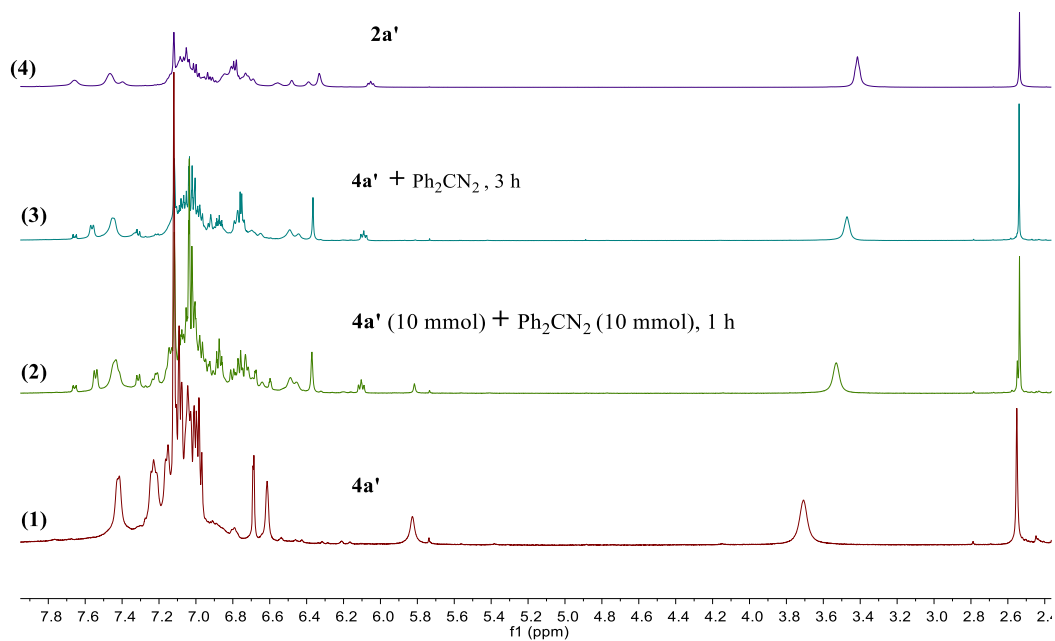


Figure S66. ^1H NMR (500 MHz, C_6D_6) monitoring the transformation of 4a' to 2a'.

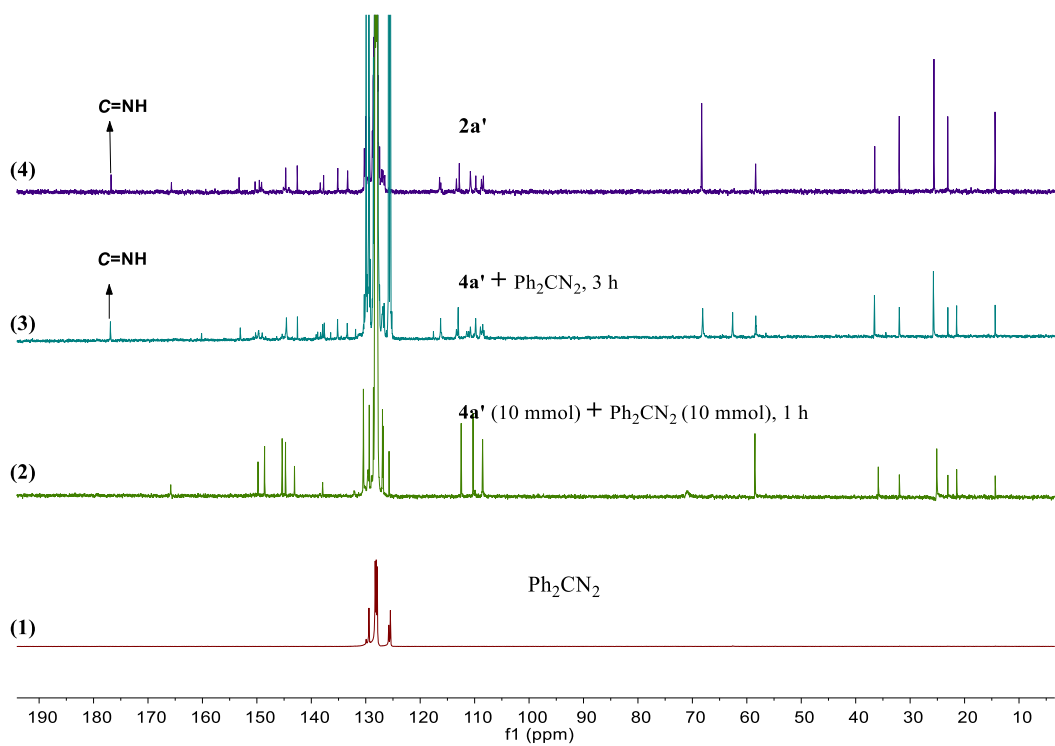


Figure S67. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6) monitoring the transformation of **4a'** to **2a**

Characterization of $(\text{NHCH}_2\text{SiMe}_3)_2$: Under an argon atmosphere, to a clear colorless solution of **1a'** (1.50 g, 1.56 mmol) in 10 mL of toluene was added a brown solution of Ph_2CN_2 (0.6 g, 3.13 mmol) in 8 mL of toluene at room temperature. The mixture was stirred for 5 h and the color of the solution gradually changed from red to dark red. Then, ^{29}Si NMR (99 MHz, C_6D_6) spectrum was performed, and a singlet -0.47 ppm was observed in the crude reaction. An aliquot (30 μL) from the mixture was diluted with C_6D_6 to 0.5 mL and the crude mixture was performed by ^1H NMR spectrum (Figure S67). Subsequently, the solvent of residual mixture was removed under vacuum, and 10 mL of *n*-hexane was added to extract organic compound. The volatiles of the extraction were removed under vacuum to give red oil. The red oil was performed by ^1H NMR (Figure S68), $^{13}\text{C}\{^1\text{H}\}$ NMR (Figure S69) and ^1H - ^{13}C HSQC (Figure S70) spectra. It is failed to obtain a pure compound of $(\text{NHCH}_2\text{SiMe}_3)_2$ by column chromatography or distillation, maybe probably because of its unstable nature.

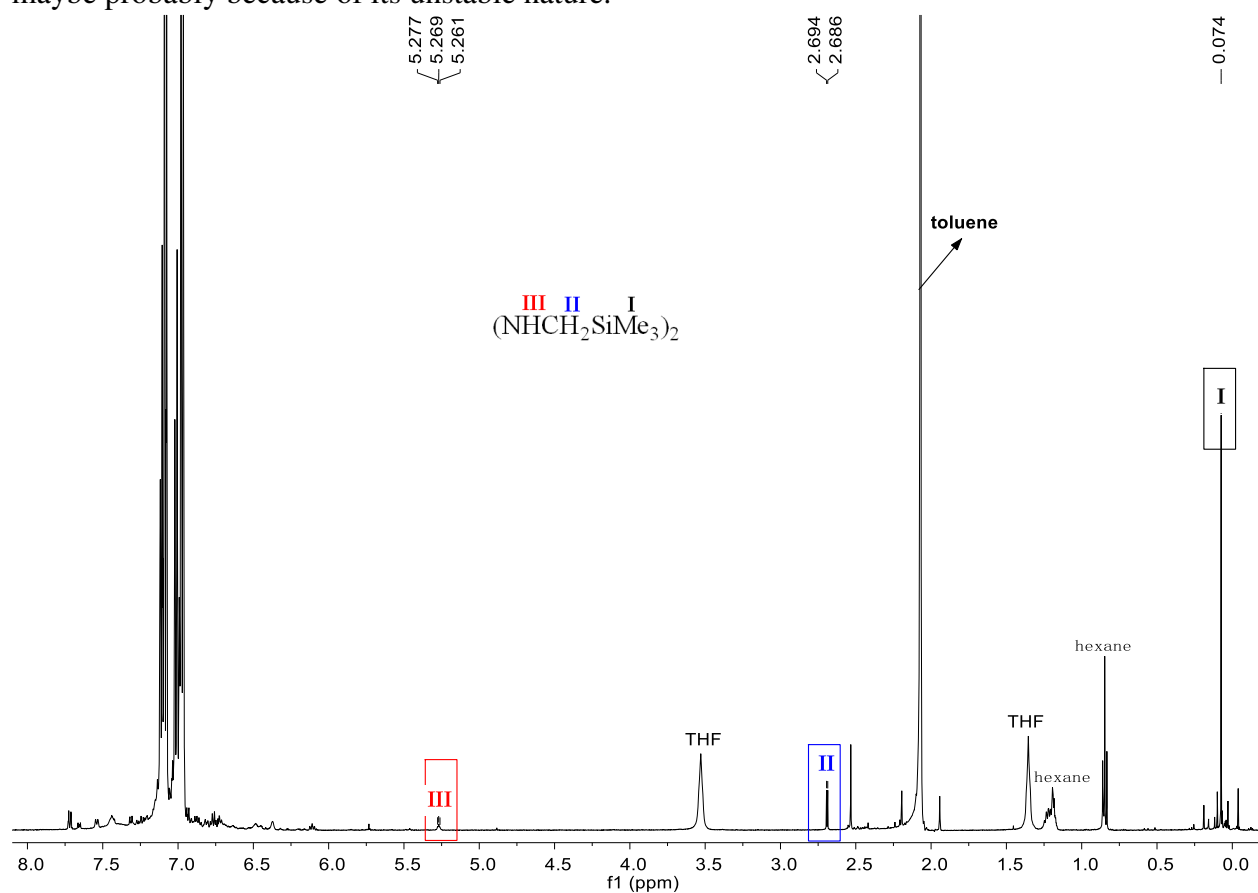


Figure S68. ^1H NMR (500 MHz, C_6D_6 , 25 $^\circ\text{C}$) spectrum of the crude mixture of **1a'** with Ph_2CN_2 in toluene after 5 h at room temperature.

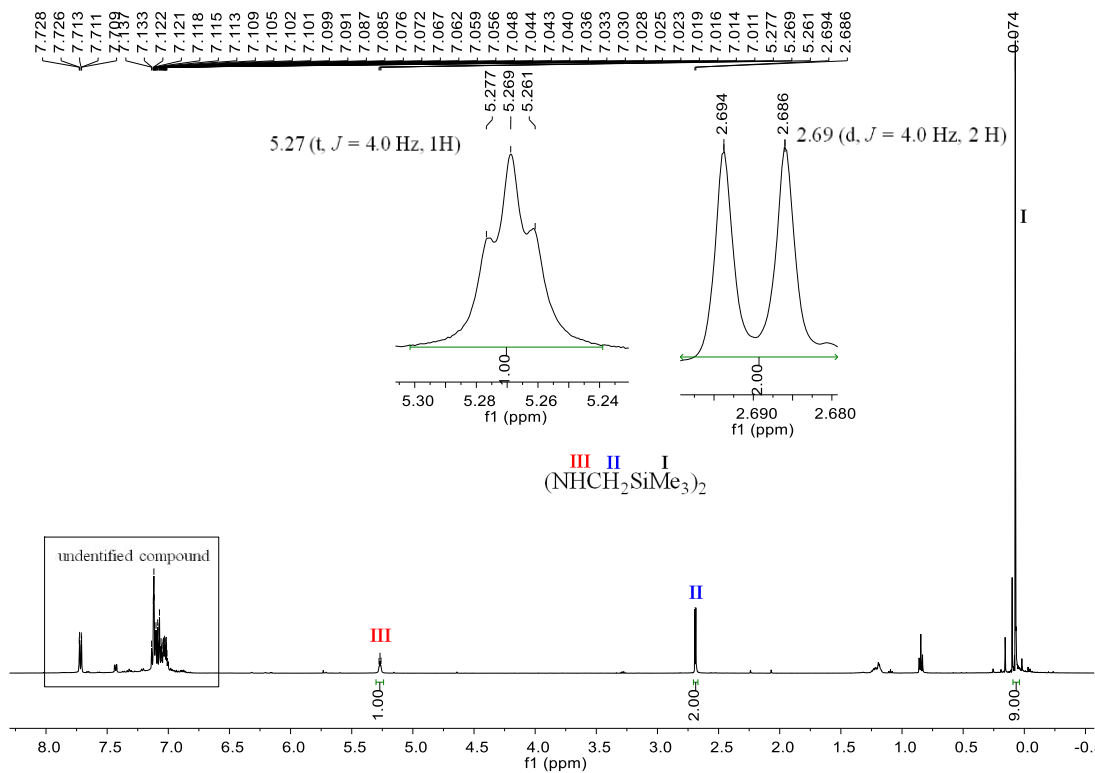


Figure S69. ¹H NMR (500 MHz, C₆D₆, 25 °C) spectrum of the red oil.

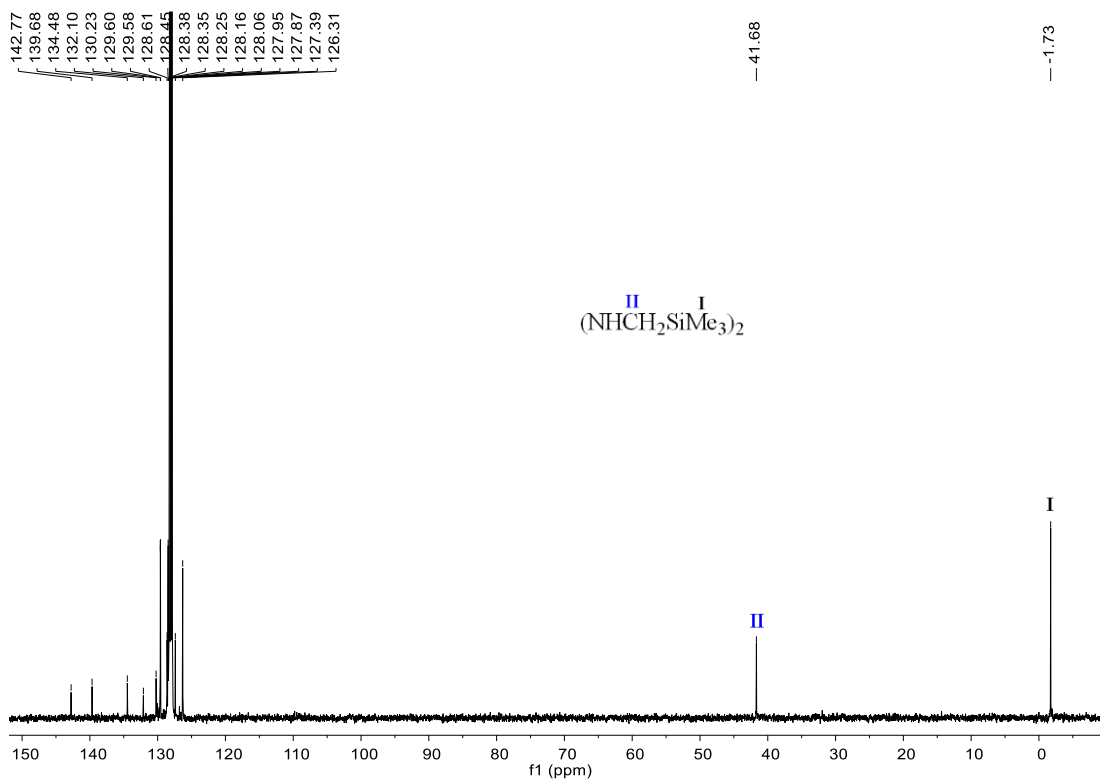


Figure S70. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C) spectrum of the red oil.

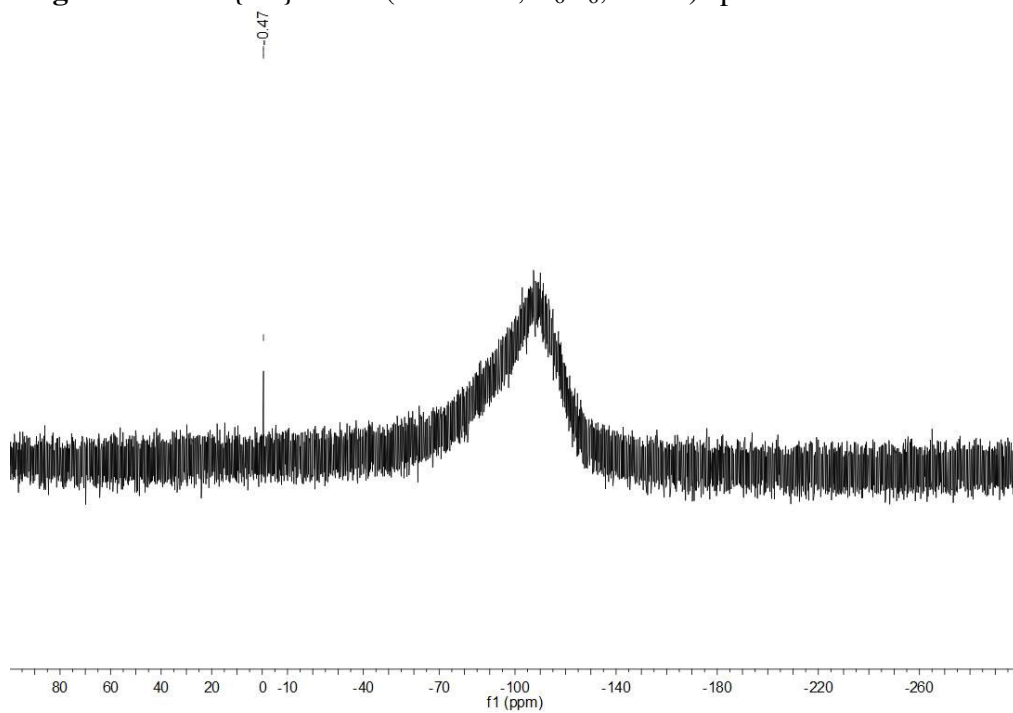


Figure S71 ^{29}Si NMR (99 MHz, C_6D_6) spectrum of the crude reaction of **1a** with Ph_2CN_2 after 5 h.

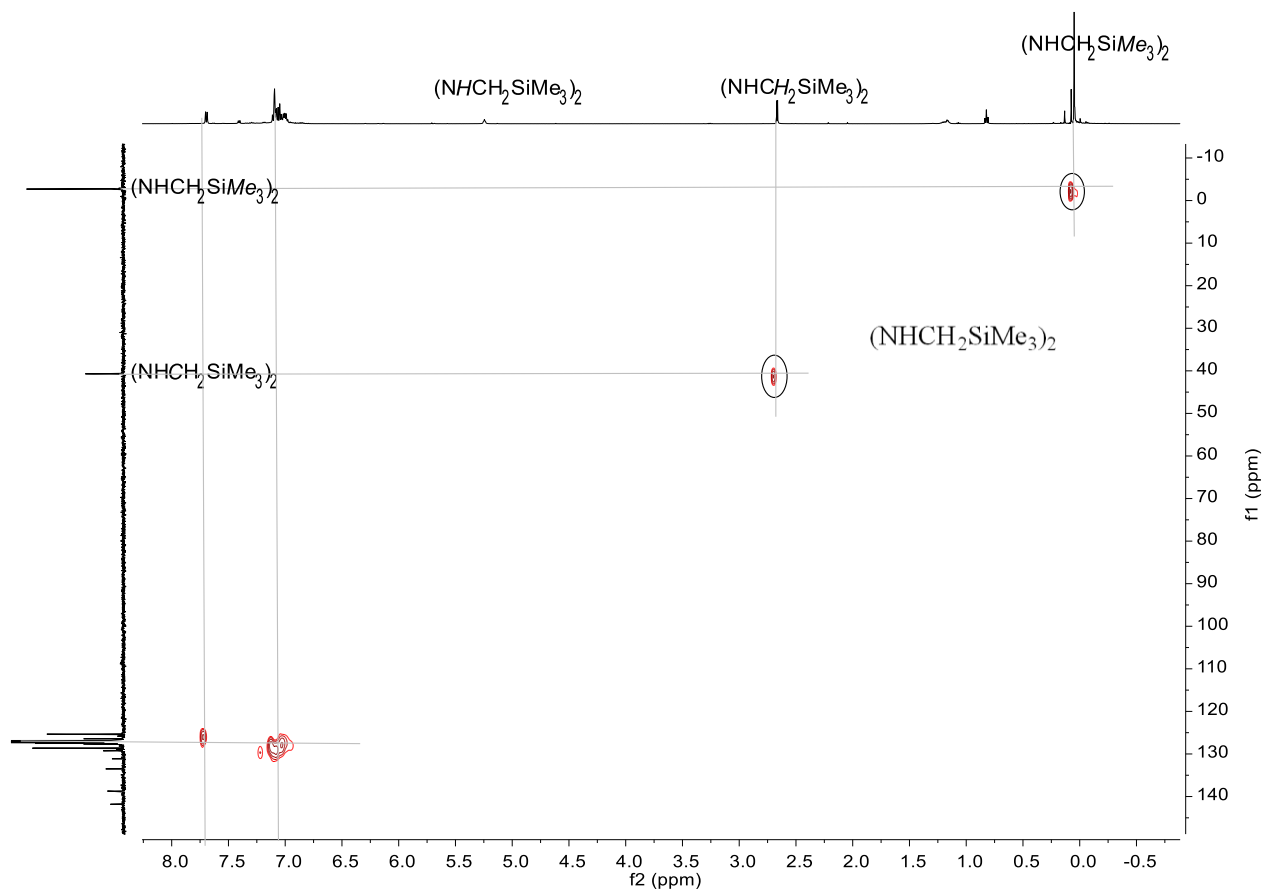


Figure S72. ^1H - ^{13}C HSQC (500 MHz, C_6D_6 , 25 $^\circ\text{C}$) spectrum of the red oil.

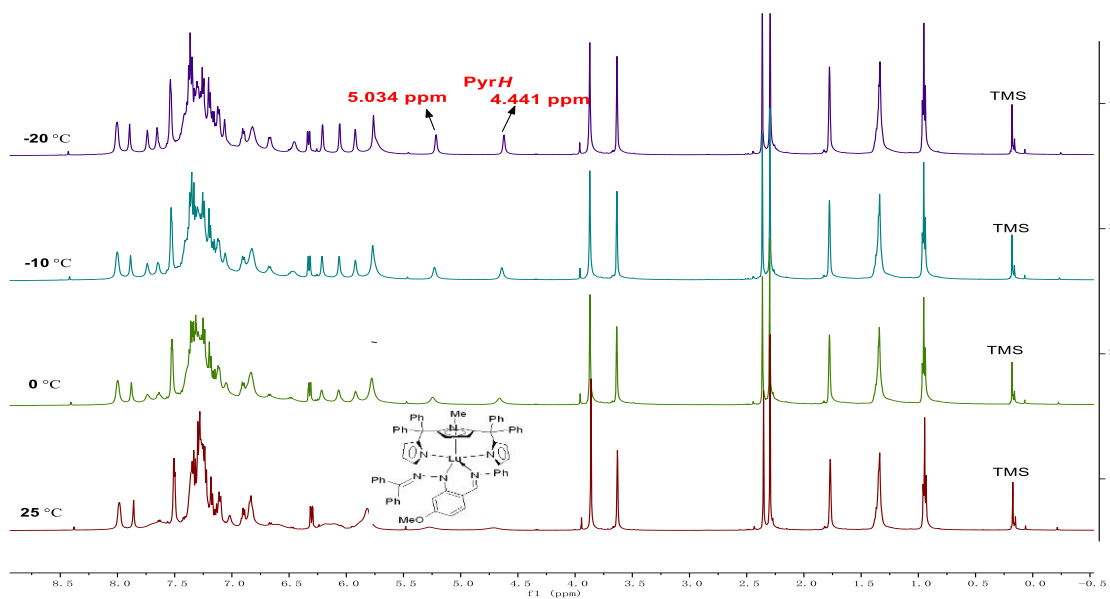


Figure S73. ^1H NMR (500 MHz, $\text{THF-}d_8$, ppm) spectrum of **2d'** at different temperature.

7. DFT Study

Computational Details

All the gas phase optimization calculations were performed using Gaussian 09 suite of programs.¹¹ For optimization, DFT hybrid functional (B3PW91)¹² along with small core pseudo potential Stuttgart basis set for yttrium, and silicon atoms with additional polarization functions¹³ for silicon atoms and Pople style basis sets¹⁴ (6-31G**) for the rest of the atoms were employed. To locate the minima of the optimized structures for reactants, intermediates, products and maxima for transition state structures, frequency calculations were carried out on the optimized structures.

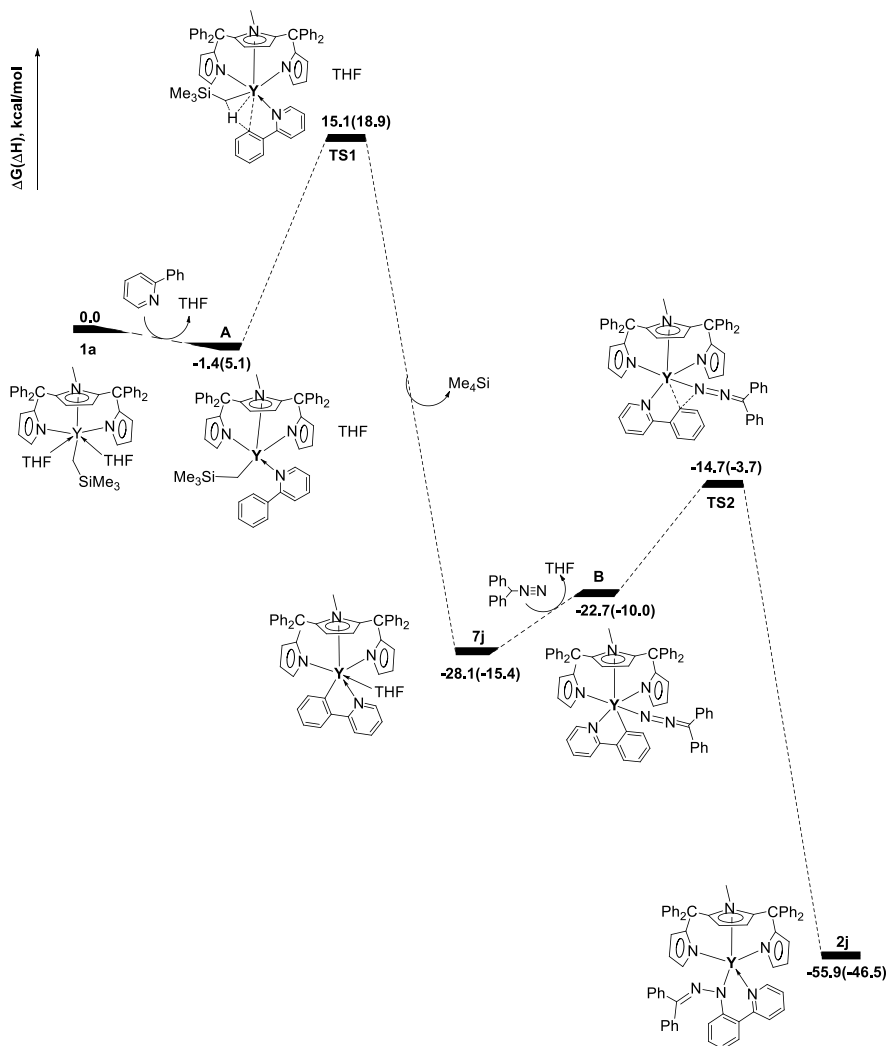


Figure S74. Energy (enthalpy between bracket) profiles for the reaction of **1a** with 2-phenylpyridine and Ph_2CN_2 .

Figure S75: DFT computed MO's (a) HOMO-2 for **7j** (b) HOMO-2 for **B** (c) HOMO-3 for **TS2**. Isovalue=0.05

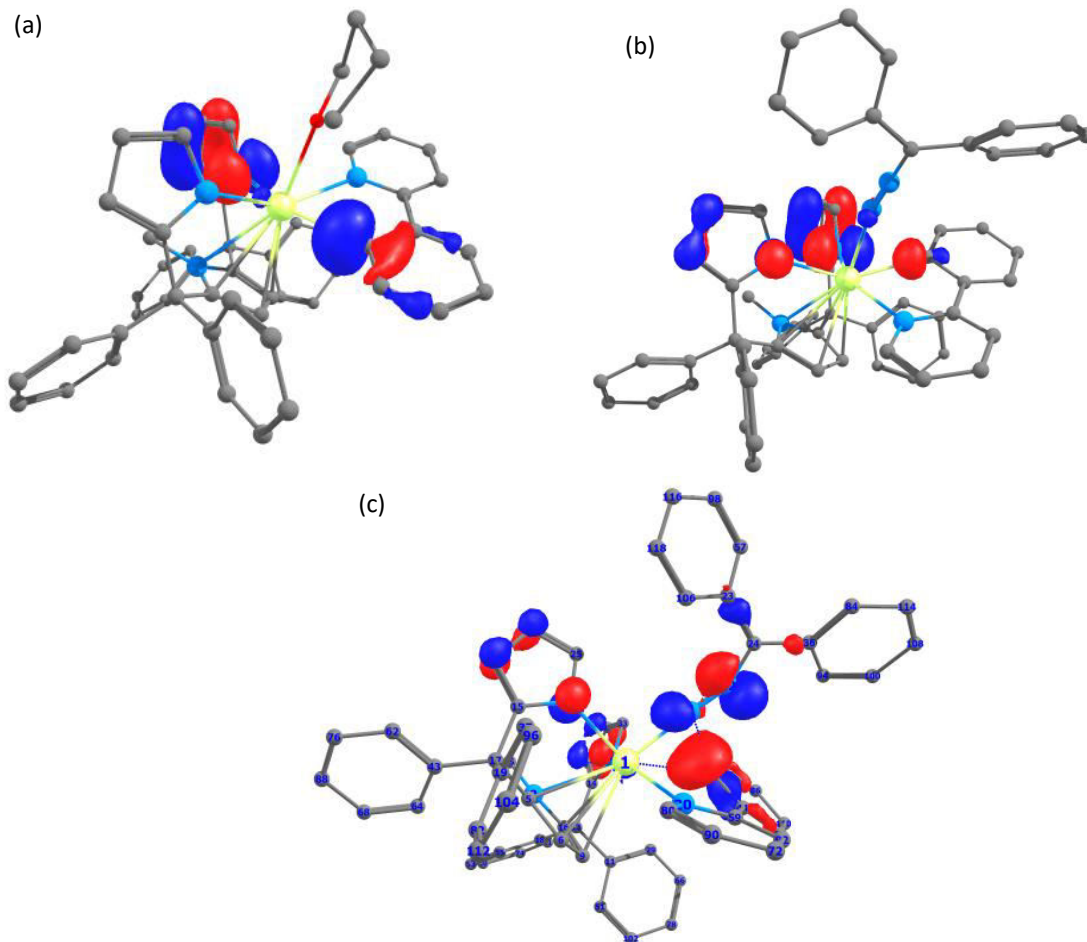


Table S8: DFT computed natural charges
Atom Natural Charges

Label	1a
Y1	1.78313
Si2	1.89939
O3	-0.62283
O4	-0.61072
N5	-0.74813
N6	-0.34988
N7	-0.74742
C78	-1.65307

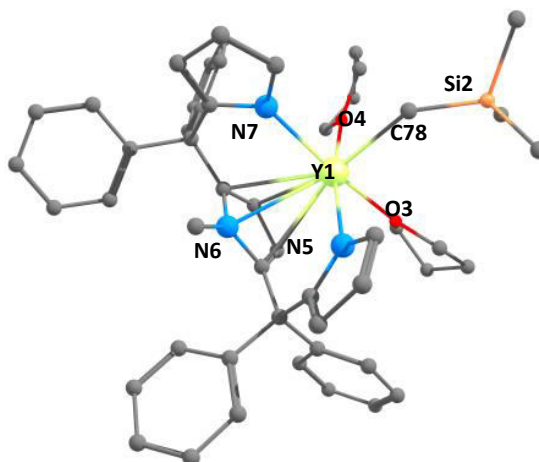


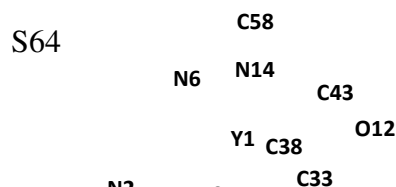
Table S9: DFT computed NBO second order perturbation analysis

1a Donor NBO	Acceptor NBO	E(2) kcal/mol
LP (1) C 78 s(16.08%)p 5.22(83.91%)d 0.00(0.01%)	LP*(1) Y 1 s(10.27%)p 0.68(6.97%)d 8.06(82.76%)	66.96
LP (1) C 78 s(16.08%)p 5.22(83.91%)d 0.00(0.01%)	LP*(2) Y 1 s(73.31%)p 0.01(0.68%)d 0.35(26.01%)	8.92
LP (2) O 3 s(39.43%)p 1.54(60.55%)d 0.00(0.02%)	LP*(2) Y 1 s(73.31%)p 0.01(0.68%)d 0.35(26.01%)	8.23
LP (2) O 3 s(39.43%)p 1.54(60.55%)d 0.00(0.02%)	LP*(3) Y 1 s(0.54%)p 6.67(3.62%)d99.99(95.84%)	15.38
LP (2) O 3 s(39.43%)p 1.54(60.55%)d 0.00(0.02%)	LP*(4) Y 1 s(5.41%)p 0.38(2.06%)d17.12(92.54%)	7.24
LP (2) O 3 s(39.43%)p 1.54(60.55%)d 0.00(0.02%)	LP*(5) Y 1 s(1.02%)p44.90(45.76%)d52.22(53.22%)	11.24
LP (2) O 3 s(39.43%)p 1.54(60.55%)d 0.00(0.02%)	LP*(7) Y 1 s(4.12%)p21.80(89.74%)d 1.49(6.15%)	8.00
LP (2) O 4 s(40.69%)p 1.46(59.29%)d 0.00(0.02%)	LP*(2) Y 1 s(73.31%)p 0.01(0.68%)d 0.35(26.01%)	11.23
LP (2) O 4 s(40.69%)p 1.46(59.29%)d 0.00(0.02%)	LP*(3) Y 1 s(0.54%)p 6.67(3.62%)d99.99(95.84%)	10.67
LP (2) O 4 s(40.69%)p 1.46(59.29%)d 0.00(0.02%)	LP*(4) Y 1 s(5.41%)p 0.38(2.06%)d17.12(92.54%)	12.21
LP (2) O 4 s(40.69%)p 1.46(59.29%)d 0.00(0.02%)	LP*(7) Y 1 s(4.12%)p21.80(89.74%)d 1.49(6.15%)	9.48
LP (1) N 5 s(27.85%)p 2.59(72.14%)d 0.00(0.01%)	LP*(2) Y 1 s(73.31%)p 0.01(0.68%)d 0.35(26.01%)	25.70
LP (1) N 5 s(27.85%)p 2.59(72.14%)d 0.00(0.01%)	LP*(3) Y 1 s(0.54%)p 6.67(3.62%)d99.99(95.84%)	19.65
LP (1) N 7 s(27.72%)p 2.61(72.26%)d 0.00(0.01%)	LP*(2) Y 1 s(73.31%)p 0.01(0.68%)d 0.35(26.01%)	17.68
LP (1) N 7 s(27.72%)p 2.61(72.26%)d 0.00(0.01%)	LP*(3) Y 1 s(0.54%)p 6.67(3.62%)d99.99(95.84%)	28.50

Table S10: DFT computed natural charges

Atom Natural Charges

Label **7j**



Y1 1.72205
 N2 -0.35799
 N6 -0.72544
 N9 -0.73450
 O12 -0.62110
 N14 -0.53609
 C33 -0.49650

SD1: Bonding analysis from NBO computation for 7j

(1.97539) BD (1) N 14 - C 43

(60.13%) 0.7754* N 14 s(37.60%)p 1.66(62.34%)d 0.00(0.06%)

(39.87%) 0.6314* C 43 s(28.74%)p 2.48(71.15%)d 0.00(0.11%)

(1.71128) BD (2) N 14 - C 43

(64.79%) 0.8049* N 14 s(0.00%)p 1.00(99.89%)d 0.00(0.11%)

(35.21%) 0.5934* C 43 s(0.00%)p 1.00(99.88%)d 0.00(0.12%)

(1.95836) BD (1) C 33 - C 38

(47.01%) 0.6856* C 33 s(35.76%)p 1.79(64.17%)d 0.00(0.06%)

(52.99%) 0.7280* C 38 s(35.47%)p 1.82(64.50%)d 0.00(0.03%)

(1.55973) BD (2) C 33 - C 38

(42.52%) 0.6521* C 33 s(0.00%)p 1.00(99.91%)d 0.00(0.09%)

(57.48%) 0.7581* C 38 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)

(1.97070) BD (1) C 38 - C 43

(49.16%) 0.7011* C 38 s(29.91%)p 2.34(70.04%)d 0.00(0.05%)

(50.84%) 0.7130* C 43 s(35.04%)p 1.85(64.93%)d 0.00(0.04%)

Table S11: DFT computed NBO second order perturbation analysis

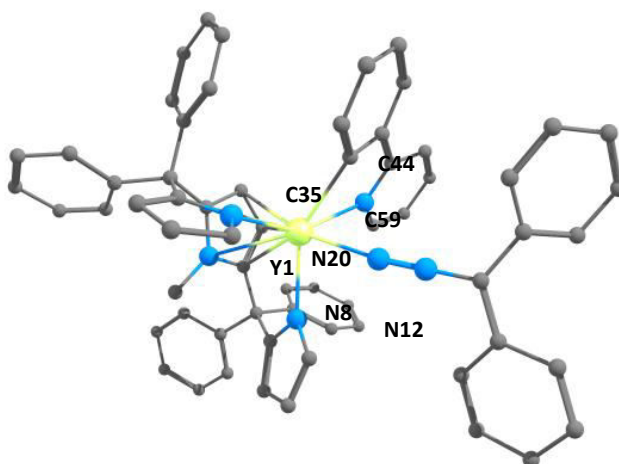
7j Donor NBO	Acceptor NBO	E(2) kcal/mol
<u>BD (1) N 14 - C 43</u>	<u>LP* (2) Y 1</u>	6.98

(60.13%) 0.7754* N 14 s(37.60%)p 1.66(62.34%)d 0.00(0.06%)	s(31.98%)p 0.08(2.54%)d 2.05(65.48%)	
(39.87%) 0.6314* C 43 s(28.74%)p 2.48(71.15%)d 0.00(0.11%)		
<u>BD (1) N 14 - C 43</u>	<u>LP*(5) Y 1</u>	8.32
(60.13%) 0.7754* N 14 s(37.60%)p 1.66(62.34%)d 0.00(0.06%)	s(0.10%)p99.99(44.83%)d99.99(55.08%)	
(39.87%) 0.6314* C 43 s(28.74%)p 2.48(71.15%)d 0.00(0.11%)		
<u>BD (1) N 14 - C 58</u>	<u>LP*(2) Y 1</u>	7.37
(60.76%) 0.7795* N 14 s(37.77%)p 1.65(62.17%)d 0.00(0.05%)	s(31.98%)p 0.08(2.54%)d 2.05(65.48%)	
(39.24%) 0.6264* C 58 s(29.53%)p 2.38(70.35%)d 0.00(0.12%)		
<u>BD (1) N 14 - C 58</u>	<u>LP*(5) Y 1</u>	8.18
(60.76%) 0.7795* N 14 s(37.77%)p 1.65(62.17%)d 0.00(0.05%)	s(0.10%)p99.99(44.83%)d99.99(55.08%)	
(39.24%) 0.6264* C 58 s(29.53%)p 2.38(70.35%)d 0.00(0.12%)		
<u>BD (1) C 33 - C 38</u>	<u>LP*(1) Y 1</u>	12.87
(47.01%) 0.6856* C 33 s(35.76%)p 1.79(64.17%)d 0.00(0.06%)	s(30.32%)p 0.43(13.10%)d 1.87(56.58%)	
(52.99%) 0.7280* C 38 s(35.47%)p 1.82(64.50%)d 0.00(0.03%)		
<u>BD (1) C 33 - C 56</u>	<u>LP*(1) Y 1</u>	13.99
(48.70%) 0.6979* C 33 s(37.52%)p 1.66(62.42%)d 0.00(0.06%)	s(30.32%)p 0.43(13.10%)d 1.87(56.58%)	
(51.30%) 0.7162* C 56 s(35.65%)p 1.80(64.32%)d 0.00(0.04%)		
<u>LP (1) N 14</u>	<u>LP*(2) Y 1</u>	27.56
s(24.56%)p 3.07(75.41%)d 0.00(0.03%)	s(31.98%)p 0.08(2.54%)d 2.05(65.48%)	
<u>LP (1) N 14</u>	<u>LP*(5) Y 1</u>	19.55
s(24.56%)p 3.07(75.41%)d 0.00(0.03%)	s(0.10%)p99.99(44.83%)d99.99(55.08%)	
<u>LP (1) C 33</u>	<u>LP*(1) Y 1</u>	83.78
s(26.48%)p 2.78(73.51%)d 0.00(0.01%)	s(30.32%)p 0.43(13.10%)d 1.87(56.58%)	

Table S12: DFT computed natural charges

Atom Natural Charges

Label	B
Y1	1.59792
N8	-0.09408
N12	0.09928
N20	-0.53473
C35	-0.41657
C44	-0.10562
C59	0.25453



SD2: Bonding analysis from NBO computation for **B**

(1.97622) BD (1) N 20 - C 59

(60.27%) 0.7763* N 20 s(37.86%)p 1.64(62.09%)d 0.00(0.06%)

(39.73%) 0.6303* C 59 s(28.67%)p 2.48(71.21%)d 0.00(0.11%)
(1.95822) BD (1) C 35 - C 44
 (47.12%) 0.6865* C 35 s(35.50%)p 1.82(64.44%)d 0.00(0.06%)
 (52.88%) 0.7272* C 44 s(35.34%)p 1.83(64.63%)d 0.00(0.03%)
(1.56314) BD (2) C 35 - C 44
 (43.09%) 0.6564* C 35 s(0.05%)p99.99(99.87%)d 1.78(0.09%)
 (56.91%) 0.7544* C 44 s(0.01%)p 1.00(99.98%)d 0.00(0.01%)
(1.97067) BD (1) C 44 - C 59
 (49.25%) 0.7018* C 44 s(30.03%)p 2.33(69.92%)d 0.00(0.05%)
 (50.75%) 0.7124* C 59 s(34.94%)p 1.86(65.03%)d 0.00(0.04%)

Table S13: DFT computed NBO second order perturbation analysis

B Donor NBO	Acceptor NBO	E(2) kcal/mol
<u>LP (1) N 8</u> s(62.67%)p 0.60(37.32%)d 0.00(0.01%)	<u>LP*(1) Y 1</u> s(48.13%)p 0.31(14.84%)d 0.77(37.03%)	22.32
<u>LP (1) N 8</u> s(62.67%)p 0.60(37.32%)d 0.00(0.01%)	<u>LP*(2) Y 1</u> s(6.24%)p 1.70(10.58%)d13.33(83.18%)	43.23
<u>LP (1) N 8</u> s(62.67%)p 0.60(37.32%)d 0.00(0.01%)	<u>LP*(3) Y 1</u> s(33.42%)p 0.23(7.55%)d 1.77(59.04%)	28.95
65. BD (1) C 35 - C 44 (47.12%) 0.6865* C 35 s(35.50%)p 1.82(64.44%)d 0.00(0.06%) (52.88%) 0.7272* C 44 s(35.34%)p 1.83(64.63%)d 0.00(0.03%)	<u>LP*(1) Y 1</u> s(48.13%)p 0.31(14.84%)d 0.77(37.03%)	11.06
<u>LP (1) N 20</u> s(24.50%)p 3.08(75.47%)d 0.00(0.03%)	<u>LP*(2) Y 1</u> s(6.24%)p 1.70(10.58%)d13.33(83.18%)	10.29
<u>LP (1) N 20</u> s(24.50%)p 3.08(75.47%)d 0.00(0.03%)	<u>LP*(1) Y 1</u> s(48.13%)p 0.31(14.84%)d 0.77(37.03%)	7.20
<u>LP (1) N 20</u> s(24.50%)p 3.08(75.47%)d 0.00(0.03%)	<u>LP*(6) Y 1</u> s(0.24%)p99.99(63.32%)d99.99(36.44%)	14.03
<u>LP (1) C 35</u> s(26.23%)p 2.81(73.76%)d 0.00(0.01%)	<u>LP*(1) Y 1</u> s(48.13%)p 0.31(14.84%)d 0.77(37.03%)	77.15

Table S14: DFT computed natural charges

Atom Natural Charges
 Label TS2



S67

C44

C35

C59

Y1 1.67650
 N8 -0.32626
 N12 -0.05994
 N20 -0.52962
 C35 -0.19446
 C44 -0.09764
 C59 0.24999

SD3: Bonding analysis from NBO computation for TS2

(1.97557) BD (1) N 20 - C 59

(60.13%) 0.7754* N 20 s(37.71%)p 1.65(62.24%)d 0.00(0.06%)

(39.87%) 0.6314* C 59 s(28.93%)p 2.45(70.96%)d 0.00(0.11%)

(1.82562) BD (1) N 8 - C 35

(42.97%) 0.6555* N 8 s(3.03%)p31.99(96.92%)d 0.01(0.05%)

(57.03%) 0.7552* C 35 s(21.08%)p 3.74(78.91%)d 0.00(0.00%)

(1.95667) BD (1) C 35 - C 44

(47.85%) 0.6918* C 35 s(37.95%)p 1.63(62.00%)d 0.00(0.06%)

(52.15%) 0.7221* C 44 s(34.72%)p 1.88(65.24%)d 0.00(0.03%)

(1.62397) BD (2) C 35 - C 44

(50.60%) 0.7114* C 35 s(1.50%)p65.47(98.45%)d 0.03(0.05%)

(49.40%) 0.7028* C 44 s(0.05%)p99.99(99.93%)d 0.50(0.02%)

(1.96808) BD (1) C 44 - C 59

(49.86%) 0.7061* C 44 s(30.61%)p 2.27(69.34%)d 0.00(0.05%)

(50.14%) 0.7081* C 59 s(34.29%)p 1.91(65.67%)d 0.00(0.04%)

Table S15: DFT computed NBO second order perturbation analysis

TS2
 Donor NBO

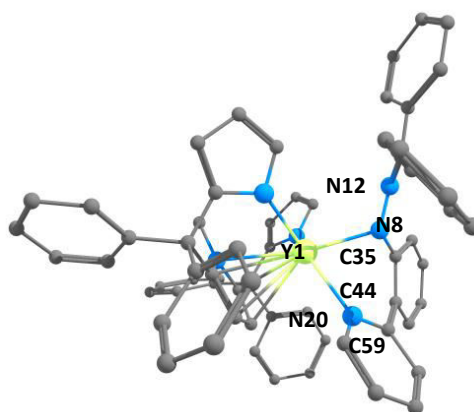
Acceptor NBO

E(2)
 kcal/mol

<u>244. LP (1) N 8</u>	<u>LP*(1) Y 1</u>	36.50
s(58.93%)p 0.70(41.06%)d 0.00(0.00%)	s(2.06%)p 1.80(3.71%)d45.65(94.23%)	
<u>244. LP (1) N 8</u>	<u>LP*(2) Y 1</u>	25.09
s(58.93%)p 0.70(41.06%)d 0.00(0.00%)	s(84.50%)p 0.04(3.70%)d 0.14(11.80%)	
<u>244. LP (1) N 8</u>	<u>LP*(3) Y 1</u>	10.07
s(58.93%)p 0.70(41.06%)d 0.00(0.00%)	s(2.13%)p13.27(28.24%)d32.72(69.63%)	
<u>244. LP (1) N 8</u>	<u>LP*(4) Y 1</u>	27.22
s(58.93%)p 0.70(41.06%)d 0.00(0.00%)	s(4.01%)p 5.92(23.72%)d18.03(72.27%)	
<u>LP (1) N 20</u>	<u>LP*(2) Y 1</u>	9.36
s(24.56%)p 3.07(75.41%)d 0.00(0.03%)	s(84.50%)p 0.04(3.70%)d 0.14(11.80%)	
<u>LP (1) N 20</u>	<u>LP*(6) Y 1</u>	19.45
s(24.56%)p 3.07(75.41%)d 0.00(0.03%)	s(0.30%)p99.99(74.40%)d83.86(25.30%)	
<u>BD (1) N 8 - C 35</u>	<u>LP*(4) Y 1</u>	34.92
(42.97%) 0.6555* N 8 s(3.03%)p31.99(96.92%)d 0.01(0.05%)	s(4.01%)p 5.92(23.72%)d18.03(72.27%)	
(57.03%) 0.7552* C 35 s(21.08%)p 3.74(78.91%)d 0.00(0.00%)		
<u>BD (1) C 35 - C 44</u>	<u>LP*(4) Y 1</u>	11.06
(47.85%) 0.6918* C 35 s(37.95%)p 1.63(62.00%)d 0.00(0.06%)	s(4.01%)p 5.92(23.72%)d18.03(72.27%)	
(52.15%) 0.7221* C 44 s(34.72%)p 1.88(65.24%)d 0.00(0.03%)		

Table S16: DFT computed natural charges

Atom	Natural Charges
Label	2j
Y1	1.83470
N8	-0.60360
N12	-0.26720
N20	-0.58936
C35	0.18268
C44	-0.16098
C59	0.25422



SD4: Bonding analysis from NBO computation for **2j**

(1.97432) BD (1) N 20 - C 59

(60.28%) 0.7764* N 20 s(38.00%)p 1.63(61.94%)d 0.00(0.05%)

(39.72%) 0.6302* C 59 s(28.80%)p 2.47(71.08%)d 0.00(0.11%)

(1.96388) BD (1) C 44 - C 59

(49.70%) 0.7050* C 44 s(31.49%)p 2.17(68.47%)d 0.00(0.05%)

(50.30%) 0.7092* C 59 s(34.98%)p 1.86(64.98%)d 0.00(0.04%)

(1.95273) BD (1) C 35 - C 44

(49.36%) 0.7026* C 35 s(34.11%)p 1.93(65.85%)d 0.00(0.04%)

(50.64%) 0.7116* C 44 s(34.16%)p 1.93(65.80%)d 0.00(0.04%)

(1.59746) BD (2) C 35 - C 44

(42.62%) 0.6528* C 35 s(0.09%)p99.99(99.87%)d 0.43(0.04%)

(57.38%) 0.7575* C 44 s(0.04%)p99.99(99.95%)d 0.29(0.01%)

(1.97057) BD (1) N 8 - C 35

(58.81%) 0.7669* N 8 s(37.64%)p 1.66(62.30%)d 0.00(0.07%)

(41.19%) 0.6418* C 35 s(29.49%)p 2.39(70.40%)d 0.00(0.10%)

Table S17: DFT computed NBO second order perturbation analysis

2j	Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.97540) BD (1) N 8 - N 12	(50.51%) 0.7107* N 8 s(25.18%)p 2.97(74.69%)d 0.01(0.13%) (49.49%) 0.7035* N 12 s(24.32%)p 3.11(75.55%)d 0.01(0.13%)	LP*(1) Y 1 s(0.63%)p13.99(8.80%)d99.99(90.57%)	11.73
(1.97057) BD (1) N 8 - C 35	(58.81%) 0.7669* N 8 s(37.64%)p 1.66(62.30%)d 0.00(0.07%) (41.19%) 0.6418* C 35 s(29.49%)p 2.39(70.40%)d 0.00(0.10%)	LP*(1) Y 1 s(0.63%)p13.99(8.80%)d99.99(90.57%)	15.03
(1.97432) BD (1) N 20 - C 59	(60.28%) 0.7764* N 20 s(38.00%)p 1.63(61.94%)d 0.00(0.05%) (39.72%) 0.6302* C 59 s(28.80%)p 2.47(71.08%)d 0.00(0.11%)	LP*(6) Y 1 s(2.29%)p30.01(68.80%)d12.61(28.91%)	9.43
LP (1) N 8	s(37.12%)p 1.69(62.84%)d 0.00(0.03%)	LP*(1) Y 1 s(0.63%)p13.99(8.80%)d99.99(90.57%)	48.78
LP (1) N 8	s(37.12%)p 1.69(62.84%)d 0.00(0.03%)	LP*(2) Y 1 s(32.98%)p 0.30(9.83%)d 1.73(57.19%)	10.50
LP (1) N 20	s(24.16%)p 3.14(75.81%)d 0.00(0.02%)	LP*(6) Y 1 s(2.29%)p30.01(68.80%)d12.61(28.91%)	16.50

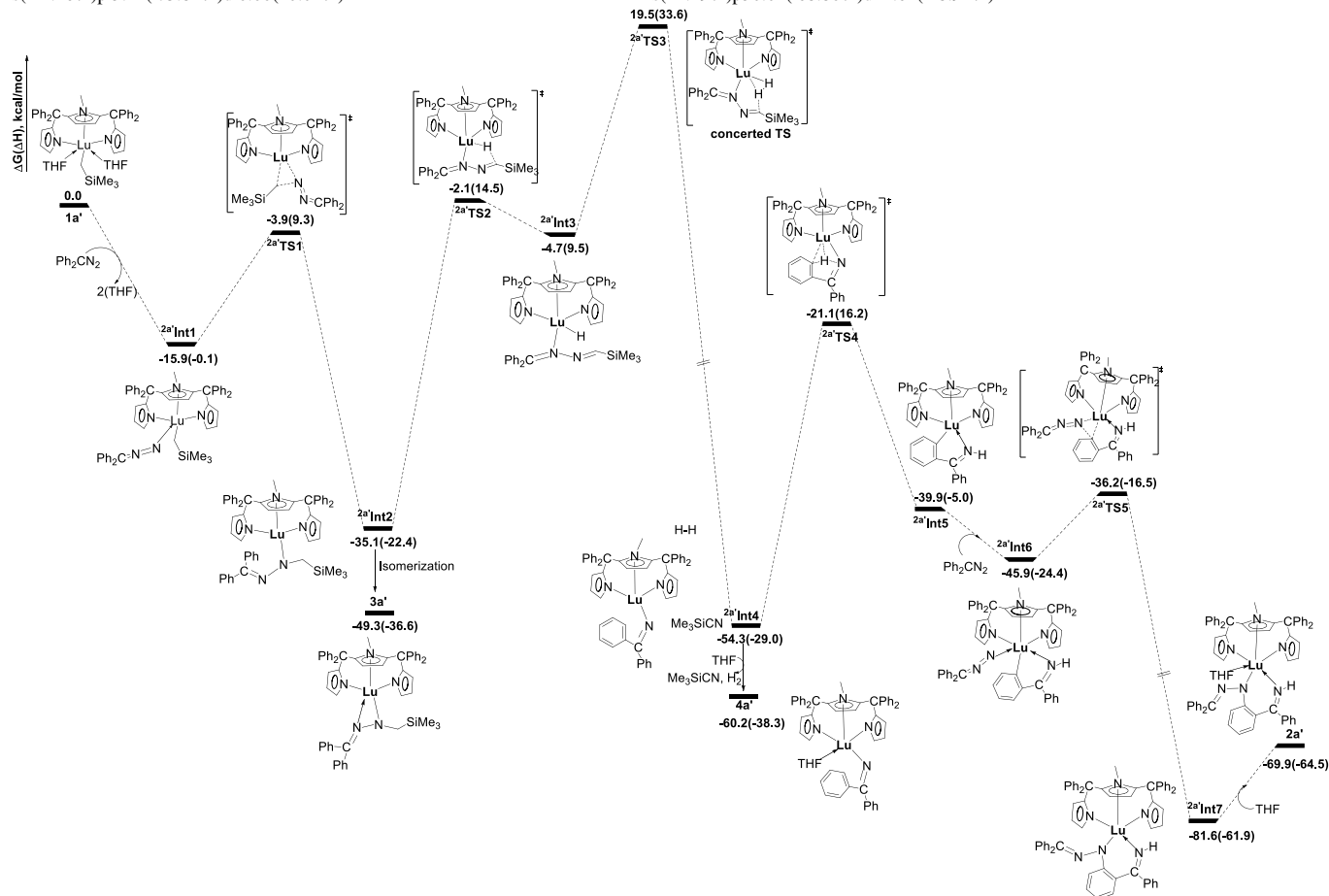


Figure S76. Energy (enthalpy between bracket) profiles for the reaction of 1a' with Ph₂CN₂.

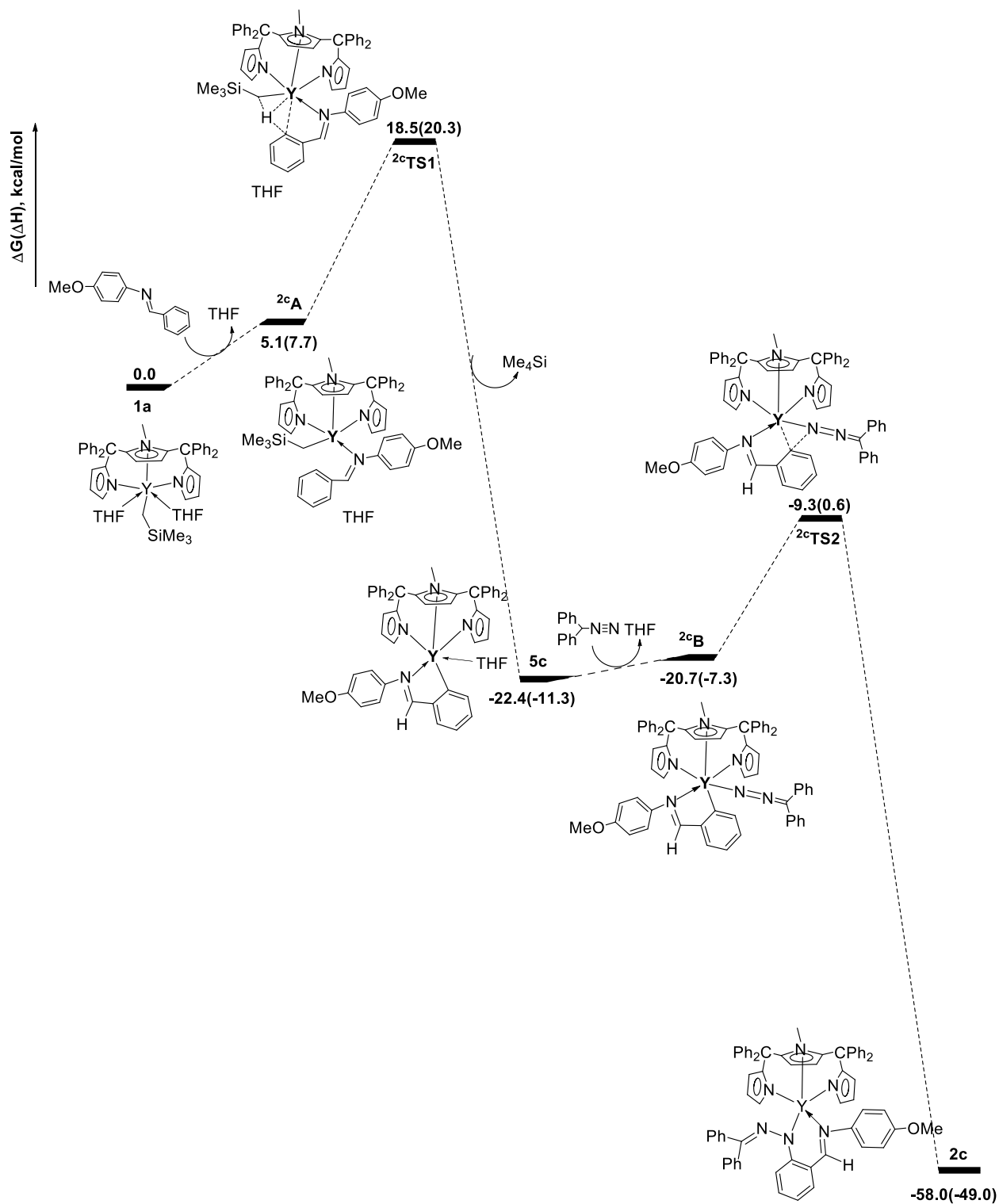


Figure S77. Energy (enthalpy between bracket) profiles for the formation of **2c**.

Optimized coordinates

Ia

Y -4.791592000 6.579289000 11.977041000
 Si -7.571838000 4.031575000 10.502462000
 O -4.968668000 7.105944000 9.543723000
 O -3.188628000 4.859771000 10.930556000
 N -6.315570000 8.350957000 12.336543000
 N -3.494633000 8.696964000 13.609852000
 N -4.235203000 5.747951000 14.126676000
 C -7.599464000 8.023539000 12.718080000
 H -7.980586000 7.023462000 12.567057000
 C -8.242776000 9.108120000 13.279482000
 H -9.249503000 9.130114000 13.677097000
 C -7.316342000 10.178564000 13.246339000
 H -7.483277000 11.174646000 13.629160000
 C -6.156421000 9.689300000 12.657926000
 C -4.860419000 10.400861000 12.268939000
 C -4.576242000 11.676153000 13.098535000
 C -5.500420000 12.731651000 13.089511000
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H	-0.622228000	2.353148000	2.779441000	C	5.657696000	1.111558000	0.077684000
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C	1.194992000	0.027360000	3.811540000	H	7.492615000	0.468912000	-2.131333000
H	1.038786000	0.353050000	4.830122000	C	6.665932000	2.418322000	-1.634649000
C	3.126133000	-2.674447000	-0.754287000	H	7.570316000	2.896428000	-2.021622000
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H	-1.622537000	0.400451000	7.605579000	C	0.307691000	-4.353661000	-3.390007000
C	2.365627000	-4.100840000	1.050147000	H	1.212973000	-4.313999000	-2.776902000
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H	9.271192000	4.839229000	17.856882000	C	14.006318000	7.240419000	12.209997000
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C	10.518755000	2.139341000	10.871739000	C	6.696651000	1.889897000	11.169932000
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C	10.234804000	3.815939000	14.883816000	Si	6.556919000	0.331183000	10.106955000
H	10.883894000	3.528804000	14.063965000	C	6.426848000	-1.200227000	11.221574000
C	4.571547000	1.133237000	17.140297000	H	7.321996000	-1.312690000	11.841027000
H	3.515103000	0.958997000	17.327089000	H	5.561772000	-1.126356000	11.890049000
C	7.276316000	1.613601000	16.680536000	H	6.309747000	-2.111588000	10.625150000
H	8.330870000	1.802483000	16.508037000	C	4.988578000	0.425981000	9.032147000
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H	4.508447000	7.312167000	14.033157000	H	4.091515000	0.516784000	9.654486000
C	6.295388000	5.494847000	19.681988000	H	5.021042000	1.295862000	8.367083000
H	6.661560000	5.283582000	20.683110000	C	8.051143000	0.138783000	8.952053000
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H	3.496535000	6.284763000	11.228543000	H	5.986995000	1.987247000	13.812410000
C	4.874565000	6.736431000	18.194671000	C	6.419759000	6.430781000	12.117629000
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H	6.374015000	5.549401000	7.267530000	C	6.292304000	5.183173000	12.987462000
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H	4.837518000	11.140023000	10.914772000	C	6.058206000	3.867429000	12.608160000
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H	3.311840000	9.401553000	14.534772000	N	9.679841000	3.586793000	10.910710000

C	5.586466000	4.020688000	17.262803000
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C	5.487649000	1.242781000	16.259609000
H	4.578519000	1.773816000	15.990297000
C	6.210321000	6.023919000	10.635216000
C	7.822599000	6.981737000	12.380458000
C	8.060089000	4.086536000	16.633327000
C	5.314062000	7.472682000	12.407484000
C	4.439441000	4.677952000	16.809460000
H	4.309972000	4.866058000	15.747742000
C	6.874920000	6.353884000	15.166324000
H	7.948091000	6.370910000	15.363358000
H	6.331931000	6.315151000	16.109363000
H	6.596605000	7.250422000	14.620005000
C	5.683534000	3.739728000	18.633977000
H	6.536392000	3.178432000	19.002222000
C	9.681295000	8.210005000	12.708517000
H	10.370574000	9.037659000	12.819964000
C	8.644471000	1.508949000	12.428275000
C	9.960430000	6.866379000	12.889707000
H	10.898511000	6.411536000	13.190287000
C	8.549908000	4.698553000	17.777696000
H	8.008976000	4.897773000	18.691800000
C	9.109901000	1.240122000	11.115284000
C	7.208730000	6.209737000	9.679352000
H	8.157045000	6.634846000	9.989487000
C	9.893994000	5.054016000	17.503679000
H	10.581444000	5.561602000	18.168781000
C	9.651326000	2.365226000	10.319026000
C	8.305134000	8.285711000	12.385503000
H	7.740461000	9.190303000	12.210919000
C	10.147528000	4.640874000	16.209192000
H	11.056279000	4.753028000	15.630571000
C	5.450485000	-0.138482000	16.426944000
H	4.518960000	-0.674789000	16.266156000
C	7.816976000	1.261995000	16.856073000
H	8.735945000	1.811129000	17.033119000
C	4.303848000	7.273790000	13.352443000
H	4.288726000	6.364663000	13.944963000
C	4.694124000	4.148508000	19.521890000
H	4.797792000	3.922835000	20.579886000
C	8.184617000	0.389716000	13.148686000
H	7.821551000	0.519502000	14.168379000
C	10.196839000	4.629137000	10.242346000
H	10.181994000	5.575747000	10.775544000
C	3.567651000	4.829595000	19.058690000
H	2.792722000	5.145123000	19.751673000
C	5.260445000	8.638334000	11.627865000
H	5.995115000	8.787414000	10.843053000
C	4.969324000	5.523363000	10.213120000
H	4.163068000	5.413950000	10.933566000
C	3.440540000	5.083396000	17.697227000
H	2.560433000	5.594277000	17.315822000
C	6.987387000	5.879942000	8.340365000
H	7.779735000	6.035934000	7.613142000
C	4.265800000	9.590126000	11.824481000
H	4.253362000	10.486193000	11.209719000
C	5.762244000	5.358033000	7.937081000
H	5.589706000	5.101228000	6.895408000
C	3.298548000	8.223223000	13.546941000
H	2.528284000	8.041179000	14.291646000
C	4.749528000	5.183694000	8.881942000
H	3.780921000	4.794764000	8.578933000
C	8.168582000	-0.906067000	12.627656000
H	7.804085000	-1.735178000	13.230665000

C	10.146771000	2.213510000	9.011122000
H	10.114441000	1.245497000	8.526963000
C	9.086071000	-0.059431000	10.574655000
H	9.433409000	-0.259473000	9.564552000
C	6.598488000	-0.829025000	16.818779000
H	6.567901000	-1.905742000	16.962170000
C	3.279787000	9.390494000	12.791386000
H	2.499546000	10.131262000	12.942307000
C	7.777273000	-0.122186000	17.039371000
H	8.674857000	-0.645477000	17.358776000
C	10.721614000	4.538444000	8.960197000
H	11.132841000	5.417149000	8.474746000
C	11.434585000	2.044571000	14.467190000
H	10.683704000	1.277001000	14.264923000
H	11.347925000	2.381836000	15.503840000
C	8.616426000	-1.129616000	11.326461000
H	8.602417000	-2.129042000	10.899305000
C	10.684588000	3.295912000	8.332338000
H	11.069890000	3.169723000	7.323876000
C	12.305799000	3.552310000	12.850597000
H	12.343545000	4.642277000	12.782513000
H	12.211291000	3.135155000	11.841759000
C	13.471124000	2.933517000	13.604523000
H	14.345859000	2.787157000	12.965277000
H	13.762649000	3.567406000	14.449089000
C	12.852634000	1.623858000	14.098781000
H	13.382735000	1.190370000	14.950737000
H	12.838270000	0.882471000	13.292641000

B

Y	-0.225498000	-0.305145000	-0.043947000
N	-0.433252000	0.758772000	2.595934000
N	-0.678441000	2.018910000	-0.246890000
N	-2.175412000	-1.082826000	0.961801000
C	0.712025000	1.358104000	2.073306000
C	1.660078000	0.353268000	1.921172000
H	2.663834000	0.491512000	1.551962000
N	-0.850414000	-0.127234000	-2.391655000
C	1.084511000	-0.870174000	2.361184000
H	1.559128000	-1.840114000	2.383457000
C	-0.668555000	-3.012332000	3.181678000
N	-0.751635000	-0.031748000	-3.541874000
C	-1.284267000	-1.588428000	3.245649000
C	-2.451472000	-1.424606000	2.269856000
C	-0.372930000	3.026652000	0.652713000
C	-0.210558000	-0.603377000	2.789538000
C	0.770827000	2.822438000	1.645605000
C	-1.709129000	-1.361928000	4.710124000
C	2.142990000	3.112289000	0.980428000
N	2.027380000	-0.754472000	-1.168375000
C	-3.823580000	-1.566382000	2.441039000
H	-4.346657000	-1.799974000	3.356997000
C	-0.929829000	1.392093000	-5.423215000
C	-0.649726000	0.066507000	-4.828350000
C	-1.707450000	2.507691000	-1.020691000
H	-2.162239000	1.897596000	-1.790091000
C	-4.420621000	-1.309032000	1.181847000
H	-5.478105000	-1.320453000	0.950051000
C	-1.035051000	-3.921627000	2.188525000
H	-1.767556000	-3.628376000	1.445149000
C	-2.655007000	-2.224778000	5.283957000
H	-3.069800000	-3.030536000	4.686996000
C	-3.384954000	-1.019252000	0.312639000
H	-3.436314000	-0.753677000	-0.737609000
C	-0.179895000	-2.434569000	-1.301788000

C	-0.269487000	-1.145660000	-5.585432000
C	2.225645000	3.577435000	-0.335367000
H	1.312639000	3.694897000	-0.910181000
C	-1.245235000	-3.348860000	-1.365658000
H	-2.234550000	-3.033791000	-1.036856000
C	-1.200357000	4.122973000	0.441566000
H	-1.214294000	5.045267000	1.004068000
C	0.701396000	3.780532000	2.855282000
C	1.076745000	-2.899314000	-1.756385000
C	-1.676944000	1.459321000	2.928909000
H	-1.821164000	2.275976000	2.221573000
H	-1.620079000	1.859560000	3.942772000
H	-2.504373000	0.753759000	2.856223000
C	-2.056238000	3.787325000	-0.635018000
H	-2.841211000	4.400545000	-1.058893000
C	0.277447000	-3.410239000	4.137966000
H	0.557107000	-2.724525000	4.933338000
C	-1.509771000	-0.252748000	6.867509000
H	-1.039691000	0.510757000	7.481746000
C	-1.126282000	-0.394324000	5.532179000
H	-0.346184000	0.250288000	5.138939000
C	-1.446006000	1.488950000	-6.725453000
H	-1.633074000	0.586107000	-7.298066000
C	2.196387000	-1.936997000	-1.811831000
C	-2.480520000	-1.087726000	7.410144000
H	-2.782661000	-0.978360000	8.447951000
C	0.766616000	5.165442000	2.640999000
H	0.849503000	5.544548000	1.627679000
C	0.688383000	3.325336000	4.176594000
H	0.699336000	2.258984000	4.381019000
C	-0.464546000	-5.195412000	2.144348000
H	-0.761663000	-5.883624000	1.358205000
C	0.684928000	4.218578000	5.249629000
H	0.671455000	3.834105000	6.265995000
C	1.259546000	-4.231232000	-2.171194000
H	2.240580000	-4.599500000	-2.460626000
C	4.374347000	-1.218589000	-2.588709000
H	5.284394000	-1.408173000	-3.151481000
C	-3.045729000	-2.082299000	6.611087000
H	-3.785744000	-2.760813000	7.026986000
C	0.755059000	6.058869000	3.707095000
H	0.798931000	7.126765000	3.510624000
C	0.480452000	-5.578251000	3.091730000
H	0.921747000	-6.570804000	3.057733000
C	2.993252000	0.174011000	-1.240019000
H	2.799365000	1.110583000	-0.725380000
C	3.329348000	2.992623000	1.720208000
H	3.282617000	2.677532000	2.759176000
C	0.483421000	-1.033423000	-6.765682000
H	0.781967000	-0.052102000	-7.121030000
C	-1.081538000	-4.661789000	-1.813064000
H	-1.932272000	-5.339834000	-1.845063000
C	0.705451000	5.590148000	5.020164000
H	0.700034000	6.287526000	5.853119000
C	4.183637000	-0.005570000	-1.930660000
H	4.923241000	0.786809000	-1.950457000
C	3.377017000	-2.180165000	-2.533604000
H	3.495277000	-3.111890000	-3.073250000
C	-0.619891000	-2.424229000	-5.125140000
H	-1.191171000	-2.535308000	-4.207836000
C	3.461709000	3.898956000	-0.902800000
H	3.500648000	4.268697000	-1.924174000
C	-1.734632000	2.733135000	-7.278634000
H	-2.135203000	2.788214000	-8.287215000
C	-0.232886000	-3.557908000	-5.833103000

H	-0.510921000	-4.537525000	-5.456082000
C	0.850354000	-4.678013000	4.092154000
H	1.578851000	-4.966660000	4.845521000
C	4.634680000	3.752217000	-0.166943000
H	5.595399000	4.006640000	-0.606644000
C	-0.729185000	2.571212000	-4.687584000
H	-0.347096000	2.521267000	-3.671674000
C	0.500324000	-3.438486000	-7.013001000
H	0.793437000	-4.325238000	-7.567967000
C	0.183326000	-5.110050000	-2.198898000
H	0.330966000	-6.138688000	-2.517789000
C	4.562714000	3.296118000	1.150912000
H	5.468108000	3.194441000	1.743466000
C	0.857150000	-2.171588000	-7.474029000
H	1.437836000	-2.066169000	-8.386500000
C	-1.528418000	3.899286000	-6.542834000
H	-1.758785000	4.868288000	-6.976233000
C	-1.031512000	3.810363000	-5.242971000
H	-0.875390000	4.709364000	-4.653473000

TS2

Y	7.354196000	3.887387000	4.606530000
N	7.010278000	4.902028000	7.237231000
N	6.926806000	6.165465000	4.391425000
N	5.382806000	3.049483000	5.511656000
C	8.174488000	5.523799000	6.783965000
C	9.146319000	4.535771000	6.685994000
H	10.167398000	4.693532000	6.377220000
N	6.998686000	3.500612000	2.410723000
C	8.568003000	3.301338000	7.088227000
H	9.058650000	2.340502000	7.136947000
C	6.803097000	1.125271000	7.803726000
N	6.958434000	3.317314000	1.213783000
C	6.165966000	2.540266000	7.836406000
C	5.048698000	2.690648000	6.802376000
C	7.145155000	7.177986000	5.311025000
C	7.246424000	3.543758000	7.442194000
C	8.235922000	6.991047000	6.363231000
C	5.661598000	2.754058000	9.278155000
C	9.639198000	7.291963000	5.770544000
N	9.679896000	3.378011000	3.664690000
C	3.672305000	2.529753000	6.905766000
H	3.109361000	2.281013000	7.793664000
C	6.576685000	5.118594000	-0.356208000
C	6.823207000	3.693841000	-0.016295000
C	5.919748000	6.610644000	3.564139000
H	5.561326000	5.993790000	2.750618000
C	3.132379000	2.794367000	5.622338000
H	2.087153000	2.775120000	5.340963000
C	6.474479000	0.198736000	6.813177000
H	5.759928000	0.474697000	6.045455000
C	4.704061000	1.871884000	9.800963000
H	4.335611000	1.059999000	9.182231000
C	4.203504000	3.107497000	4.806642000
H	4.198546000	3.392463000	3.760491000
C	7.419097000	1.737588000	3.225544000
C	6.933457000	2.648158000	-1.060593000
C	9.791184000	7.723960000	4.449623000
H	8.911399000	7.814258000	3.820813000
C	6.345178000	0.845093000	3.183263000
H	5.331448000	1.221385000	3.296366000
C	6.285332000	8.238605000	5.059488000
H	6.204269000	9.157540000	5.622175000
C	8.086018000	7.946710000	7.565262000
C	8.728487000	1.247202000	3.060375000

C	5.741138000	5.584214000	7.507610000
H	5.613592000	6.389412000	6.783759000
H	5.748565000	5.999547000	8.516994000
H	4.929646000	4.863724000	7.409658000
C	5.500048000	7.871718000	3.937604000
H	4.720410000	8.458835000	3.469687000
C	7.720608000	0.747982000	8.795589000
H	7.967710000	1.446877000	9.590271000
C	5.728297000	3.861263000	11.444506000
H	6.151099000	4.632238000	12.083235000
C	6.182594000	3.730725000	10.130472000
H	6.968518000	4.392090000	9.778971000
C	5.710707000	5.467063000	-1.406336000
H	5.219724000	4.683102000	-1.975285000
C	9.857887000	2.193711000	3.034438000
C	4.747243000	3.006423000	11.935123000
H	4.390053000	3.107299000	12.956140000
C	8.125738000	9.332265000	7.350161000
H	8.244676000	9.711381000	6.340339000
C	8.019612000	7.491957000	8.885043000
H	8.046340000	6.426014000	9.091245000
C	7.052947000	-1.072427000	6.808555000
H	6.781210000	-1.777603000	6.028373000
C	7.941897000	8.386025000	9.954578000
H	7.888127000	8.002838000	10.970095000
C	8.938309000	-0.133360000	2.901628000
H	9.948350000	-0.527694000	2.822170000
C	12.066710000	2.862518000	2.325702000
H	12.991498000	2.657192000	1.793884000
C	4.242877000	2.003430000	11.106435000
H	3.495428000	1.310024000	11.482516000
C	8.040785000	10.226150000	8.412608000
H	8.066450000	11.294640000	8.216289000
C	7.970760000	-1.434083000	7.790267000
H	8.417273000	-2.424860000	7.787113000
C	10.661841000	4.290790000	3.620188000
H	10.466632000	5.234962000	4.120551000
C	10.782839000	7.206020000	6.579074000
H	10.680544000	6.915993000	7.621390000
C	7.369615000	2.953453000	-2.360094000
H	7.616188000	3.979727000	-2.614771000
C	6.559693000	-0.521631000	3.010323000
H	5.714841000	-1.206034000	2.988225000
C	7.939882000	9.757455000	9.722809000
H	7.876697000	10.455405000	10.552885000
C	11.871066000	4.081791000	2.969746000
H	12.624556000	4.861383000	2.968360000
C	11.051349000	1.916767000	2.352832000
H	11.160529000	0.978162000	1.821889000
C	6.643927000	1.307188000	-0.756899000
H	6.305088000	1.055599000	0.244348000
C	11.054030000	8.046330000	3.944841000
H	11.146814000	8.390972000	2.918175000
C	5.468631000	6.802725000	-1.713982000
H	4.789125000	7.051554000	-2.524930000
C	6.785129000	0.310864000	-1.716216000
H	6.550537000	-0.718534000	-1.457579000
C	8.304028000	-0.515600000	8.786974000
H	9.009875000	-0.787746000	9.567491000
C	12.184908000	7.933405000	4.749470000
H	13.166067000	8.188994000	4.358274000
C	7.182677000	6.147686000	0.377960000
H	7.845326000	5.898280000	1.201505000
C	7.213049000	0.627667000	-3.006378000
H	7.316097000	-0.150477000	-3.757650000

C	7.861277000	-1.011406000	2.874104000
H	8.035991000	-2.076456000	2.750022000
C	12.043229000	7.510669000	6.072775000
H	12.914458000	7.436199000	6.718244000
C	7.505113000	1.953682000	-3.320527000
H	7.848488000	2.214217000	-4.318415000
C	6.084392000	7.817199000	-0.980825000
H	5.893354000	8.859503000	-1.220622000
C	6.939139000	7.483222000	0.068424000
H	7.411966000	8.264174000	0.656812000

3

Y	7.407166000	3.888210000	4.306091000
N	6.836818000	4.916225000	6.869834000
N	6.375299000	5.935604000	6.053865000
N	5.827395000	2.497835000	5.232286000
C	7.825694000	5.777027000	6.388039000
C	9.007070000	5.049324000	6.345063000
H	9.963614000	5.437583000	6.034242000
N	7.298457000	2.851072000	2.231983000
C	8.737120000	3.732941000	6.803754000
H	9.442999000	2.922080000	6.904047000
C	7.558371000	1.242029000	7.684386000
N	6.167495000	2.992184000	1.445800000
C	6.589664000	2.454920000	7.608211000
C	5.508007000	2.240920000	6.552670000
C	6.440699000	7.071134000	4.842668000
C	7.392396000	3.667110000	7.145966000
C	7.563490000	7.190504000	5.870227000
C	6.015163000	2.636023000	9.026591000
C	8.877950000	7.704094000	5.222692000
N	9.712476000	3.473043000	3.544723000
C	4.204644000	1.772036000	6.637404000
H	3.664025000	1.507096000	7.534466000
C	7.308560000	4.853290000	0.274036000
C	6.145829000	3.973336000	0.598994000
C	5.258424000	6.081573000	3.260677000
H	4.968228000	5.307804000	2.561841000
C	3.698449000	1.728666000	5.313062000
H	2.709458000	1.411024000	5.007984000
C	7.489369000	0.191097000	6.767506000
H	6.754099000	0.223541000	5.970585000
C	5.255882000	1.600678000	9.591729000
H	5.079374000	0.696857000	9.017877000
C	4.713587000	2.173971000	4.489688000
H	4.727794000	2.271779000	3.410291000
C	7.650125000	1.533518000	2.445102000
C	4.875836000	4.172506000	-0.144942000
C	9.013119000	7.824909000	3.836895000
H	8.180461000	7.559232000	3.193773000
C	6.818484000	0.445270000	2.063919000
H	5.886659000	0.679048000	1.564401000
C	5.383926000	7.917215000	4.540172000
H	5.154534000	8.862672000	5.010101000
C	7.208529000	8.176337000	6.999909000
C	8.927791000	1.213780000	3.019998000
C	5.435083000	5.277405000	7.102519000
H	5.150002000	6.056788000	6.396365000
H	5.307212000	5.641587000	8.123500000
H	4.818122000	4.390837000	6.951183000
C	4.627898000	7.281120000	3.522904000
H	3.724121000	7.651185000	3.056195000
C	8.515707000	1.176683000	8.707864000
H	8.566690000	1.972897000	9.445749000
C	5.809261000	3.846766000	11.128264000

H	6.049849000	4.721962000	11.725999000
C	6.304772000	3.744503000	9.826757000
H	6.943708000	4.535099000	9.444303000
C	7.181753000	6.248715000	0.284601000
H	6.245550000	6.697531000	0.602842000
C	10.000352000	2.208518000	3.149437000
C	5.020027000	2.832026000	11.658991000
H	4.630624000	2.909899000	12.670183000
C	7.011094000	9.529293000	6.685545000
H	7.108308000	9.855624000	5.654762000
C	7.153933000	7.801620000	8.344370000
H	7.357448000	6.773649000	8.628114000
C	8.356776000	-0.898863000	6.871626000
H	8.280639000	-1.705787000	6.148770000
C	6.863996000	8.734375000	9.342356000
H	6.826074000	8.414079000	10.380101000
C	9.241293000	-0.137065000	3.282545000
H	10.192285000	-0.361267000	3.758550000
C	12.319495000	2.830730000	2.821825000
H	13.336064000	2.570447000	2.539998000
C	4.753487000	1.702258000	10.884762000
H	4.162267000	0.887747000	11.294543000
C	6.715327000	10.459953000	7.675968000
H	6.560334000	11.500605000	7.404164000
C	9.309384000	-0.950719000	7.884917000
H	9.980467000	-1.801789000	7.965792000
C	10.678358000	4.410294000	3.520056000
H	10.376803000	5.418597000	3.790627000
C	9.962641000	8.070102000	6.033747000
H	9.866309000	8.009432000	7.114415000
C	4.859863000	4.797347000	-1.401709000
H	5.787585000	5.161321000	-1.831820000
C	7.166698000	-0.861837000	2.332809000

H	6.484754000	-1.659948000	2.049569000
C	6.632507000	10.065369000	9.011859000
H	6.404723000	10.792422000	9.786243000
C	11.990551000	4.142712000	3.171879000
H	12.726692000	4.938903000	3.173867000
C	11.322605000	1.871275000	2.796334000
H	11.536198000	0.863843000	2.458409000
C	3.661381000	3.702348000	0.382852000
H	3.665253000	3.225326000	1.357145000
C	10.205380000	8.290648000	3.275369000
H	10.283734000	8.377403000	2.195355000
C	8.248875000	7.060810000	-0.099280000
H	8.131240000	8.141249000	-0.089751000
C	2.473987000	3.850426000	-0.324588000
H	1.544280000	3.487293000	0.105238000
C	9.387625000	0.096230000	8.804644000
H	10.118930000	0.065225000	9.608234000
C	11.280224000	8.638798000	4.089081000
H	12.204445000	9.006996000	3.651706000
C	8.526772000	4.288271000	-0.131595000
H	8.630397000	3.208167000	-0.151025000
C	2.471593000	4.470814000	-1.574859000
H	1.542023000	4.590383000	-2.124698000
C	8.379381000	-1.170018000	2.969501000
H	8.645490000	-2.198394000	3.193295000
C	11.153279000	8.526507000	5.474891000
H	11.978620000	8.807764000	6.123748000
C	3.669325000	4.940993000	-2.109920000
H	3.679766000	5.421418000	-3.084599000
C	9.452047000	6.489241000	-0.509994000
H	10.277523000	7.120905000	-0.827941000
C	9.587146000	5.099702000	-0.524815000
H	10.518232000	4.646194000	-0.854025000

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Y	-0.074179000	-0.290426000	-0.532096000
N	-1.553031000	1.311057000	1.189256000
C	-2.367958000	-0.765050000	0.994468000
H	-2.587075000	-1.802540000	1.190394000
C	-2.395254000	2.447598000	-0.976940000
N	0.029289000	1.901667000	-1.315341000
C	-1.610411000	0.063324000	1.811276000
C	-2.306199000	1.283813000	0.008322000
N	1.099142000	-0.322314000	1.517617000
C	-2.809013000	-0.002705000	-0.119323000
H	-3.411294000	-0.355974000	-0.940977000
O	6.063212000	-1.680236000	-0.041973000
C	-1.111103000	-1.771871000	3.446175000
N	2.132871000	-1.226110000	-1.584343000
C	-1.368398000	0.508235000	4.307774000
C	-0.851310000	-0.284133000	3.087225000
C	-2.403483000	-2.192670000	3.795997000
H	-3.223375000	-1.479723000	3.777433000
C	-3.115972000	1.948648000	-2.257490000
C	-0.958781000	2.871016000	-1.266823000
C	0.622739000	-0.022679000	2.780406000
C	-3.239237000	3.614823000	-0.426941000
C	-2.506578000	1.317485000	4.254020000
H	-3.042576000	1.433727000	3.316760000
C	-0.875277000	2.487990000	1.741354000
H	-0.560518000	3.132301000	0.921046000
H	-0.006930000	2.154324000	2.310110000
H	-1.553583000	3.035675000	2.398346000
C	-0.757965000	0.321347000	5.556820000
H	0.078947000	-0.363705000	5.642910000
C	0.991074000	3.934272000	-1.629341000
H	1.738278000	4.699621000	-1.796243000
C	1.189208000	-3.663212000	-0.047509000
C	1.211104000	2.575213000	-1.533145000
H	2.149684000	2.043135000	-1.611074000

C	1.645642000	0.494091000	3.566857000
H	1.571186000	0.844186000	4.585977000
C	2.516602000	-3.313215000	-0.336478000
C	-2.436933000	1.810007000	-3.470211000
H	-1.378349000	2.044744000	-3.513100000
C	2.808318000	0.515082000	2.759403000
H	3.789926000	0.872039000	3.045210000
C	-0.402348000	4.127378000	-1.457134000
H	-0.920915000	5.075203000	-1.442447000
C	2.433254000	0.011619000	1.526836000
H	3.041420000	-0.115851000	0.640661000
C	-2.647693000	-3.503128000	4.193516000
H	-3.657298000	-3.805640000	4.458665000
C	-0.068176000	-2.695949000	3.521007000
H	0.936824000	-2.383786000	3.257219000
C	-3.860092000	3.579557000	0.823683000
H	-3.749039000	2.704864000	1.456958000
C	-1.229428000	0.972822000	6.691819000
H	-0.731816000	0.814407000	7.644862000
C	0.921268000	-4.768934000	0.751014000
H	-0.107091000	-5.043023000	0.962317000
C	-2.344179000	1.808097000	6.614758000
H	-2.715062000	2.313779000	7.501856000
C	-3.469770000	4.731789000	-1.244013000
H	-3.047774000	4.753963000	-2.243898000
C	-4.489142000	1.665770000	-2.224397000
H	-5.041665000	1.801059000	-1.298255000
C	-2.988810000	1.965917000	5.392533000
H	-3.874954000	2.590624000	5.317944000
C	-3.110007000	1.388065000	-4.618891000
H	-2.564315000	1.293168000	-5.553989000
C	-4.247894000	5.796064000	-0.801237000
H	-4.405668000	6.651697000	-1.452388000
C	-4.469845000	1.094616000	-4.571911000
H	-4.992397000	0.767065000	-5.466389000

H	12.766729000	3.252186000	14.175779000
C	9.483003000	-0.776609000	13.454245000
H	9.945563000	-1.660774000	13.884048000
C	14.865428000	1.555195000	12.603465000
H	15.086398000	1.696904000	11.541131000
H	15.047158000	0.496928000	12.855002000
C	15.646932000	2.473073000	13.534929000
H	16.661543000	2.119161000	13.738614000
H	15.713550000	3.476910000	13.101140000
C	14.744765000	2.476105000	14.775006000
H	14.841199000	3.386272000	15.372473000
H	14.991232000	1.627478000	15.422048000
C	6.954359000	2.809693000	10.107842000
H	7.645683000	2.153877000	11.327883000
H	5.906442000	3.077379000	10.312270000
Si	6.897647000	1.345023000	8.920284000
C	5.839588000	-0.054846000	9.651553000
H	6.277706000	-0.437410000	10.578568000
H	4.825531000	0.296059000	9.873752000
H	5.756152000	-0.890798000	8.948517000
C	6.120928000	1.858870000	7.259128000
H	6.061954000	1.011758000	6.566011000
H	5.108225000	2.247938000	7.406479000
H	6.712815000	2.644584000	6.776309000
C	8.637806000	0.673746000	8.551650000
H	9.096292000	0.244867000	9.448103000
H	8.597241000	-0.110439000	7.787529000
H	9.295440000	1.467470000	8.180906000
H	7.366331000	3.649283000	9.523248000
C	10.460072000	2.197215000	11.428680000
H	11.466920000	1.858479000	11.170571000
C	10.905870000	4.060859000	10.124457000
C	12.275528000	4.180743000	10.384600000
C	10.381712000	4.664084000	8.971382000
H	12.698931000	3.724074000	11.276141000
H	9.321677000	4.577222000	8.757057000
C	13.107940000	4.882083000	9.513266000
C	11.206859000	5.350162000	8.095089000
H	14.162518000	4.968698000	9.749583000
H	10.808388000	5.810643000	7.196897000
C	12.578144000	5.468713000	8.359483000
O	13.298291000	6.168286000	7.446464000
C	14.684519000	6.324177000	7.670028000
H	14.886421000	6.865368000	8.603566000
H	15.202690000	5.356546000	7.695571000
H	15.062028000	6.908867000	6.829884000

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Y	-0.744852000	12.715560000	16.361957000
N	-0.532622000	11.593296000	13.709320000
O	0.883864000	14.492587000	17.230394000
N	-2.658507000	11.449937000	15.907669000
N	-0.966081000	14.392323000	14.724664000
C	-0.467419000	10.492729000	14.560787000
C	2.153134000	14.326354000	13.584015000
C	-0.388155000	14.544857000	13.478955000
C	0.821308000	13.684726000	13.111252000
C	0.741444000	10.570752000	15.237997000
H	1.093116000	9.855037000	15.964925000
C	1.421355000	11.735488000	14.785125000
H	2.400666000	12.074000000	15.086250000
N	0.299680000	11.636757000	18.489634000
C	0.623822000	12.355648000	13.830640000
C	0.988023000	13.511418000	11.582969000
C	-2.835142000	10.353444000	15.082811000
C	-1.273220000	8.524067000	15.891982000
C	2.177299000	15.591328000	14.173517000
H	1.236630000	16.109495000	14.331616000
C	-4.174412000	10.209809000	14.756508000
H	-4.611271000	9.460580000	14.111650000
C	-1.615312000	9.507662000	14.738595000
C	-4.866587000	11.258982000	15.413041000
H	-5.930708000	11.456338000	15.379959000
C	-1.835075000	8.623819000	13.492631000
C	-0.264436000	7.564356000	15.724763000

H	0.301666000	7.538970000	14.797182000
C	-2.015796000	8.509972000	17.075716000
H	-2.805677000	9.241040000	17.213369000
C	-3.913990000	11.983407000	16.102159000
H	-4.050292000	12.848269000	16.737161000
C	3.375944000	13.684716000	13.335948000
H	3.382102000	12.722903000	12.829848000
C	1.250533000	14.642362000	10.794692000
H	1.324495000	15.615869000	11.268426000
C	-1.684985000	11.930198000	12.863335000
H	-2.460873000	12.415168000	13.458408000
H	-2.080991000	11.017177000	12.422819000
H	-1.359772000	12.605275000	12.077268000
C	-1.051430000	15.534385000	12.764889000
H	-0.847553000	15.856922000	11.753860000
C	0.981540000	12.264245000	10.951672000
H	0.823632000	11.363062000	11.535679000
C	-1.015864000	8.683919000	12.361843000
H	-0.196139000	9.395383000	12.326667000
C	1.298278000	10.644767000	18.682712000
C	-0.003815000	6.619117000	16.712777000
H	0.778276000	5.880412000	16.558141000
C	1.445051000	14.533140000	9.421996000
H	1.639480000	15.427586000	8.836214000
C	-2.842278000	7.647347000	13.521664000
H	-3.451937000	7.540984000	14.413082000
C	1.407569000	13.283984000	8.801613000
H	1.563589000	13.197328000	7.729972000
C	-1.993775000	15.302347000	14.782000000
H	-2.624426000	15.372478000	15.660222000
C	4.595072000	15.538034000	14.295013000
H	5.537080000	16.010191000	14.560728000
C	-2.081563000	16.023445000	13.605679000
H	-2.806420000	16.791813000	13.367939000
C	-1.426721000	12.981315000	19.570503000
C	4.583111000	14.275126000	13.700285000
H	5.517716000	13.758781000	13.496710000
C	-0.759750000	6.604949000	17.885331000
H	-0.571529000	5.854451000	18.648498000
C	3.388392000	16.196251000	14.518283000
H	3.384585000	17.194023000	14.950344000
C	1.184552000	12.149902000	9.574984000
H	1.170100000	11.166643000	9.112372000
C	-1.893313000	13.562701000	18.359832000
O	4.229695000	7.747439000	19.347481000
C	-0.343839000	12.017810000	19.551257000
H	-0.044325000	11.601606000	20.521821000
C	-1.763943000	7.553131000	18.061261000
H	-2.368732000	7.546611000	18.964812000
C	-1.966192000	13.297834000	20.833573000
H	-1.575670000	12.815625000	21.729034000
C	1.073113000	9.516764000	19.490249000
H	0.091994000	9.357971000	19.926200000
C	-1.220504000	7.831322000	11.274660000
H	-0.569077000	7.903471000	10.407698000
C	-2.996188000	14.222376000	20.936555000
H	-3.420282000	14.471945000	21.905104000
C	0.391306000	15.838228000	17.426060000
H	0.525398000	16.403398000	16.497779000
H	-0.672324000	15.767398000	17.654889000
C	-2.934695000	14.491136000	18.526302000
H	-3.362583000	14.986210000	17.653814000
C	2.068293000	8.574109000	19.691438000
H	1.888610000	7.694615000	20.301205000
C	2.545185000	10.770912000	18.065131000
H	2.740745000	11.628134000	17.431086000
C	3.322910000	8.724427000	19.087300000
C	-2.246566000	6.892970000	11.303294000
H	-2.409126000	6.229789000	10.458242000
C	-3.053614000	6.801635000	12.438056000
H	-3.845406000	6.058760000	12.485279000
C	-3.479505000	14.821675000	19.771951000
H	-4.288834000	15.546399000	19.835075000
C	3.555689000	9.831106000	18.265205000
H	4.513021000	9.975246000	17.777000000

C	2.234597000	14.394511000	17.729758000
H	2.888951000	14.078262000	16.910529000
H	2.244492000	13.637010000	18.519731000
C	2.600167000	15.779280000	18.264393000
H	3.253058000	15.721472000	19.139621000
H	3.115307000	16.358091000	17.491703000
C	1.231028000	16.392469000	18.563665000
H	0.845001000	16.036269000	19.524933000
H	1.241975000	17.485729000	18.579839000
C	5.498364000	7.839902000	18.732958000
H	5.420310000	7.825149000	17.637945000
H	6.059126000	6.964121000	19.062826000
H	6.034724000	8.746492000	19.042698000

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Y	-0.676100000	-0.481871000	-0.046820000
N	-0.848961000	0.786277000	2.563247000
N	-1.421067000	1.725112000	-0.353936000
N	-2.512299000	-1.231911000	1.179373000
C	0.153708000	1.502558000	1.917877000
C	1.220812000	0.635913000	1.727399000
H	2.158137000	0.891172000	1.258665000
N	-0.619775000	0.003825000	-2.505921000
C	0.858503000	-0.629496000	2.265591000
H	1.468842000	-1.519664000	2.288840000
C	-0.560367000	-2.973908000	3.180403000
N	-0.559234000	0.145912000	-3.648135000
C	-1.321303000	-1.630752000	3.341263000
C	-2.599990000	-1.601373000	2.506432000
C	-1.246230000	2.846168000	0.437549000
C	-0.427472000	-0.524592000	2.782672000
C	-0.035603000	2.913849000	1.369747000
C	-1.611889000	-1.448201000	4.842737000
C	1.246019000	3.324920000	0.594512000
N	1.574343000	-1.550400000	-0.800323000
C	-3.925795000	-1.838029000	2.846884000
H	-4.309300000	-2.110921000	3.819541000
C	-0.575050000	1.686178000	-5.447670000
C	-0.504180000	0.301621000	-4.934219000
C	-2.544536000	1.963232000	-1.112624000
H	-2.902838000	1.223368000	-1.819228000
C	-4.692797000	-1.602461000	1.678397000
H	-5.768633000	-1.674355000	1.581282000
C	-0.924801000	-3.903113000	2.202625000
H	-1.762778000	3.687012000	1.547964000
C	-2.356284000	-2.428481000	5.516132000
H	-2.712632000	-3.295046000	4.967750000
C	-3.795687000	-1.234356000	0.693179000
H	-4.004032000	-0.936320000	-0.327827000
C	-1.051436000	-2.530423000	-1.395389000
C	-0.380288000	-0.915244000	-5.763459000
C	1.218916000	3.574479000	-0.780121000
H	0.284638000	3.451427000	-1.318264000
C	-2.254312000	-3.161826000	-1.752137000
H	-3.203351000	-2.681930000	-1.522715000
C	-2.254651000	3.767072000	0.180023000
H	-2.399513000	4.723965000	0.660360000
C	-0.191878000	3.964869000	2.487975000
C	0.122285000	-3.261329000	-1.711792000
C	-2.140827000	1.341777000	2.971953000
H	-2.465936000	2.062872000	2.221649000
H	-2.043059000	1.839023000	3.938947000
H	-2.866625000	0.533235000	3.044759000
C	-3.087066000	3.197779000	-0.815236000
H	-3.975964000	3.637271000	-1.249318000
C	0.515379000	-3.279846000	4.026742000
H	0.795871000	-2.579932000	4.809298000
C	-1.367264000	-0.270368000	6.957219000
H	-0.961121000	0.570442000	7.513393000
C	-1.105296000	-0.382293000	5.590073000
H	-0.482772000	0.366742000	5.110005000
C	-1.173929000	1.947661000	-6.690254000
H	-1.577473000	1.126964000	-7.274845000
C	-2.136871000	-1.231206000	7.604522000
H	-2.343609000	-1.145299000	8.667666000

C	-0.373814000	5.313057000	2.145771000
H	-0.420139000	5.594808000	1.098861000
C	-0.042698000	3.649772000	3.841478000
H	0.162244000	2.624939000	4.136930000
C	-0.226258000	-5.105452000	2.068195000
H	-0.531813000	-5.815155000	1.304304000
C	-0.127879000	4.634848000	4.827190000
H	-0.011393000	4.358684000	5.871838000
C	0.099200000	-4.528192000	-2.325590000
H	1.031681000	-5.048159000	-2.540970000
C	-2.625374000	-2.316623000	6.876092000
H	-3.209961000	-3.087080000	7.371765000
C	-0.466822000	6.296531000	3.125195000
H	-0.615226000	7.332192000	2.831295000
C	0.846866000	-5.395420000	2.906491000
H	1.384730000	-6.334542000	2.805897000
C	2.450704000	3.524448000	1.283771000
H	2.484125000	3.368582000	2.358624000
C	0.298203000	-0.862494000	-6.992193000
H	0.727343000	0.075781000	-7.329420000
C	-2.297214000	-4.420381000	-2.362869000
H	-3.257744000	-4.869401000	-2.608418000
C	-0.353235000	5.961374000	4.474699000
H	-0.422809000	6.729638000	5.239692000
C	-0.901067000	-2.144553000	-5.329881000
H	-1.427045000	-2.212004000	-4.381347000
C	2.367692000	4.003864000	-1.449835000
H	2.323626000	4.204863000	-2.517352000
C	-1.266300000	3.251931000	-7.166995000
H	-1.734577000	3.435711000	-8.130075000
C	-0.750649000	-3.286731000	-6.110179000
H	-1.159383000	-4.227187000	-5.753074000
C	1.215887000	-4.475267000	3.889430000
H	2.042314000	-4.694499000	4.560783000
C	3.561353000	4.188184000	-0.756924000
H	4.451491000	4.532187000	-1.276964000
C	-0.086662000	2.764416000	-4.694089000
H	0.380005000	2.580195000	-3.730647000
C	-0.089666000	-3.224202000	-7.336206000
H	0.019023000	-4.116332000	-7.946411000
C	-1.117549000	-5.112487000	-2.650995000
H	-1.151900000	-6.093257000	-3.117723000
C	3.597980000	3.944082000	0.616781000
H	4.518936000	4.094446000	1.173698000
C	0.433459000	-2.007199000	-7.771778000
H	0.960685000	-1.947765000	-8.720077000
C	-0.778977000	4.317403000	-6.411320000
H	-0.858230000	5.334587000	-6.783678000
C	-0.194300000	4.066889000	-5.170487000
H	0.183129000	4.889695000	-4.569910000
C	1.415306000	-2.695276000	-1.386914000
H	2.305048000	-3.270925000	-1.671866000
C	2.912547000	-1.164435000	-0.525226000
C	3.793116000	-2.015933000	0.147450000
C	3.370832000	0.101319000	-0.921288000
H	3.439436000	-2.983220000	0.494694000
H	2.697226000	0.781642000	-1.433784000
C	5.109466000	-1.632612000	0.408979000
C	4.679349000	0.484699000	-0.675143000
H	5.761145000	-2.315285000	0.942595000
H	5.038168000	1.460231000	-0.984354000
C	5.561560000	-0.378503000	-0.009018000
O	6.818875000	0.097276000	0.186859000
C	7.746680000	-0.735758000	0.850690000
H	7.423038000	-0.970359000	1.873352000
H	7.914648000	-1.672891000	0.303851000
H	8.681436000	-0.174670000	0.892546000

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Y	7.363935000	3.852072000	4.609822000
N	7.057199000	4.981163000	7.239525000
N	6.772767000	6.071471000	4.294256000
N	5.454748000	3.060024000	5.668579000
C	8.119454000	5.695507000	6.691525000
C	9.177495000	4.808949000	6.545440000

H	10.149889000	5.060584000	6.151012000
N	7.060026000	3.508254000	2.402508000
C	8.751397000	3.536596000	7.018336000
H	9.338088000	2.631110000	7.050316000
C	7.209865000	1.197898000	7.774162000
N	7.044475000	3.335646000	1.202080000
C	6.473466000	2.557341000	7.901994000
C	5.263794000	2.642876000	6.971353000
C	6.870823000	7.136714000	5.175492000
C	7.435034000	3.655037000	7.448027000
C	8.002041000	7.135544000	6.202843000
C	6.070444000	2.706521000	9.382482000
C	9.345317000	7.567138000	5.551321000
N	9.633072000	2.780554000	3.932159000
C	3.912084000	2.422829000	7.203225000
H	3.451805000	2.122624000	8.133568000
C	7.106132000	5.222812000	-0.311612000
C	7.053464000	3.769567000	-0.017215000
C	5.717251000	6.362739000	3.457114000
H	5.444679000	5.683518000	2.659984000
C	3.237071000	2.719306000	5.992219000
H	2.169726000	2.677341000	5.816079000
C	6.859214000	0.267478000	6.793252000
H	6.054597000	0.499782000	6.103078000
C	5.250668000	1.729322000	9.966728000
H	4.915524000	0.888672000	9.367214000
C	4.209797000	3.106146000	5.089918000
H	4.085252000	3.451484000	4.070066000
C	7.045510000	1.694208000	3.194890000
C	7.008842000	2.750656000	-1.093775000
C	9.421994000	7.899013000	4.196142000
H	8.534304000	7.801522000	3.579748000
C	5.847126000	1.019377000	2.961544000
H	4.907907000	1.564777000	2.978370000
C	5.883809000	8.071956000	4.895378000
H	5.692567000	8.994341000	5.424526000
C	7.776969000	8.130260000	7.360224000
C	8.246332000	0.957116000	3.161604000
C	5.755854000	5.559571000	7.582439000
H	5.496134000	6.305814000	6.830786000
H	5.807434000	6.034795000	8.563751000
H	5.007474000	4.768754000	7.592994000
C	5.145497000	7.572822000	3.792963000
H	4.300874000	8.045964000	3.308860000
C	8.238270000	0.870914000	8.670453000
H	8.501860000	1.570745000	9.459015000
C	6.185463000	3.812929000	11.546053000
H	6.571295000	4.624364000	12.157505000
C	6.547878000	3.733745000	10.199757000
H	7.226432000	4.477411000	9.793279000
C	6.464075000	5.747474000	-1.446254000
H	5.930238000	5.078898000	-2.114646000
C	5.342048000	2.857335000	12.102617000
H	5.057014000	2.917969000	13.149216000
C	7.615217000	9.494242000	7.075995000
H	7.628671000	9.828216000	6.043806000
C	7.850510000	7.748088000	8.702876000
H	8.037796000	6.708816000	8.958219000
C	7.525547000	-0.957348000	6.704572000
H	7.231340000	-1.667891000	5.937389000
C	7.710523000	8.683046000	9.730142000
H	7.768205000	8.354949000	10.764634000
C	8.233307000	-0.420897000	2.872419000
H	9.171771000	-0.970959000	2.834200000
C	4.881197000	1.809028000	11.305164000
H	4.239849000	1.041663000	11.730402000
C	7.467786000	10.427990000	8.096602000
H	7.336364000	11.477342000	7.846574000
C	8.554241000	-1.266794000	7.589937000
H	9.067311000	-2.222686000	7.523865000
C	10.493851000	7.720561000	6.341386000
H	10.446994000	7.497649000	7.403913000
C	7.639585000	2.965361000	-2.329721000
H	8.155507000	3.903376000	-2.511453000
C	5.832651000	-0.354805000	2.719673000

H	4.884553000	-0.865196000	2.567367000
C	7.505477000	10.026147000	9.431995000
H	7.393179000	10.755648000	10.229152000
C	6.370731000	1.518163000	-0.880127000
H	5.881613000	1.337514000	0.072930000
C	10.613863000	8.377058000	3.645728000
H	10.648372000	8.644930000	2.592699000
C	6.493061000	7.113133000	-1.712675000
H	5.982520000	7.498246000	-2.591437000
C	6.362731000	0.537339000	-1.865907000
H	5.858884000	-0.407329000	-1.678213000
C	8.909282000	-0.344973000	8.576543000
H	9.699354000	-0.579901000	9.285239000
C	11.747780000	8.526199000	4.439882000
H	12.670586000	8.911543000	4.014217000
C	7.764989000	6.111311000	0.550468000
H	8.249830000	5.730176000	1.443942000
C	6.986847000	0.765071000	-3.092950000
H	6.974723000	0.001056000	-3.865348000
C	7.029401000	-1.077066000	2.657972000
H	7.017174000	-2.141348000	2.441565000
C	11.684000000	8.188420000	5.792617000
H	12.559122000	8.305448000	6.426176000
C	7.626016000	1.983207000	-3.317230000
H	8.125673000	2.170048000	-4.264241000
C	7.163395000	7.984202000	-0.854699000
H	7.185068000	9.050314000	-1.062338000
C	7.796044000	7.475827000	0.278579000
H	8.309685000	8.147480000	0.960209000
C	9.517737000	1.588663000	3.443271000
H	10.421371000	1.008494000	3.223011000
C	10.952872000	3.234910000	4.191129000
C	11.879010000	2.440451000	4.873273000
C	11.342474000	4.515263000	3.770590000
H	11.576950000	1.466252000	5.248537000
H	10.631422000	5.154654000	3.256643000
C	13.177104000	2.891432000	5.112451000
C	12.633678000	4.964217000	3.991981000
H	13.865645000	2.253762000	5.655296000
H	12.939758000	5.951140000	3.664291000
C	13.564349000	4.156559000	4.662010000
O	14.798397000	4.694509000	4.832572000
C	15.775905000	3.918439000	5.495297000
H	15.479406000	3.686885000	6.526736000
H	15.979999000	2.981437000	4.960920000
H	16.682676000	4.524690000	5.512390000

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Y	1.247490000	11.434131000	16.665002000
N	2.453561000	12.925793000	18.724484000
N	-0.207260000	13.148878000	17.253484000
N	1.113432000	9.000697000	16.705718000
N	3.089636000	12.449019000	15.749792000
N	0.589341000	10.785675000	14.503061000
N	-0.044080000	11.720614000	13.686157000
O	-0.257540000	6.069031000	21.262827000
C	3.389938000	11.933083000	18.428694000
C	4.904941000	13.790323000	15.547829000
H	5.835391000	14.299243000	15.754653000
C	1.587926000	10.992350000	19.452186000
H	0.919496000	10.269022000	19.893191000
C	0.337422000	14.139589000	20.880960000
C	1.351737000	12.356588000	19.367371000
C	0.090547000	13.126472000	19.743767000
C	4.274239000	12.845267000	16.343226000
C	2.854139000	10.728294000	18.864835000
H	3.336438000	9.767117000	18.781984000
C	5.704076000	13.004356000	18.449733000
C	-0.391518000	13.799643000	18.461507000
C	2.629005000	14.355261000	18.451450000
H	3.237746000	14.466841000	17.553750000
H	3.127254000	14.839125000	19.293511000
H	1.648428000	14.805873000	18.297947000
C	1.569650000	14.268031000	21.526709000
H	2.408290000	13.651120000	21.218764000

C	4.682004000	12.173770000	17.651105000	H	6.255435000	14.446503000	21.491264000
C	5.341558000	10.791062000	17.389001000	C	7.922916000	13.993384000	18.571894000
C	1.435082000	9.977039000	13.809262000	H	8.880571000	14.197094000	18.100420000
C	-0.961502000	12.122559000	20.289468000	C	2.549570000	9.335032000	11.724424000
C	-1.007796000	15.024949000	18.250968000	H	2.741350000	9.539368000	10.673713000
H	-1.253280000	15.765934000	18.997634000	C	-3.944073000	9.105007000	15.842048000
C	-1.968286000	12.838530000	12.890773000	H	-4.620472000	8.429629000	16.359117000
C	4.078758000	13.983773000	14.410368000	C	6.540944000	8.850602000	18.231778000
H	4.264341000	14.655519000	13.581904000	H	7.006465000	8.328249000	19.063621000
C	-2.136921000	9.462862000	14.277333000	C	3.168406000	8.229049000	12.343600000
H	-1.407378000	9.068118000	13.577375000	H	3.825551000	7.573321000	11.781719000
C	-2.215178000	10.846980000	14.485507000	C	-4.022983000	10.479716000	16.061129000
C	5.365563000	10.223215000	16.112721000	H	-4.761784000	10.882268000	16.748882000
H	4.912352000	10.754933000	15.282927000	C	-3.096077000	10.979674000	20.117259000
C	5.945901000	10.091233000	18.443800000	H	-4.001546000	10.776332000	19.551928000
H	5.962304000	10.530115000	19.437864000	C	-1.749401000	10.690578000	22.090213000
C	-1.216452000	15.144162000	16.854680000	H	-1.597713000	10.264581000	23.078665000
H	-1.662890000	15.980004000	16.331556000	C	-2.915678000	10.411815000	21.375593000
C	-0.738423000	14.898782000	21.365403000	H	-3.681704000	9.770371000	21.803889000
H	-1.722897000	14.766434000	20.928177000	C	-1.537577000	6.197410000	21.847235000
C	1.670078000	7.370246000	18.486795000	H	-2.330856000	5.875664000	21.159626000
H	2.680447000	7.265878000	18.100227000	H	-1.735040000	7.229455000	22.163875000
C	1.691723000	10.158352000	12.416090000	H	-1.537546000	5.545661000	22.722290000
H	1.209755000	10.991413000	11.919862000	C	-3.878964000	13.711142000	11.727231000
C	-1.335214000	11.779817000	13.720678000	H	-4.916644000	13.612761000	11.363392000
C	5.971143000	8.982895000	15.897456000				
H	5.982474000	8.566023000	14.894193000				
C	0.767275000	8.243588000	17.857544000				
C	-0.713837000	13.990924000	16.286931000				
H	-0.661330000	13.728494000	15.240180000				
C	6.954641000	13.277909000	17.875569000				
H	7.175047000	12.905812000	16.880245000				
C	2.044900000	8.829984000	14.435800000				
C	2.989470000	13.150610000	14.567775000				
H	2.139691000	13.002372000	13.912180000				
C	-0.569630000	15.796443000	22.414288000				
H	-1.419129000	16.376877000	22.764077000				
C	1.726703000	8.358232000	15.743037000				
H	1.992083000	7.311110000	15.924709000				
C	-0.894041000	7.678386000	19.538304000				
H	-1.891555000	7.825542000	19.934245000				
C	5.482826000	13.422160000	19.764539000				
H	4.548739000	13.175400000	20.260320000				
C	-2.999176000	8.599500000	14.947836000				
H	-2.936725000	7.529826000	14.767875000				
C	0.009325000	6.805426000	20.152602000				
C	0.676094000	15.939867000	23.026263000				
H	0.807793000	16.638063000	23.848061000				
C	-0.510170000	8.389837000	18.401981000				
H	-1.221249000	9.054696000	17.920018000				
C	-1.216553000	13.942354000	12.453632000				
H	-0.179501000	14.023393000	12.761936000				
C	-3.167638000	11.347619000	15.383451000				
H	-3.229723000	12.419023000	15.552074000				
C	1.741462000	15.162205000	22.585486000				
H	2.712607000	15.241952000	23.066673000				
C	-3.308060000	12.737840000	12.487197000				
H	-3.902863000	11.887305000	12.804406000				
C	-2.125902000	11.826809000	19.576704000				
H	-2.280814000	12.279328000	18.602683000				
C	2.887851000	7.984829000	13.666157000				
H	3.315474000	7.114775000	14.160023000				
C	1.296198000	6.660073000	19.617638000				
H	1.992508000	5.991500000	20.114170000				
C	-0.786332000	11.539637000	21.552954000				
H	0.101574000	11.775475000	22.133319000				
C	6.556094000	8.289707000	16.953612000				
H	7.031852000	7.327384000	16.783714000				
C	-1.790478000	14.914086000	11.642948000				
H	-1.196006000	15.765165000	11.322064000				
C	7.675499000	14.433142000	19.872755000				
H	8.433016000	14.988689000	20.418463000				
C	-3.124898000	14.803523000	11.247659000				
H	-3.572922000	15.566086000	10.616428000				
C	6.455641000	14.133578000	20.469942000				
				Ia'			
				Lu	-4.785002000	6.582730000	11.986092000
				Si	-7.558980000	4.108396000	10.487730000
				O	-4.939905000	7.108189000	9.619571000
				O	-3.178166000	4.872251000	10.931541000
				N	-6.284143000	8.292120000	12.359227000
				N	-3.482586000	8.704365000	13.599642000
				N	-4.254452000	5.769265000	14.086699000
				C	-7.567007000	7.954755000	12.740304000
				H	-7.932792000	6.947130000	12.611842000
				C	-8.233124000	9.039152000	13.269315000
				H	-9.243466000	9.051213000	13.657617000
				C	-7.326226000	10.124325000	13.218028000
				H	-7.512554000	11.125642000	13.577111000
				C	-6.153478000	9.643746000	12.649883000
				C	-4.872259000	10.379444000	12.255805000
				C	-4.599888000	11.660589000	13.082040000
				C	-5.535326000	12.706092000	13.079497000
				H	-6.452237000	12.602124000	12.509960000
				C	-5.291579000	13.893435000	13.762424000
				H	-6.040222000	14.681027000	13.748295000
				C	-4.089091000	14.082895000	14.443115000
				H	-3.896801000	15.011422000	14.973285000
				C	-3.130240000	13.075871000	14.413258000
				H	-2.175798000	13.214440000	14.914278000
				C	-3.383480000	11.882710000	13.734833000
				H	-2.609776000	11.121973000	13.703039000
				C	-4.939678000	10.893830000	10.791125000
				C	-6.144719000	10.897655000	10.084293000
				H	-7.031171000	10.489945000	10.561971000
				C	-6.223296000	11.446613000	8.801987000
				H	-7.176763000	11.450364000	8.279655000
				C	-5.094909000	11.998069000	8.200739000
				H	-5.155581000	12.427971000	7.204573000
				C	-3.889263000	12.016966000	8.904646000
				H	-3.005413000	12.467567000	8.460352000
				C	-3.818374000	11.484607000	10.189307000
				H	-2.885287000	11.548149000	10.742229000
				C	-3.758300000	9.356258000	12.402005000
				C	-2.944929000	8.795143000	11.432994000
				H	-2.916221000	9.102324000	10.400022000
				C	-2.149594000	7.797139000	12.053919000
				H	-1.373293000	7.208177000	11.594995000
				C	-2.484542000	7.757149000	13.398889000
				C	-4.141955000	8.983630000	14.876677000
				H	-3.619880000	9.782360000	15.406619000
				H	-4.135827000	8.076468000	15.480461000
				H	-5.170178000	9.287963000	14.679453000
				C	-2.000613000	6.810542000	14.486051000

C	-1.242063000	7.550061000	15.612501000
C	-0.972974000	8.920626000	15.567883000
H	-1.327089000	9.512093000	14.729612000
C	-0.234633000	9.547377000	16.573614000
H	-0.045265000	10.615776000	16.511694000
C	0.261100000	8.809762000	17.643313000
H	0.833709000	9.295236000	18.428638000
C	0.031700000	7.434249000	17.683384000
H	0.434797000	6.837671000	18.497396000
C	-0.697416000	6.812898000	16.674910000
H	-0.826490000	5.735888000	16.697265000
C	-0.960325000	5.820435000	13.897369000
C	0.257960000	6.292041000	13.384887000
H	0.451655000	7.361228000	13.366737000
C	1.235704000	5.410867000	12.929783000
H	2.171737000	5.801098000	12.538520000
C	1.027224000	4.032518000	13.004171000
H	1.797880000	3.342373000	12.671383000
C	-0.169920000	3.553177000	13.530784000
H	-0.334833000	2.482201000	13.620620000
C	-1.159584000	4.439344000	13.964466000
H	-2.086992000	4.064165000	14.385773000
C	-3.243142000	6.077153000	14.982960000
C	-3.552604000	5.587735000	16.244851000
H	-2.969073000	5.700344000	17.147008000
C	-4.804569000	4.936933000	16.133085000
H	-5.357338000	4.446038000	16.923873000
C	-5.192660000	5.067973000	14.816491000
H	-6.096552000	4.706128000	14.348583000
C	-6.411120000	4.885931000	11.753575000
H	-5.860962000	4.032601000	12.184933000
H	-7.105595000	5.156645000	12.568894000
C	-8.157192000	2.387370000	11.062591000
H	-7.316502000	1.695834000	11.191317000
H	-8.850141000	1.937769000	10.341837000
H	-8.673985000	2.455990000	12.026034000
C	-6.761675000	3.804262000	8.775454000
H	-6.340443000	4.712947000	8.335676000
H	-7.504938000	3.405312000	8.075664000
H	-5.953271000	3.066598000	8.839957000
C	-9.141865000	5.146746000	10.246872000
H	-9.730789000	5.136188000	11.171009000
H	-9.768232000	4.723660000	9.453626000
H	-8.952034000	6.196264000	10.002656000
C	-6.243915000	7.516818000	9.107395000
H	-6.508015000	8.441761000	9.619437000
H	-6.964124000	6.740917000	9.367327000
C	-6.063870000	7.701796000	7.603771000
H	-6.334505000	6.788453000	7.062937000
H	-6.681762000	8.518094000	7.221824000
C	-4.565377000	7.978587000	7.470823000
H	-4.348174000	9.025272000	7.707220000
H	-4.168702000	7.754972000	6.476686000
C	-3.991583000	7.064776000	8.541068000
H	-3.897300000	6.030000000	8.187471000
H	-3.026023000	7.399375000	8.927234000
C	-1.861178000	4.935843000	10.348903000
H	-1.111090000	5.015561000	11.144214000
H	-1.814040000	5.822990000	9.715712000
C	-1.709186000	3.629594000	9.590150000
H	-0.663386000	3.391681000	9.378409000
H	-2.255261000	3.669412000	8.640953000
C	-2.367693000	2.649176000	10.562078000
H	-2.731346000	1.738642000	10.078870000
H	-1.653501000	2.362769000	11.339104000
C	-3.510466000	3.472319000	11.158316000
H	-4.461047000	3.286588000	10.656616000
H	-3.636032000	3.319260000	12.233396000

^{2a}IntI

Lu	0.044731000	-0.225563000	-0.067838000
N	-0.050939000	0.650763000	2.413877000
N	-0.019714000	2.033605000	-0.333740000
N	-1.964047000	-0.929312000	0.627432000
C	1.192615000	1.098532000	1.956645000

C	1.987688000	-0.027478000	1.783818000
H	3.003505000	-0.021093000	1.419866000
N	-0.637799000	-0.177228000	-2.337806000
C	1.231754000	-1.166570000	2.162970000
H	1.558166000	-2.194659000	2.138612000
C	-0.831437000	-3.081785000	2.800113000
N	-1.062954000	-0.389179000	-3.390910000
C	-1.244860000	-1.589336000	2.930055000
C	-2.338837000	-1.231797000	1.925392000
C	0.429301000	2.969128000	0.582800000
C	-0.027609000	-0.740822000	2.561507000
C	1.499270000	2.549300000	1.587152000
C	-1.689342000	-1.378415000	4.389938000
C	2.915634000	2.599629000	0.950855000
C	-3.721353000	-1.204513000	2.034758000
H	-4.307617000	-1.377849000	2.925381000
C	-2.296650000	0.478651000	-5.217574000
C	-1.528941000	-0.611076000	-4.576612000
C	-0.935722000	2.690491000	-1.125126000
H	-1.466802000	-1.378415000	-1.911052000
C	-4.227487000	-0.878292000	0.750925000
H	-5.267398000	-0.764626000	0.473299000
C	-1.304722000	-3.884154000	1.759326000
H	-1.980242000	-3.459090000	1.024604000
C	-2.766764000	-2.126275000	4.887947000
H	-3.266320000	-2.836925000	4.237676000
C	-3.132705000	-0.720154000	-0.072218000
H	-3.108396000	-0.451740000	-1.120808000
C	-1.263703000	-1.932369000	-5.185887000
C	3.098001000	2.896010000	-0.402212000
H	2.231765000	3.083921000	-1.027688000
C	-0.198609000	4.188000000	0.366545000
H	-0.067440000	5.097640000	0.934378000
C	1.545415000	3.465313000	2.825575000
C	-1.188747000	1.513548000	2.750822000
H	-1.176986000	2.381331000	2.090311000
H	-1.112966000	1.841576000	3.788819000
H	-2.108447000	0.945921000	2.608271000
C	-1.074457000	4.005637000	-0.731748000
H	-1.732842000	4.745928000	-1.167730000
C	0.028182000	-3.654032000	3.748802000
H	0.387749000	-3.051208000	4.578413000
C	-1.417021000	-0.414411000	6.607774000
H	-0.867842000	0.243646000	7.275844000
C	-1.007662000	-0.543602000	5.278985000
H	-0.129424000	0.001301000	4.946060000
C	-3.359104000	0.172913000	-6.082027000
H	-3.609795000	-0.864958000	-6.278064000
C	-2.514456000	-1.129194000	7.075531000
H	-2.836492000	-1.028793000	8.108171000
C	1.849839000	4.824520000	2.658660000
H	2.042243000	5.208085000	1.661968000
C	1.396671000	2.985117000	4.129338000
H	1.225623000	1.926481000	4.301347000
C	-0.921060000	-5.223354000	1.664456000
H	-1.304278000	-5.831678000	0.849549000
C	1.493633000	3.838708000	5.230186000
H	1.372364000	3.436137000	6.232282000
C	-3.182822000	-1.994256000	6.208506000
H	-4.024581000	-2.581289000	6.565783000
C	1.939159000	5.679623000	3.751980000
H	2.170250000	6.729404000	3.592636000
C	-0.057764000	-5.779300000	2.604120000
H	0.239334000	-6.821714000	2.528354000
C	4.049638000	2.385192000	1.747628000
H	3.928437000	2.182394000	2.808432000
C	-1.045158000	-2.035447000	-6.568380000
H	-1.070636000	-1.141106000	-7.183245000
C	1.752780000	5.192587000	5.046189000
H	1.826848000	5.859528000	5.900482000
C	-1.214719000	-3.093887000	-4.400384000
H	-1.404594000	-3.032555000	-3.332349000
C	4.382030000	2.967872000	-0.946954000
H	4.502239000	3.205489000	-2.000463000
C	-4.096036000	1.192950000	-6.676024000

H	-4.917464000	0.940939000	-7.340932000
C	-0.943448000	-4.327757000	-4.984230000
H	-0.908923000	-5.217722000	-4.362526000
C	0.416903000	-4.986955000	3.649897000
H	1.084056000	-5.409569000	4.396568000
C	5.500633000	2.740520000	-0.150578000
H	6.498539000	2.796079000	-0.576626000
C	-1.993747000	1.824925000	-4.961638000
H	-1.162835000	2.080628000	-4.309424000
C	-0.731463000	-4.423723000	-6.358967000
H	-0.525624000	-5.388313000	-6.813756000
C	5.328914000	2.447060000	1.202717000
H	6.193376000	2.276118000	1.838710000
C	-0.786770000	-3.274284000	-7.146978000
H	-0.617053000	-3.339048000	-8.218092000
C	-3.794764000	2.528625000	-6.411034000
H	-4.375098000	3.321917000	-6.873128000
C	-2.743259000	2.839186000	-5.549660000
H	-2.495946000	3.875944000	-5.340392000
C	1.192520000	-1.965728000	-1.200045000
H	0.492219000	-2.482714000	-1.875959000
H	1.334374000	-2.672175000	-0.361764000
Si	2.818941000	-1.862220000	-2.131460000
C	3.350646000	-3.568243000	-2.802781000
H	3.485805000	-4.287590000	-1.987487000
H	2.591891000	-3.974325000	-3.480675000
H	4.295438000	-3.506940000	-3.355276000
C	2.690547000	-0.685508000	-3.622994000
H	3.648407000	-0.622025000	-4.151212000
H	1.940895000	-1.032344000	-4.342484000
H	2.414236000	0.326505000	-3.308450000
C	4.230926000	-1.234072000	-1.018578000
H	4.311372000	-1.826255000	-0.099772000
H	5.192675000	-1.306575000	-1.538567000
H	4.090023000	-0.183836000	-0.742312000

2a⁺ TSI

Lu	6.969594000	4.037833000	4.725525000
N	6.924538000	4.882153000	7.272358000
N	6.728259000	6.268520000	4.585229000
N	5.044340000	3.252698000	5.480284000
C	8.125906000	5.377688000	6.761890000
C	8.949332000	4.281141000	6.530363000
H	9.954506000	4.333360000	6.140460000
N	6.929960000	3.625146000	2.613604000
C	8.246502000	3.111011000	6.924082000
H	8.610529000	2.095032000	6.893428000
C	6.267633000	1.126221000	7.613391000
N	6.667429000	3.201634000	1.499608000
C	5.810592000	2.603468000	7.770076000
C	4.692050000	2.939002000	6.782843000
C	7.219071000	7.225756000	5.456745000
C	6.993466000	3.492760000	7.387253000
C	8.365603000	6.839698000	6.386410000
C	5.388180000	2.782111000	9.240249000
C	9.737537000	6.922464000	5.663324000
C	3.310730000	2.911367000	6.897059000
H	2.734483000	2.715154000	7.789391000
C	5.464075000	4.744882000	0.054409000
C	6.109447000	3.443482000	0.354012000
C	5.716584000	6.876023000	3.876404000
H	5.158664000	6.327247000	3.129648000
C	2.784740000	3.212583000	5.613623000
H	1.739444000	3.281542000	5.342198000
C	5.792831000	0.318739000	6.576880000
H	5.082369000	0.726961000	5.865894000
C	4.327855000	2.013658000	9.743085000
H	3.822834000	1.310453000	9.089117000
C	3.865931000	3.410895000	4.782478000
H	3.878490000	3.664698000	3.729055000
C	6.160642000	2.359791000	-0.655416000
C	9.826976000	7.161246000	4.289413000
H	8.917733000	7.299901000	3.714129000
C	6.523983000	8.414905000	5.292325000
H	6.665239000	9.331817000	5.846178000

C	8.453556000	7.754722000	7.621566000
C	5.773050000	5.699286000	7.671675000
H	5.743244000	6.591239000	7.045628000
H	5.869023000	5.988067000	8.719540000
H	4.865023000	5.112170000	7.531866000
C	5.561364000	8.187524000	4.276637000
H	4.835353000	8.896118000	3.899668000
C	7.170345000	0.573220000	8.533272000
H	7.530430000	1.178444000	9.360959000
C	5.695505000	3.702508000	11.472119000
H	6.251606000	4.351743000	12.143042000
C	6.080255000	3.604270000	10.133499000
H	6.947264000	4.164183000	9.795295000
C	4.310573000	4.808393000	-0.745888000
H	3.882717000	3.890910000	-1.139004000
C	4.613097000	2.968618000	11.945503000
H	4.309610000	3.045359000	12.985716000
C	8.719237000	9.119804000	7.438269000
H	8.853946000	9.504855000	6.432439000
C	8.368075000	7.274064000	8.930681000
H	8.221973000	6.213018000	9.110867000
C	6.217908000	-1.006167000	6.457340000
H	5.831849000	-1.618970000	5.647200000
C	8.493214000	8.132668000	10.024788000
H	8.421098000	7.731102000	11.031960000
C	3.936165000	2.115122000	11.073865000
H	3.106734000	1.513163000	11.434952000
C	8.837639000	9.979186000	8.525436000
H	9.037616000	11.033566000	8.355062000
C	7.124272000	-1.542182000	7.367633000
H	7.452670000	-2.573593000	7.273331000
C	10.924277000	6.774077000	6.395810000
H	10.874032000	6.615391000	7.469794000
C	6.238760000	2.647506000	-2.027842000
H	6.246665000	3.682306000	-2.356669000
C	8.717398000	9.490915000	9.827122000
H	8.813640000	10.161445000	10.676343000
C	6.168210000	1.011734000	-0.260718000
H	6.086958000	0.774871000	0.796392000
C	11.072297000	7.237954000	3.661274000
H	11.120595000	7.431614000	2.593052000
C	3.708678000	6.030841000	-1.028151000
H	2.811754000	6.058227000	-1.641303000
C	6.261074000	-0.009518000	-1.200853000
H	6.259775000	-1.045138000	-0.870864000
C	7.600111000	-0.744971000	8.409337000
H	8.299473000	-1.153054000	9.134288000
C	12.244125000	7.075335000	4.395131000
H	13.211733000	7.136741000	3.904814000
C	5.989665000	5.940561000	0.563184000
H	6.878558000	5.912736000	1.186744000
C	6.337735000	0.290566000	-2.561203000
H	6.402824000	-0.506957000	-3.296064000
C	12.165146000	6.843232000	5.768834000
H	13.072067000	6.725727000	6.355947000
C	6.325379000	1.623895000	-2.967834000
H	6.392477000	1.871642000	-4.023943000
C	4.245794000	7.214342000	-0.520884000
H	3.774330000	8.168034000	-0.741288000
C	5.387572000	7.163352000	0.277129000
H	5.809739000	8.074890000	0.690270000
C	7.968663000	2.054328000	3.529321000
H	7.258709000	1.366124000	3.069766000
H	8.000154000	1.788762000	4.604327000
Si	9.697159000	1.914251000	2.766610000
C	10.190117000	0.076406000	2.747253000
H	10.192406000	-0.349154000	3.756054000
H	9.493006000	-0.508281000	2.138164000
H	11.193064000	-0.051379000	2.324581000
C	9.770950000	2.585198000	0.998896000
H	10.781609000	2.444961000	0.599289000
H	9.069858000	2.071190000	0.335712000
H	9.541145000	3.654259000	0.967567000
C	10.972566000	2.854471000	3.815834000
H	11.005027000	2.483398000	4.846020000

H	11.972844000	2.717210000	3.390473000
H	10.777478000	3.931939000	3.837354000

2a⁺Int2

Lu	-0.187504000	0.434131000	-0.420782000
N	-0.138288000	1.328713000	2.094795000
N	0.222078000	2.589866000	-0.768271000
N	-2.284619000	0.248747000	0.294387000
C	1.148485000	1.580436000	1.615571000
C	1.749662000	0.345399000	1.401778000
H	2.752168000	0.202568000	1.028882000
N	0.569979000	-0.875349000	-1.979757000
C	0.819879000	-0.668004000	1.757623000
H	0.973562000	-1.736228000	1.712104000
C	-1.526320000	-2.226908000	2.307546000
N	0.177230000	-2.045553000	-2.530715000
C	-1.689485000	-0.699513000	2.534708000
C	-2.703857000	-0.086388000	1.572516000
C	0.705752000	3.492049000	0.166057000
C	-0.347238000	-0.048519000	2.196041000
C	1.664652000	2.968341000	1.236372000
C	-2.094826000	-0.491674000	4.004613000
C	3.102448000	2.816586000	0.665968000
C	-4.037981000	0.252058000	1.731292000
H	-4.633768000	0.134793000	2.625158000
C	-2.016379000	-1.140341000	-3.301662000
C	-1.002368000	-2.206538000	-3.058946000
C	-0.527125000	3.320304000	-1.664859000
H	-1.022100000	2.831600000	-2.496059000
C	-4.466071000	0.818672000	0.502657000
H	-5.452543000	1.200049000	0.273536000
C	-2.053963000	-2.857620000	1.178136000
H	-2.615529000	-2.275092000	0.455587000
C	-3.269472000	-1.098566000	4.473250000
H	-3.863455000	-1.700957000	3.792930000
C	-3.375031000	0.801929000	-0.339443000
H	-3.300556000	1.153294000	-1.360495000
C	-1.295568000	-3.584422000	-3.528828000
C	3.400684000	3.137590000	-0.660431000
H	2.607430000	3.475187000	-1.318649000
C	0.255870000	4.767603000	-0.142284000
H	0.449166000	5.677321000	0.407068000
C	1.795654000	3.899908000	2.456925000
C	-1.115055000	2.366506000	2.442017000
H	-0.973973000	3.213838000	1.769555000
H	-0.964436000	2.688287000	3.473548000
H	-2.118294000	1.957437000	2.323393000
C	-0.531939000	4.654404000	-1.316430000
H	-1.042222000	5.456605000	-1.833389000
C	-0.821708000	-3.001524000	3.240297000
H	-0.422285000	-2.531613000	4.135045000
C	-1.703427000	0.349934000	6.252624000
H	-1.073575000	0.904060000	6.943358000
C	-1.309670000	0.213013000	4.919810000
H	-0.366607000	0.648412000	4.603368000
C	-3.382832000	-1.385071000	-3.092900000
H	-3.690800000	-2.331176000	-2.657793000
C	-2.889331000	-0.226140000	6.695276000
H	-3.198510000	-0.119971000	7.731224000
C	2.225135000	5.221653000	2.268767000
H	2.446919000	5.572458000	1.266528000
C	1.621699000	3.450605000	3.769207000
H	1.355478000	2.414206000	3.957457000
C	-1.871659000	-4.227613000	0.977911000
H	-2.283969000	-4.696811000	0.089233000
C	1.811084000	4.304545000	4.857299000
H	1.666067000	3.927076000	5.865928000
C	-3.668118000	-0.958685000	5.798294000
H	-4.585359000	-1.434210000	6.134790000
C	2.405777000	6.078203000	3.349831000
H	2.732006000	7.099615000	3.173894000
C	-1.162165000	-4.985996000	1.904794000
H	-1.021909000	-6.052016000	1.748520000
C	4.147057000	2.403256000	1.505906000
H	3.940493000	2.179910000	2.549340000

C	-2.158280000	-3.834840000	-4.609352000
H	-2.644885000	-3.003943000	-5.111004000
C	2.190095000	5.626963000	4.652085000
H	2.334869000	6.294911000	5.496376000
C	-0.671038000	-4.685556000	-2.915895000
H	-0.006694000	-4.499450000	-2.078546000
C	4.710866000	3.044057000	-1.136088000
H	4.924126000	3.312211000	-2.167397000
C	-4.346956000	-0.447708000	-3.457937000
H	-5.397696000	-0.663795000	-3.286203000
C	-0.895805000	-5.980986000	-3.369886000
H	-0.402800000	-6.815367000	-2.877089000
C	-0.638403000	-4.367102000	3.040449000
H	-0.091028000	-4.949510000	3.776920000
C	5.738000000	2.618169000	-0.298646000
H	6.755869000	2.545263000	-0.671266000
C	-1.645815000	0.092197000	-3.871603000
H	-0.595688000	0.294253000	-4.055516000
C	-1.756400000	-6.214264000	-4.443428000
H	-1.937370000	-7.227044000	-4.793102000
C	5.449547000	2.295571000	1.027968000
H	6.242995000	1.972587000	1.696636000
C	-2.384094000	-5.133156000	-5.060004000
H	-3.049792000	-5.298501000	-5.903287000
C	-3.966957000	0.760630000	-4.038634000
H	-4.717653000	1.488948000	-4.332345000
C	-2.611085000	1.027693000	-4.239433000
H	-2.304033000	1.960170000	-4.706330000
C	2.039099000	-0.870029000	-1.818141000
H	2.375479000	-1.565342000	-1.027132000
H	2.347608000	0.143205000	-1.509203000
Si	3.079139000	-1.259589000	-3.395077000
C	4.839270000	-0.632260000	-3.046807000
H	4.852556000	0.441341000	-2.834491000
H	5.280042000	-1.147003000	-2.186036000
H	5.491106000	-0.815140000	-3.908102000
C	3.158797000	-3.119258000	-3.731100000
H	3.785157000	-3.330714000	-4.604935000
H	3.589801000	-3.649492000	-2.874904000
H	2.158945000	-3.522991000	-3.907342000
C	2.351104000	-0.339614000	-4.881529000
H	2.227807000	0.727560000	-4.669508000
H	3.006962000	-0.435256000	-5.753511000
H	1.374373000	-0.752106000	-5.150788000

2a⁺TS2

Lu	0.211476000	0.266499000	-0.762079000
N	-0.240207000	1.581278000	1.509920000
N	0.179609000	2.390340000	-1.482493000
N	-1.854791000	-0.341947000	-0.069378000
C	0.988193000	2.106547000	1.100674000
C	1.919235000	1.083125000	1.187761000
H	2.958621000	1.160901000	0.909289000
N	-0.051135000	-0.832664000	-2.996425000
C	1.264331000	-0.070466000	1.693051000
H	1.708142000	-1.039500000	1.856192000
C	-0.625117000	-2.125243000	2.402985000
N	-1.171035000	-1.662062000	-3.121452000
C	-1.206272000	-0.688489000	2.318816000
C	-2.268395000	-0.565564000	1.232232000
C	0.265615000	3.543302000	-0.720527000
C	-0.068861000	0.243338000	1.901634000
C	1.156265000	3.507712000	0.520640000
C	-1.773317000	-0.340925000	3.707166000
C	2.648852000	3.724240000	0.144349000
C	-3.653869000	-0.553156000	1.299933000
H	-4.260737000	-0.671933000	2.186026000
C	-2.012135000	-0.151611000	-4.893580000
C	-2.077026000	-1.326699000	-3.978373000
C	-0.583709000	2.708766000	-2.585285000
H	-0.792821000	1.963358000	-3.342470000
C	-4.122810000	-0.304499000	-0.014203000
H	-5.153954000	-0.219021000	-0.331784000
C	-0.879440000	-3.074387000	1.410374000
H	-1.509545000	-2.805996000	0.569152000

H	1.292847000	3.985105000	5.750541000	H	-4.012948000	-1.135474000	3.455580000
C	-2.999349000	-1.465686000	6.377754000	C	-1.028179000	-0.404100000	-4.656788000
H	-3.816401000	-2.026460000	6.823798000	C	-1.135328000	-0.869913000	-3.239484000
C	1.616325000	6.027254000	3.061768000	C	-1.298008000	2.544666000	-1.342832000
H	1.751700000	7.073463000	2.800885000	H	-1.783735000	1.872135000	-2.038616000
C	-0.035718000	-5.557763000	3.040991000	C	-4.183946000	-0.771101000	1.257580000
H	0.252437000	-6.605314000	3.058489000	H	-5.249961000	-0.692574000	1.088035000
C	3.975231000	2.567856000	1.484547000	C	-0.945706000	-3.607428000	2.152800000
H	3.811633000	2.335260000	2.533324000	H	-1.721927000	-3.290605000	1.464171000
C	-3.547784000	-2.030900000	-3.468709000	C	-2.257732000	-1.735230000	5.278237000
H	-3.725853000	-1.302787000	-4.254734000	H	-2.753446000	-2.529714000	4.729492000
C	1.496311000	5.649554000	4.399353000	C	-3.189834000	-0.647379000	0.310898000
H	1.525802000	6.397381000	5.186812000	H	-3.290147000	-0.464707000	-0.750964000
C	-2.033390000	-3.106132000	-1.913567000	C	-2.284145000	-1.776348000	-2.928245000
H	-1.032544000	-3.214455000	-1.502161000	C	2.703796000	3.266857000	-0.885541000
C	4.412542000	3.248741000	-1.170281000	H	1.793212000	3.289596000	-1.474427000
H	4.574122000	3.530187000	-2.207328000	C	-0.650828000	4.292660000	-0.098434000
C	-0.705672000	0.177134000	-6.881408000	H	-0.585712000	5.280696000	0.333553000
H	-0.504817000	1.147780000	-7.326021000	C	1.274244000	4.018883000	2.358026000
C	-3.074262000	-3.920037000	-1.474435000	C	-1.208307000	1.841105000	2.718544000
H	-2.886237000	-4.668959000	-0.711260000	H	-1.308239000	2.660733000	2.006490000
C	0.512585000	-4.661730000	3.959329000	H	-1.094064000	2.242880000	3.726987000
H	1.228955000	-5.008159000	4.699649000	H	-2.090401000	1.201747000	2.676709000
C	5.500488000	3.049941000	-0.324679000	C	-1.542950000	3.884727000	-1.121912000
H	6.514465000	3.172031000	-0.695721000	H	-2.278787000	4.499513000	-1.624174000
C	-1.261591000	-2.298961000	-5.734589000	C	0.542159000	-3.124934000	3.979902000
H	-1.492039000	-3.260884000	-5.286501000	H	0.925214000	-2.434463000	4.726566000
C	-4.352186000	-3.777471000	-2.010888000	C	-0.913962000	0.214041000	6.730499000
H	-5.163207000	-4.408378000	-1.658313000	H	-0.368248000	0.967451000	7.292317000
C	5.275789000	2.702499000	1.007973000	C	-0.616954000	0.011756000	5.381231000
H	6.114501000	2.552978000	1.682792000	H	0.172774000	0.598873000	4.922148000
C	-4.588923000	-2.827525000	-3.005154000	C	-0.671203000	0.922657000	-4.935262000
H	-5.584512000	-2.712379000	-3.424017000	H	-0.448779000	1.590757000	-4.109930000
C	-0.922755000	-0.934756000	-7.696760000	C	-1.895716000	-0.548961000	7.353518000
H	-0.882614000	-0.833444000	-8.777773000	H	-2.130378000	-0.392665000	8.402683000
C	-1.195306000	-2.173754000	-7.120133000	C	1.397688000	5.378241000	2.034473000
H	-1.365695000	-3.043542000	-7.748186000	H	1.470038000	5.672664000	0.992652000
C	1.876048000	-0.944469000	-3.181723000	C	1.281930000	3.666941000	3.710457000
H	1.791551000	-2.001068000	-2.894758000	H	1.250930000	2.620001000	3.997765000
H	1.186739000	-1.860821000	-0.596127000	C	-0.462121000	-4.916841000	2.112252000
Si	3.515891000	-0.284575000	-3.906911000	H	-0.868165000	-5.615156000	1.384943000
C	4.848676000	-0.380695000	-2.570682000	C	1.354379000	4.638876000	4.710351000
H	4.649461000	0.329886000	-1.763968000	H	1.355892000	4.334610000	5.753657000
H	4.896146000	-1.386083000	-2.140534000	C	-2.561737000	-1.531971000	6.620284000
H	5.832232000	-0.147308000	-2.992761000	H	-3.313581000	-2.153508000	7.099194000
C	3.946189000	-1.467680000	-5.324699000	C	1.461429000	6.350117000	3.027510000
H	4.888601000	-1.169902000	-5.796904000	H	1.549334000	7.396395000	2.747392000
H	4.065322000	-2.493733000	-4.961775000	C	0.528520000	-5.331885000	2.997468000
H	3.167930000	-1.467131000	-6.094014000	H	0.902733000	-6.351519000	2.964938000
C	3.243164000	1.469394000	-4.542265000	C	3.810532000	3.082569000	1.242914000
H	2.840137000	2.104254000	-3.749119000	H	3.763665000	2.978589000	2.323582000
H	4.180986000	1.907497000	-4.899081000	C	-3.564733000	-1.536088000	-3.447878000
H	2.528304000	1.470776000	-5.370273000	H	-3.726601000	-0.680816000	-4.097524000
2a' TS3				C	1.431118000	5.986233000	4.374022000
Lu	-0.056992000	-0.111000000	-0.104017000	H	1.484170000	6.744729000	5.149939000
N	-0.032600000	1.045623000	2.354629000	C	-2.081129000	-2.888274000	-2.099415000
N	-0.299294000	2.090062000	-0.510601000	H	-1.084292000	-3.082646000	-1.714134000
N	-1.947148000	-0.800997000	0.886108000	C	3.944389000	3.417208000	-1.509578000
C	1.116393000	1.548162000	1.743084000	H	3.984662000	3.566135000	-2.585443000
C	1.991435000	0.483597000	1.580534000	C	-0.613042000	1.372303000	-6.250191000
H	2.966173000	0.545020000	1.121324000	H	-0.348331000	2.406161000	-6.454246000
N	1.415505000	-0.150802000	-3.218867000	C	-3.137508000	-3.741677000	-1.795498000
C	1.381220000	-0.677068000	2.126215000	H	-2.967898000	-4.608741000	-1.163613000
H	1.797591000	-1.671691000	2.148994000	C	1.029880000	-4.427928000	3.934713000
C	-0.445870000	-2.693457000	3.083369000	H	1.795980000	-4.740335000	4.639553000
N	-0.316380000	-0.536155000	-2.314004000	C	5.119876000	3.390774000	-0.763292000
C	-0.968761000	-1.232540000	3.149690000	H	6.083356000	3.514894000	-1.250404000
C	-2.172544000	-1.027022000	2.235152000	C	-1.319947000	-1.269572000	-5.720117000
C	0.094800000	3.174654000	0.249196000	H	-1.602459000	-2.297709000	-5.512243000
C	0.131294000	-0.321546000	2.608410000	C	-4.412310000	-3.483363000	-2.297819000
C	1.252908000	2.976587000	1.223553000	H	-5.238553000	-4.144054000	-2.050616000
C	-1.298566000	-0.946055000	4.626447000	C	5.047737000	3.217979000	0.620021000
C	2.621729000	3.099307000	0.498790000	H	5.955656000	3.204687000	1.217299000
C	-3.534133000	-1.013614000	2.494719000	C	-4.625036000	-2.376777000	-3.120005000
				H	-5.617990000	-2.170228000	-3.509607000

C	-0.888824000	0.499724000	-7.303893000
H	-0.837171000	0.852343000	-8.330620000
C	-1.236258000	-0.823872000	-7.037087000
H	-1.450804000	-1.507659000	-7.853823000
C	2.270917000	-0.791067000	-2.619066000
H	1.941477000	-1.269263000	-1.480870000
H	1.501001000	-1.449258000	-0.475988000
Si	4.059091000	-0.971591000	-3.285741000
C	5.214342000	-0.697067000	-1.818424000
H	5.128460000	0.323795000	-1.434443000
H	4.987028000	-1.393331000	-1.005333000
H	6.254525000	-0.859159000	-2.121832000
C	4.169090000	-2.751493000	-3.913047000
H	5.180788000	-2.961816000	-4.276865000
H	3.938559000	-3.465819000	-3.117048000
H	3.469524000	-2.920173000	-4.737107000
C	4.380271000	0.267320000	-4.670461000
H	4.298767000	1.292111000	-4.297618000
H	5.385358000	0.131669000	-5.084201000
H	3.653715000	0.142305000	-5.478217000

2a⁺Int4

Lu	-1.018947000	0.386676000	-0.138480000
N	-0.280720000	1.275859000	2.244772000
N	-1.951875000	2.402141000	-0.080712000
N	-2.152218000	-0.974395000	1.222817000
C	0.382643000	2.103840000	1.333343000
C	1.322096000	1.313927000	0.677580000
H	2.012562000	1.640660000	-0.085730000
N	3.847180000	-0.308256000	-0.996948000
C	1.232732000	-0.003310000	1.201257000
H	1.839828000	-0.844470000	0.902875000
C	0.435342000	-2.483424000	2.457650000
N	-1.076088000	-0.334717000	-2.088121000
C	-0.339637000	-1.218924000	2.924438000
C	-1.813090000	-1.301517000	2.524101000
C	-1.505739000	3.497599000	0.638450000
C	0.241607000	-0.017951000	2.177026000
C	-0.028837000	3.545845000	1.030480000
C	-0.137391000	-1.117433000	4.447939000
C	0.843621000	4.043333000	-0.155864000
C	-2.941103000	-1.732034000	3.208075000
H	-2.999001000	-2.038223000	4.242504000
C	-0.104726000	-0.648808000	-4.285701000
C	-1.217839000	-0.748087000	-3.279630000
C	-3.272901000	2.644301000	-0.385458000
H	-3.850180000	1.922441000	-0.951716000
C	-4.022455000	-1.674480000	2.291994000
H	-5.054224000	-1.934049000	2.490831000
C	-0.161010000	-3.448470000	1.641928000
H	-1.188017000	-3.313355000	1.320089000
C	-0.599592000	-2.156588000	5.269094000
H	-1.095684000	-3.010026000	4.818587000
C	-3.503088000	-1.211650000	1.100492000
H	-4.013402000	-1.024224000	0.162842000
C	-2.514702000	-1.352531000	-3.741677000
C	0.299677000	4.256845000	-1.425223000
H	-0.756726000	4.075126000	-1.591196000
C	-2.539559000	4.409916000	0.787580000
H	-2.505120000	5.352734000	1.314130000
C	0.243525000	4.496730000	2.210674000
C	-1.358450000	1.702857000	3.143269000
H	-1.914585000	2.507812000	2.661676000
H	-0.940536000	2.057853000	4.086536000
H	-2.015943000	0.852458000	3.328857000
C	-3.670238000	3.860776000	0.128133000
H	-4.653846000	4.305520000	0.050441000
C	1.758826000	-2.685226000	2.874775000
H	2.232218000	-1.956465000	3.526927000
C	0.785655000	-0.048026000	6.429731000
H	1.346580000	0.772650000	6.868791000
C	0.580474000	-0.080004000	5.048948000
H	1.008697000	0.708382000	4.436919000
C	0.818151000	0.401313000	-4.190091000
H	0.686465000	1.138316000	-3.403620000

C	0.282820000	-1.063225000	7.236442000
H	0.438391000	-1.039489000	8.311315000
C	-0.049989000	5.861021000	2.067705000
H	-0.463617000	6.220307000	1.131012000
C	0.861620000	4.081205000	3.392952000
H	1.161069000	3.044072000	3.512078000
C	0.549057000	-4.585763000	1.250837000
H	0.061885000	-5.329884000	0.626245000
C	1.130830000	4.984069000	4.423515000
H	1.611703000	4.631932000	5.332210000
C	-0.404537000	-2.124099000	6.645911000
H	-0.779594000	-2.939213000	7.258876000
C	0.209276000	6.761959000	3.095105000
H	-0.034151000	7.812356000	2.960069000
C	1.864996000	-4.774322000	1.665865000
H	2.411531000	-5.666143000	1.370661000
C	2.207185000	4.302856000	0.041228000
H	2.642340000	4.162701000	1.026990000
C	-3.033651000	-1.099175000	-5.018831000
H	-2.469969000	-0.484199000	-5.714626000
C	0.794279000	6.326338000	4.284616000
H	1.000466000	7.030620000	5.085635000
C	-3.264335000	-2.135379000	-2.852994000
H	-2.864976000	-2.324493000	-1.860590000
C	1.102585000	4.710810000	-2.473951000
H	0.658285000	4.877768000	-3.451644000
C	1.873906000	0.504148000	-5.089733000
H	2.569911000	1.334805000	-5.010984000
C	-4.495038000	-2.660978000	-3.234039000
H	-5.058405000	-3.276413000	-2.537635000
C	2.469484000	-3.815153000	2.480149000
H	3.491765000	-3.953208000	2.822392000
C	2.458175000	4.953482000	-2.271234000
H	3.081093000	5.307275000	-3.088314000
C	0.067080000	-1.606428000	-5.296061000
H	-0.635163000	-2.430959000	-5.378171000
C	-5.007112000	-2.395163000	-4.505586000
H	-5.971663000	-2.799278000	-4.800830000
C	3.009080000	4.746907000	-1.006159000
H	4.064379000	4.938193000	-0.831403000
C	-4.276567000	-1.607523000	-5.393242000
H	-4.674259000	-1.386544000	-6.380181000
C	2.036654000	-0.454825000	-6.092276000
H	2.857668000	-0.371428000	-6.799763000
C	1.135775000	-1.515055000	-6.187026000
H	1.259666000	-2.269057000	-6.959981000
C	4.037026000	-1.318685000	-1.542722000
H	-2.729913000	-5.725028000	-3.691698000
H	-2.501670000	-6.431431000	-3.734803000
Si	4.342987000	-2.966833000	-2.418853000
C	5.516752000	-3.934532000	-1.305143000
H	6.462063000	-3.401696000	-1.167741000
H	5.069502000	-4.100998000	-0.321105000
H	5.737241000	-4.911008000	-1.749399000
C	2.665926000	-3.800329000	-2.591568000
H	2.778966000	-4.773743000	-3.081015000
H	2.205914000	-3.960611000	-1.612193000
H	1.989372000	-3.189591000	-3.195966000
C	5.119905000	-2.546419000	-4.081806000
H	6.056011000	-1.995377000	-3.953500000
H	5.337493000	-3.464437000	-4.638062000
H	4.436652000	-1.937249000	-4.680159000

2a⁺TS4

Lu	7.876856000	4.095284000	4.881140000
N	7.291077000	4.990904000	7.313806000
N	6.801989000	6.031297000	4.550452000
N	6.388857000	2.592870000	5.545941000
C	8.276266000	5.864938000	6.838033000
C	9.457855000	5.138606000	6.764377000
H	10.400578000	5.517021000	6.399827000
C	9.195745000	3.818751000	7.213446000
H	9.904272000	3.007236000	7.265952000
C	8.018098000	1.286704000	8.018589000
C	7.047456000	2.499646000	7.953861000

C	6.009209000	2.309376000	6.848788000
C	6.871746000	7.172798000	5.329803000
C	7.854521000	3.736032000	7.561880000
C	8.005422000	7.287250000	6.345025000
C	6.429309000	2.619616000	9.360210000
C	9.311226000	7.806651000	5.684336000
N	9.836955000	3.366578000	3.969434000
C	4.717917000	1.804533000	6.858087000
H	4.140032000	1.509912000	7.721897000
C	5.693522000	6.181760000	3.746308000
H	5.391946000	5.394160000	3.068821000
C	4.280916000	1.764936000	5.508732000
H	3.317919000	1.425601000	5.149899000
C	7.921842000	0.224045000	7.117030000
H	7.170654000	0.253369000	6.335174000
C	5.644486000	1.568343000	9.856103000
H	5.476514000	0.692372000	9.238447000
C	5.320378000	2.248509000	4.743751000
H	5.377418000	2.371777000	3.668903000
C	7.908286000	3.425867000	2.319177000
C	9.435665000	7.910778000	4.296633000
H	8.596085000	7.641764000	3.664162000
C	6.887414000	3.614636000	1.387907000
H	6.291348000	4.524161000	1.392281000
C	5.826546000	8.026137000	5.012444000
H	5.606455000	8.980958000	5.467564000
C	7.656962000	8.251492000	7.493282000
C	8.682101000	2.253831000	2.219728000
C	5.889909000	5.343972000	7.566279000
H	5.615006000	6.173504000	6.915412000
H	5.760328000	5.633923000	8.610167000
H	5.267163000	4.475214000	7.348346000
C	5.072839000	7.387508000	3.994729000
H	4.177315000	7.763522000	3.517345000
C	8.987387000	1.221019000	9.030351000
H	9.057931000	2.025389000	9.757604000
C	6.181861000	3.733989000	11.509959000
H	6.416477000	4.577117000	12.154159000
C	6.711187000	3.685825000	10.218949000
H	7.370282000	4.484788000	9.891457000
C	9.797440000	2.296187000	3.251728000
C	5.366313000	2.706018000	11.971211000
H	4.950344000	2.742008000	12.974062000
C	7.453624000	9.608102000	7.199553000
H	7.549864000	9.949816000	6.173770000
C	7.606241000	7.855901000	8.831916000
H	7.815499000	6.824952000	9.101288000
C	8.774737000	-0.876974000	7.223414000
H	8.678809000	-1.695846000	6.515833000
C	7.315080000	8.772576000	9.844479000
H	7.281536000	8.437002000	10.877546000
C	8.393195000	1.244049000	1.304191000
H	8.958614000	0.316776000	1.285471000
C	5.108320000	1.616600000	11.138752000
H	4.497787000	0.791180000	11.494674000
C	7.156550000	10.522502000	8.204418000
H	6.997675000	11.566613000	7.948768000
C	9.739651000	-0.928584000	8.225425000
H	10.398126000	-1.788902000	8.309965000
C	10.399717000	8.181840000	6.484601000
H	10.312607000	8.129308000	7.566530000
C	6.616808000	2.633557000	0.423665000
H	5.823906000	2.792266000	-0.303490000
C	7.078146000	10.107542000	9.534399000
H	6.849855000	10.822039000	10.320213000
C	10.623575000	8.367365000	3.722015000
H	10.698356000	8.443496000	2.640666000
C	9.845286000	0.129657000	9.129394000
H	10.587312000	0.099075000	9.922878000
C	11.702896000	8.725792000	4.524355000
H	12.626421000	9.081194000	4.075723000
C	7.349832000	1.447899000	0.397106000
H	7.116916000	0.682690000	-0.338530000
C	11.585726000	8.632212000	5.911562000
H	12.417089000	8.918043000	6.550536000

C	10.771260000	1.189193000	3.410592000
C	11.111670000	0.726267000	4.687473000
C	11.413810000	0.639232000	2.292352000
C	12.057374000	-0.281771000	4.842194000
C	12.378716000	-0.353262000	2.451713000
C	12.696130000	-0.821885000	3.725270000
H	10.614569000	1.150765000	5.553018000
H	11.184380000	1.016293000	1.300220000
H	12.297441000	-0.643505000	5.837821000
H	12.883488000	-0.758746000	1.579227000
H	13.441681000	-1.602762000	3.848053000
H	8.942077000	3.912982000	3.172089000

2a⁺Int5

Lu	-0.383305000	-0.130837000	-1.053294000
N	-0.713411000	0.858977000	1.448077000
N	-1.244469000	1.885173000	-1.397291000
N	-1.931834000	-1.471670000	-0.158206000
C	0.261416000	1.683521000	0.876930000
C	1.398385000	0.907992000	0.703966000
H	2.318625000	1.242382000	0.252175000
C	1.119179000	-0.399457000	1.181739000
H	1.795541000	-1.241271000	1.192181000
C	-0.086611000	-2.861240000	2.116117000
C	-1.001236000	-1.606002000	2.154340000
C	-2.166829000	-1.748994000	1.178440000
C	-1.165389000	3.009751000	-0.592098000
C	-0.186110000	-0.415580000	1.657992000
C	0.000672000	3.107186000	0.388966000
C	-1.455978000	-1.444025000	3.617183000
C	1.286630000	3.605571000	-0.327255000
N	1.922040000	-0.238349000	-2.166019000
C	-3.467226000	-2.199590000	1.344131000
H	-3.946891000	-2.475740000	2.271944000
C	-2.314751000	2.087099000	-2.243190000
H	-2.575859000	1.343681000	-2.984746000
C	-4.063378000	-2.211687000	0.056544000
H	-5.075796000	-2.507611000	-0.186243000
C	-0.296815000	-3.891954000	1.196935000
H	-1.113694000	-3.814804000	0.487378000
C	-2.200983000	-2.469344000	4.218329000
H	-2.449723000	-3.354505000	3.642014000
C	-3.101458000	-1.767194000	-0.825262000
H	-3.164736000	-1.647767000	-1.898803000
C	-0.562462000	-0.992567000	-3.293817000
C	1.328326000	3.796742000	-1.710637000
H	0.441972000	3.597387000	-2.303531000
C	-1.629998000	-1.154494000	-4.196311000
H	-2.606739000	-0.730716000	-3.962295000
C	-2.177258000	3.895793000	-0.924822000
H	-2.384948000	4.849453000	-0.461565000
C	-0.269250000	4.090090000	1.543605000
C	0.654507000	-1.604196000	-3.701079000
C	-2.073903000	1.277454000	1.797597000
H	-2.379658000	2.071918000	1.116277000
H	-2.103963000	1.641875000	2.825758000
H	-2.739310000	0.419723000	1.692342000
C	-2.911166000	3.302013000	-1.985177000
H	-3.774016000	3.718246000	-2.488736000
C	0.961964000	-2.990407000	3.038397000
H	1.124314000	-2.210934000	3.778076000
C	-1.460897000	-0.276074000	5.752570000
H	-1.147957000	0.577997000	6.347250000
C	-1.071785000	-0.362597000	4.414379000
H	-0.442495000	0.418982000	3.999043000
C	1.765262000	-1.403478000	-2.746956000
C	-2.236976000	-1.279575000	6.322683000
H	-2.543663000	-1.213802000	7.362761000
C	-0.496094000	5.442946000	1.250108000
H	-0.481105000	5.772737000	0.216330000
C	-0.202927000	3.714878000	2.887935000
H	0.033039000	2.688192000	3.151338000
C	0.526586000	-5.019690000	1.194383000
H	0.341366000	-5.813152000	0.475405000
C	-0.408178000	4.645124000	3.908752000

H	-0.352209000	4.324107000	4.945487000
C	0.799665000	-2.329040000	-4.895215000
H	1.755970000	-2.775671000	-5.157736000
C	-2.598031000	-2.382820000	5.548591000
H	-3.180547000	-3.188833000	5.986602000
C	-0.708387000	6.371241000	2.263947000
H	-0.888018000	7.411931000	2.007985000
C	1.572293000	-5.133067000	2.105564000
H	2.210955000	-6.012147000	2.102700000
C	2.435092000	3.895814000	0.422987000
H	2.412588000	3.778348000	1.503109000
C	-1.500883000	-1.840793000	-5.404552000
H	-2.352735000	-1.923896000	-6.076131000
C	-0.674200000	5.975239000	3.601419000
H	-0.836553000	6.700684000	4.393593000
C	2.493371000	4.254409000	-2.329959000
H	2.502600000	4.402085000	-3.406641000
C	1.787796000	-4.110678000	3.030167000
H	2.594057000	-4.189858000	3.754706000
C	3.632737000	4.525637000	-1.578078000
H	4.537923000	4.882586000	-2.061695000
C	-0.283752000	-2.429664000	-5.758855000
H	-0.184110000	-2.958761000	-6.702724000
C	3.598641000	4.344780000	-0.194972000
H	4.477102000	4.563474000	0.406478000
C	2.652558000	-2.511336000	-2.336901000
C	2.284014000	-3.854727000	-2.511058000
C	3.897724000	-2.212489000	-1.758143000
C	3.144281000	-4.874775000	-2.114939000
C	4.754056000	-3.233799000	-1.366482000
C	4.379228000	-4.567033000	-1.545736000
H	1.316473000	-4.093433000	-2.940699000
H	4.173896000	-1.169671000	-1.639916000
H	2.848575000	-5.911446000	-2.247581000
H	5.718821000	-2.993929000	-0.928466000
H	5.051395000	-5.365275000	-1.242709000
H	1.401540000	0.452170000	-2.724190000

2a¹ Int6

Lu	-0.428703000	-0.197611000	0.162620000
N	-0.610300000	0.811519000	2.689806000
N	-0.722948000	2.077545000	-0.074733000
N	-2.440152000	-0.936101000	0.963133000
C	0.616501000	1.269903000	2.200984000
C	1.441118000	0.159376000	2.082885000
H	2.454244000	0.174046000	1.714528000
N	-1.195349000	-0.150834000	-2.101872000
C	0.710601000	-0.985395000	2.497449000
H	1.061310000	-2.006104000	2.520746000
C	-1.323428000	-2.898155000	3.348572000
N	-1.111797000	-0.056420000	-3.251464000
C	-1.752648000	-1.405580000	3.320942000
C	-2.834786000	-1.152483000	2.269849000
C	-0.238402000	3.061219000	0.767884000
C	-0.553902000	-0.565629000	2.892646000
C	0.871311000	2.710188000	1.757261000
C	-2.207926000	-1.084698000	4.760053000
C	2.268017000	2.775461000	1.083161000
N	1.709692000	-0.202351000	-0.958546000
C	-4.222501000	-1.173139000	2.349067000
H	-4.824995000	-1.297330000	3.237066000
C	-1.464282000	1.298963000	-5.161249000
C	-1.028599000	0.026370000	-4.541292000
C	-1.690837000	2.682348000	-0.842089000
H	-2.270468000	2.110740000	-1.555147000
C	-4.708163000	-0.973132000	1.033432000
H	-5.744620000	-0.923638000	0.724670000
C	-1.903044000	-3.837696000	2.495174000
H	-2.652095000	-3.510848000	1.782124000
C	-3.303404000	-1.773197000	5.301814000
H	-3.817605000	-2.512880000	4.697644000
C	-3.596408000	-0.836059000	0.225421000
H	-3.551570000	-0.659879000	-0.842489000
C	-0.026294000	-2.298063000	-0.993712000
C	-0.513153000	-1.144075000	-5.280305000

C	2.408966000	3.077195000	-0.274548000
H	1.518805000	3.254982000	-0.869889000
C	-0.834479000	-3.443958000	-0.982016000
H	-1.847099000	-3.374208000	-0.589263000
C	-0.891864000	4.263432000	0.525653000
H	-0.745471000	5.199677000	1.044686000
C	0.926737000	3.686912000	2.950060000
C	1.267708000	-2.456450000	-1.554788000
C	-1.772836000	1.652279000	2.991822000
H	-1.765684000	2.515024000	2.326320000
H	-1.732005000	1.986224000	4.030024000
H	-2.676570000	1.063610000	2.830365000
C	-1.824115000	4.017038000	-0.511040000
H	-2.523381000	4.723771000	-0.939265000
C	-0.376225000	-3.339540000	4.284337000
H	0.060740000	-2.628960000	4.981136000
C	-1.910246000	0.002226000	6.918720000
H	-1.343372000	0.684145000	7.547100000
C	-1.504125000	-0.218223000	5.601217000
H	-0.611145000	0.281247000	5.237166000
C	-2.103755000	1.292333000	-6.411194000
H	-2.271524000	0.350161000	-6.923761000
C	2.109618000	-1.246627000	-1.616817000
C	-3.027775000	-0.651885000	7.426126000
H	-3.348482000	-0.480128000	8.449796000
C	1.224261000	5.037858000	2.716084000
H	1.404502000	5.375082000	1.700363000
C	0.782494000	3.270078000	4.275706000
H	0.608235000	2.221555000	4.496385000
C	-1.537319000	-5.183351000	2.565176000
H	-2.004567000	-5.899096000	1.894123000
C	0.881230000	4.176297000	5.333307000
H	0.761964000	3.822969000	6.354046000
C	1.745394000	-3.701027000	-1.998526000
H	2.759605000	-3.802509000	-2.374875000
C	-3.717294000	-1.549831000	6.610836000
H	-4.574238000	-2.092633000	7.000651000
C	1.316494000	5.945117000	3.766332000
H	1.541821000	6.987095000	3.555473000
C	-0.583823000	-5.609058000	3.484806000
H	-0.299683000	-6.656605000	3.537300000
C	3.428328000	2.584440000	1.847127000
H	3.340152000	2.387183000	2.912197000
C	0.137258000	-0.965753000	-6.512807000
H	0.256048000	0.034364000	-6.917180000
C	-0.381309000	-4.684046000	-1.446089000
H	-1.036945000	-5.552104000	-1.410788000
C	1.137818000	5.520113000	5.083310000
H	1.213416000	6.227688000	5.904184000
C	-0.630861000	-2.443150000	-4.760206000
H	-1.120951000	-2.606771000	-3.804595000
C	3.675766000	3.166635000	-0.857710000
H	3.763141000	3.410967000	-1.913125000
C	-2.536343000	2.483330000	-6.986729000
H	-3.031316000	2.460137000	-7.953761000
C	-0.116784000	-3.531082000	-5.459590000
H	-0.215202000	-4.525725000	-5.035524000
C	-0.002372000	-4.678483000	4.347045000
H	0.734529000	-4.997837000	5.079482000
C	4.820762000	2.956108000	-0.092746000
H	5.805266000	3.032688000	-0.546097000
C	-1.282510000	2.523265000	-4.500406000
H	-0.798132000	2.552253000	-3.528198000
C	0.514274000	-3.348043000	-6.689931000
H	0.906083000	-4.200880000	-7.236968000
C	0.917399000	-4.817934000	-1.938428000
H	1.283414000	-5.785263000	-2.272376000
C	4.691228000	2.664687000	1.265942000
H	5.575954000	2.514820000	1.879241000
C	0.638502000	-2.060322000	-7.211089000
H	1.135555000	-1.902777000	-8.164560000
C	-2.353071000	3.696122000	-6.322891000
H	-2.696382000	4.623210000	-6.772967000
C	-1.730775000	3.708633000	-5.075487000
H	-1.585785000	4.644679000	-4.543794000

C	3.360747000	-1.203275000	-2.421372000
C	4.529343000	-0.658926000	-1.870215000
C	3.374985000	-1.645093000	-3.752700000
C	5.692109000	-0.569477000	-2.630303000
C	4.535067000	-1.534650000	-4.515071000
C	5.696787000	-1.004252000	-3.955224000
H	4.529190000	-0.319435000	-0.838067000
H	2.470725000	-2.053363000	-4.193773000
H	6.595563000	-0.160643000	-2.186751000
H	4.528864000	-1.864547000	-5.549981000
H	6.603261000	-0.929540000	-4.549538000
H	2.316306000	0.607474000	-1.084849000

2a⁺TSS

Lu	7.396048000	3.923257000	4.605330000
N	7.043665000	4.822032000	7.163403000
N	7.120607000	6.159962000	4.434165000
N	5.368878000	3.103615000	5.261595000
C	8.295974000	5.311616000	6.777725000
C	9.141830000	4.216171000	6.681970000
H	10.179971000	4.255727000	6.394414000
N	7.049284000	3.430284000	2.486242000
C	8.399373000	3.048562000	7.000772000
H	8.763345000	2.032320000	7.023404000
C	6.332617000	1.084764000	7.660075000
N	6.866708000	3.145902000	1.323982000
C	5.892534000	2.574324000	7.645221000
C	4.883624000	2.847483000	6.529727000
C	7.512649000	7.129337000	5.341661000
C	7.105543000	3.440090000	7.322891000
C	8.558131000	6.768008000	6.393920000
C	5.337992000	2.848824000	9.058948000
C	9.994795000	6.864674000	5.812407000
N	9.646330000	3.844391000	3.714413000
C	3.494281000	2.813112000	6.507821000
H	2.830117000	2.657242000	7.345544000
C	6.053389000	4.790605000	-0.254970000
C	6.513719000	3.424793000	0.109277000
C	6.193691000	6.756915000	3.611125000
H	5.715204000	6.194017000	2.821245000
C	3.102669000	3.047845000	5.166669000
H	2.090780000	3.099106000	4.785456000
C	5.801000000	0.161343000	6.758728000
H	5.089120000	0.501297000	6.014174000
C	4.212580000	2.138932000	9.502552000
H	3.745881000	1.415868000	8.842365000
C	4.267529000	3.216916000	4.444206000
H	4.386823000	3.428907000	3.388678000
C	7.842483000	1.815388000	3.322656000
C	6.606198000	2.339945000	-0.893250000
C	10.215440000	7.171011000	4.466117000
H	9.361758000	7.337482000	3.816671000
C	6.986957000	0.714043000	3.354553000
H	5.920303000	0.872182000	3.495893000
C	6.841368000	8.316584000	5.084204000
H	6.919573000	9.241124000	5.638041000
C	8.519407000	7.711577000	7.612097000
C	9.221009000	1.609654000	3.102397000
C	5.853525000	5.640762000	7.414657000
H	5.892594000	6.522561000	6.775326000
H	5.824346000	5.945502000	8.462207000
H	4.968926000	5.047922000	7.179649000
C	5.996147000	8.074205000	3.972028000
H	5.315056000	8.775871000	3.508173000
C	7.229980000	0.625774000	8.635702000
H	7.626397000	1.322782000	9.369381000
C	5.480118000	3.868529000	11.265578000
H	5.997849000	4.533191000	11.952112000
C	5.977447000	3.691192000	9.973049000
H	6.889929000	4.206240000	9.687165000
C	4.956996000	4.973835000	-1.113898000
H	4.441129000	4.105287000	-1.512873000
C	10.098954000	2.793171000	3.110207000
C	4.334635000	3.194010000	11.674440000
H	3.943136000	3.332536000	12.678302000

C	8.795249000	9.074992000	7.430371000
H	9.024349000	9.443768000	6.435646000
C	8.309616000	7.254788000	8.915521000
H	8.150378000	6.196445000	9.098592000
C	6.162144000	-1.185895000	6.824708000
H	5.726794000	-1.890676000	6.121186000
C	8.324434000	8.133869000	10.000260000
H	8.155645000	7.750229000	11.002913000
C	9.722535000	0.307147000	2.945325000
H	10.787456000	0.148561000	2.798704000
C	3.708595000	2.319014000	10.786407000
H	2.830305000	1.760758000	11.099255000
C	8.803908000	9.955018000	8.507491000
H	9.013917000	11.007550000	8.337281000
C	7.066705000	-1.628750000	7.784790000
H	7.346380000	-2.677624000	7.834828000
C	11.107596000	6.685432000	6.646441000
H	10.955314000	6.482743000	7.703168000
C	6.734974000	2.619129000	-2.263916000
H	6.752163000	3.650843000	-2.601020000
C	7.493074000	-0.579052000	3.214328000
H	6.822190000	-1.432933000	3.267818000
C	8.560635000	9.489841000	9.800312000
H	8.570516000	10.176361000	10.642200000
C	6.612755000	0.993197000	-0.490570000
H	6.515061000	0.759480000	0.565891000
C	11.514698000	7.278116000	3.962699000
H	11.663981000	7.528254000	2.915557000
C	4.521087000	6.253358000	-1.445592000
H	3.665612000	6.374580000	-2.104946000
C	6.741125000	-0.031166000	-1.421291000
H	6.739150000	-1.064427000	-1.083447000
C	7.602335000	-0.713878000	8.692414000
H	8.299659000	-1.046823000	9.456810000
C	12.612864000	7.080223000	4.796946000
H	13.622603000	7.172120000	4.406129000
C	6.692505000	5.925019000	0.262783000
H	7.539566000	5.802518000	0.931637000
C	6.859846000	0.259160000	-2.781577000
H	6.952228000	-0.542614000	-3.508980000
C	8.859790000	-0.782112000	3.007099000
H	9.251880000	-1.789151000	2.897686000
C	12.403166000	6.783299000	6.144494000
H	13.250117000	6.643449000	6.811187000
C	6.857255000	1.589960000	-3.194565000
H	6.958576000	1.833287000	-4.249149000
C	5.168119000	7.374639000	-0.925771000
H	4.824714000	8.372845000	-1.182854000
C	6.253131000	7.204792000	-0.067436000
H	6.757316000	8.068604000	0.356118000
C	11.421299000	2.778850000	2.436826000
C	12.522266000	3.407851000	3.036309000
C	11.575484000	2.187791000	1.173725000
C	13.753614000	3.438181000	2.389148000
C	12.805030000	2.235864000	0.522516000
C	13.896863000	2.854834000	1.130326000
H	12.416831000	3.858995000	4.019301000
H	10.723120000	1.714926000	0.695351000
H	14.603155000	3.915162000	2.869341000
H	12.909087000	1.790180000	-0.462499000
H	14.857786000	2.882411000	0.624267000
H	10.261585000	4.654878000	3.638263000

2a⁺Int7

Lu	-0.155849000	-0.270174000	-0.148480000
N	-0.795611000	0.831191000	2.271547000
N	-1.119158000	1.732641000	-0.567271000
N	-1.726256000	-1.649532000	0.660825000
C	0.236381000	1.652661000	1.807900000
C	1.400686000	0.902698000	1.851825000
H	2.374382000	1.266675000	1.561222000
N	-0.156551000	-1.277817000	-2.198260000
C	1.082004000	-0.385765000	2.350341000
H	1.759326000	-1.210863000	2.506835000
C	-0.151318000	-2.819660000	3.235759000

N	-1.318174000	-1.088957000	-2.964118000	H	-3.783235000	-0.821368000	-3.139635000
C	-1.114457000	-1.607512000	3.078487000	C	2.909014000	3.757219000	-1.273725000
C	-2.131107000	-1.857266000	1.968501000	H	3.076322000	3.690034000	-2.345084000
C	-1.026440000	2.916901000	0.145271000	C	1.157636000	2.558872000	-4.769964000
C	-0.276592000	-0.416452000	2.623890000	H	1.186212000	3.644557000	-4.731656000
C	0.048157000	3.049131000	1.219906000	C	-4.944252000	-0.163692000	-4.830118000
C	-1.765549000	-1.379678000	4.455022000	H	-5.891956000	-0.457659000	-4.387447000
C	1.415308000	3.476134000	0.618722000	C	1.599199000	-3.950469000	4.488903000
N	2.036819000	-0.801066000	-0.607653000	H	2.260780000	-3.981000000	5.350862000
C	-3.418661000	-2.372830000	1.985535000	C	3.928683000	4.187597000	-0.428972000
H	-4.011499000	-2.619101000	2.854386000	H	4.898436000	4.463608000	-0.834291000
C	-0.029814000	0.484730000	-4.367113000	C	1.066528000	-0.225427000	-4.872250000
C	-1.264268000	-0.234863000	-3.930544000	H	1.024824000	-1.309657000	-4.920833000
C	-2.188093000	1.887869000	-1.422829000	C	-4.915187000	0.422980000	-6.096842000
H	-2.499085000	1.080675000	-2.069285000	H	-5.839182000	0.584645000	-6.645331000
C	-3.825827000	-2.500063000	0.633351000	C	1.517137000	-5.120235000	-2.723171000
H	-4.778649000	-2.869928000	0.276522000	H	1.922874000	-6.120701000	-2.833147000
C	-0.121131000	-3.857701000	2.300909000	C	3.691019000	4.268869000	0.943465000
H	-0.791416000	-3.827422000	1.448945000	H	4.474248000	4.612140000	1.614396000
C	-2.563517000	-2.390483000	5.011150000	C	-3.695407000	0.803307000	-6.651397000
H	-2.714101000	-3.312317000	4.459252000	H	-3.662247000	1.257237000	-7.638020000
C	-2.773401000	-2.055620000	-0.139706000	C	2.244563000	1.845961000	-5.275288000
H	-2.687301000	-1.998806000	-1.217998000	H	3.124045000	2.373550000	-5.634784000
C	0.398062000	-2.508305000	-2.366568000	C	2.194845000	0.453178000	-5.326905000
C	-2.528478000	0.014970000	-4.672652000	H	3.035435000	-0.107191000	-5.727190000
C	1.661006000	3.406232000	-0.755008000	C	4.021212000	-2.031578000	-1.193766000
H	0.870423000	3.079493000	-1.422463000	C	4.754346000	-1.807966000	-0.019540000
C	-0.246564000	-3.511887000	-3.154848000	C	4.711709000	-2.339632000	-2.374738000
H	-1.203552000	-3.265501000	-3.598291000	C	6.144052000	-1.894575000	-0.023550000
C	-2.015328000	3.797779000	-0.266001000	C	6.101820000	-2.410612000	-2.380265000
H	-2.209110000	4.785090000	0.127305000	C	6.821178000	-2.191540000	-1.205398000
C	-0.332077000	4.092577000	2.286486000	H	4.227407000	-1.595680000	0.907033000
C	1.699808000	-2.843806000	-1.832947000	H	4.150303000	-2.506976000	-3.288539000
C	-2.199533000	1.226274000	2.418910000	H	6.697372000	-1.736024000	0.897767000
H	-2.421120000	2.009439000	1.694395000	H	6.625303000	-2.636291000	-3.305076000
H	-2.381473000	1.596788000	3.429313000	H	7.905699000	-2.255131000	-1.210582000
H	-2.827561000	0.353765000	2.232666000	H	2.777076000	-0.167898000	-0.312757000
C	-2.757788000	3.135782000	-1.274818000				
H	-3.617307000	3.519249000	-1.809227000				
C	0.717120000	-2.884387000	4.334987000				
H	0.694212000	-2.096793000	5.083174000				
C	-2.077928000	-0.098021000	6.501240000				
H	-1.863153000	0.794758000	7.082565000				
C	-1.510218000	-0.247947000	5.234366000				
H	-0.840878000	0.523131000	4.864192000				
C	0.021986000	1.884085000	-4.324522000				
H	-0.824793000	2.438381000	-3.929009000				
C	2.538440000	-1.867618000	-1.186314000				
C	-2.905541000	-1.088431000	7.019434000				
H	-3.351282000	-0.973556000	8.003488000				
C	-0.454116000	5.438665000	1.910143000				
H	-0.276086000	5.719755000	0.876846000				
C	-0.488042000	3.774723000	3.637590000				
H	-0.344021000	2.752397000	3.973352000				
C	0.760295000	-4.929382000	2.457547000				
H	0.764842000	-5.726357000	1.718897000				
C	-0.803266000	4.756620000	4.579211000				
H	-0.920045000	4.479319000	5.623463000				
C	2.205015000	-4.155539000	-2.024038000				
H	3.166633000	-4.398322000	-1.583097000				
C	-3.137175000	-2.241991000	6.269692000				
H	-3.757236000	-3.038430000	6.672294000				
C	-0.774608000	6.418639000	2.843722000				
H	-0.868953000	7.452861000	2.523721000				
C	1.624615000	-4.980152000	3.547751000				
H	2.307658000	-5.816678000	3.668916000				
C	2.446151000	3.918420000	1.460253000				
H	2.267852000	3.995340000	2.529204000				
C	-2.511080000	0.604338000	-5.945174000				
H	-1.565314000	0.900109000	-6.387525000				
C	0.282095000	-4.773062000	-3.303017000				
H	-0.273589000	-5.512713000	-3.874765000				
C	-0.958821000	6.081256000	4.185267000				
H	-1.205843000	6.846818000	4.915399000				
C	-3.764535000	-0.368650000	-4.125380000				
				2a'			
				Lu	8.362058000	5.877346000	4.529646000
				O	8.382439000	6.368948000	2.125007000
				N	6.184683000	5.181965000	4.170907000
				N	8.145926000	3.044285000	5.243907000
				N	10.551804000	6.749361000	4.309901000
				H	11.296729000	6.221074000	4.765438000
				N	8.590446000	5.595392000	6.787909000
				N	8.178951000	8.166457000	4.601783000
				C	9.195803000	4.612000000	7.548860000
				C	7.164419000	2.730536000	6.284135000
				H	6.182016000	3.060943000	5.945087000
				H	7.437378000	3.261102000	7.195773000
				H	7.144966000	1.655699000	6.473525000
				C	9.475568000	3.389191000	5.467607000
				C	10.078753000	3.578529000	6.853685000
				C	10.128522000	8.896950000	3.297440000
				C	8.773248000	9.059211000	3.754485000
				C	9.045399000	3.444404000	3.238423000
				H	9.157991000	3.532523000	2.170355000
				C	6.489706000	2.845016000	3.296349000
				C	7.878905000	3.059903000	3.879446000
				N	7.041939000	8.576755000	5.281817000
				C	5.620186000	3.944490000	3.907368000
				C	8.856308000	4.767295000	8.886704000
				H	9.153182000	4.135434000	9.711240000
				C	12.478179000	8.139206000	3.867567000
				C	11.008435000	7.877963000	3.837011000
				C	7.647109000	7.533476000	0.198351000
				H	8.088291000	8.531543000	0.290706000
				H	6.812158000	7.587850000	-0.505414000
				C	8.004506000	5.895726000	8.962027000
				H	7.533429000	6.298004000	9.849698000
				C	5.963682000	1.413221000	3.553602000
				C	5.796727000	9.969750000	6.730055000
				C	4.577016000	9.690955000	6.092220000
				H	4.594042000	9.223644000	5.113051000

C	3.368867000	10.013766000	6.699986000
H	2.434800000	9.793313000	6.190490000
C	3.354457000	10.624918000	7.954393000
H	2.409878000	10.879406000	8.427372000
C	4.558811000	10.911403000	8.595287000
H	4.556695000	11.382067000	9.574661000
C	5.770225000	10.592439000	7.987802000
H	6.703687000	10.811306000	8.496890000
C	10.180290000	2.255486000	7.642280000
C	8.303357000	10.364663000	6.458987000
C	5.680971000	3.800261000	1.053521000
H	4.998589000	4.426846000	1.620787000
C	10.043055000	3.648331000	4.227691000
H	11.075576000	3.911192000	4.059377000
C	11.919895000	5.351455000	7.141654000
H	11.169985000	6.000367000	7.583008000
C	11.537343000	4.083207000	6.696578000
C	3.983141000	5.257337000	4.726872000
H	3.209849000	5.618056000	5.092006000
C	9.425965000	9.708777000	6.981836000
H	9.407821000	8.628794000	7.093477000
C	13.249057000	5.771278000	7.041766000
H	13.526571000	6.759739000	7.397279000
C	4.271234000	3.958142000	4.243945000
H	3.574969000	3.134413000	4.184373000
C	9.809481000	1.020567000	7.103939000
H	9.411749000	0.968216000	6.095260000
C	6.543725000	2.949446000	1.747655000
C	12.520544000	3.241219000	6.155834000
H	12.247341000	2.239555000	5.834917000
C	7.081594000	9.589456000	6.092698000
C	7.866890000	6.365589000	7.671377000
H	7.256794000	7.183740000	7.313831000
C	10.649263000	9.801640000	2.340190000
H	11.668328000	9.650576000	1.997180000
C	5.166477000	5.965397000	4.667069000
H	5.372673000	6.982467000	4.975444000
C	13.375272000	7.148933000	3.445995000
H	12.990914000	6.210106000	3.056387000
C	8.057903000	10.180708000	3.238663000
H	7.038134000	10.335490000	3.571543000
C	6.766720000	0.406144000	4.097657000
H	7.787035000	0.631256000	4.393496000
C	9.414816000	6.269638000	1.122391000
H	9.880067000	5.284506000	1.203444000
H	10.169156000	7.038836000	1.319634000
C	10.761984000	2.263725000	8.919116000
H	11.124266000	3.199088000	9.333180000
C	12.985026000	9.353309000	4.354337000
H	12.293668000	10.119299000	4.691950000
C	7.207425000	7.017341000	1.561009000
H	6.419830000	6.264862000	1.490117000
H	6.894968000	7.804382000	2.250041000
C	7.377132000	2.100614000	1.004090000
H	8.016485000	1.390368000	1.521272000
C	10.909040000	1.089763000	9.650301000
H	11.356493000	1.128040000	10.639933000
C	10.501388000	-0.131652000	9.113136000
H	10.618831000	-1.049479000	9.682457000
C	4.682518000	1.053527000	3.109915000
H	4.065918000	1.789846000	2.606247000
C	6.523545000	3.000261000	-1.070692000
H	6.512182000	3.016521000	-2.157218000
C	8.321378000	11.760839000	6.343619000
H	7.448631000	12.275715000	5.951643000
C	14.214433000	4.930923000	6.494510000
H	15.247491000	5.258478000	6.420275000
C	8.598612000	11.028352000	2.297047000
H	7.991683000	11.843953000	1.910685000
C	13.843487000	3.661110000	6.049580000
H	14.589057000	2.989387000	5.631720000
C	9.445378000	12.488861000	6.726522000
H	9.448091000	13.570795000	6.625662000
C	8.710650000	6.510515000	-0.204036000
H	8.240314000	5.588614000	-0.561458000

H	9.396938000	6.874850000	-0.973545000
C	9.909200000	10.843646000	1.823306000
H	10.332311000	11.508092000	1.076803000
C	9.961904000	-0.161415000	7.831705000
H	9.660752000	-1.106198000	7.386903000
C	6.291846000	-0.897452000	4.251503000
H	6.940407000	-1.655764000	4.682338000
C	5.001004000	-1.225816000	3.851005000
H	4.627143000	-2.238577000	3.972733000
C	10.558380000	11.830581000	7.247640000
H	11.431010000	12.398395000	7.559665000
C	14.359304000	9.563137000	4.424381000
H	14.740866000	10.501896000	4.816309000
C	10.541927000	10.441387000	7.379807000
H	11.399068000	9.924762000	7.803122000
C	5.668122000	3.823906000	-0.343244000
H	4.978037000	4.485777000	-0.860616000
C	7.379327000	2.134425000	-0.387490000
H	8.036638000	1.468206000	-0.940409000
C	4.201500000	-0.242022000	3.269294000
H	3.201089000	-0.486839000	2.922480000
C	14.749451000	7.368963000	3.498283000
H	15.432631000	6.598577000	3.152210000
C	15.244373000	8.575532000	3.990407000
H	16.316372000	8.747182000	4.034525000

3a'

Lu	3.777311000	7.078210000	4.749662000
Si	8.000429000	9.231190000	4.482796000
N	1.582974000	6.068168000	5.901384000
N	4.645370000	8.700177000	3.400865000
N	4.355184000	6.940542000	6.905152000
N	3.661023000	5.019374000	3.899864000
N	5.574176000	7.814183000	3.783164000
C	1.257779000	6.145940000	4.544660000
C	1.689479000	7.353930000	6.437692000
C	1.456587000	8.245655000	5.398096000
H	1.473928000	9.321150000	5.481049000
C	2.163080000	7.657706000	7.859552000
C	1.185372000	4.940387000	3.607792000
C	1.763547000	4.822304000	6.654037000
H	2.127704000	4.054127000	5.971064000
H	0.814507000	4.507044000	7.090519000
H	2.493139000	4.994931000	7.446360000
C	1.191895000	7.496367000	4.220633000
H	0.970611000	7.894090000	3.241389000
C	3.522851000	6.976826000	8.008843000
C	2.536305000	4.235339000	3.718635000
C	0.953499000	5.480223000	2.168915000
C	1.150239000	7.207666000	8.928311000
C	4.649822000	9.666411000	2.505888000
C	5.637119000	9.847804000	1.417052000
C	2.292201000	9.200696000	7.988946000
C	4.161944000	6.401003000	9.097895000
H	3.761647000	6.266334000	10.092197000
C	3.489600000	10.585974000	2.545917000
C	-0.095107000	6.659806000	8.609749000
H	-0.377295000	6.523624000	7.569918000
C	3.538920000	9.827274000	8.068810000
H	4.440564000	9.224317000	8.046803000
C	1.138975000	9.996297000	8.043370000
H	0.160834000	9.524302000	8.008227000
C	1.229428000	11.381046000	8.157236000
H	0.321815000	11.977306000	8.202116000
C	5.522504000	6.338213000	7.317266000
H	6.335448000	6.176516000	6.619624000
C	6.133004000	11.125124000	1.101068000
H	5.824557000	11.975881000	1.702339000
C	1.437295000	7.443280000	10.281040000
H	2.367099000	7.934202000	10.549545000
C	-0.000545000	4.010970000	3.927390000
C	6.986467000	7.912624000	3.479108000
H	7.193185000	8.055189000	2.411536000
H	7.418819000	6.940677000	3.748475000
C	-0.292236000	6.020108000	1.818363000

H	-1.092045000	6.043068000	2.553730000	N	7.293443000	1.540025000	5.110252000
C	2.479088000	11.998295000	8.229519000	C	3.348347000	4.145711000	4.935040000
H	2.552364000	13.077993000	8.327052000	C	6.691885000	4.426473000	2.377598000
C	-0.688628000	6.505163000	10.947419000	C	5.568460000	4.939107000	4.303292000
H	-1.393820000	6.228378000	11.725997000	C	5.888598000	3.015368000	0.553082000
C	3.630065000	11.215867000	8.189062000	C	6.911604000	4.093345000	0.902739000
H	4.609010000	11.682698000	8.256605000	C	4.878523000	5.152814000	6.699416000
C	5.444782000	5.993612000	8.651350000	C	7.575764000	4.304528000	3.440337000
H	6.208616000	5.499672000	9.237803000	H	8.607357000	3.996042000	3.365015000
C	4.740181000	4.165297000	3.876894000	C	8.212212000	1.129214000	5.879058000
H	5.747154000	4.546446000	3.999988000	C	8.362019000	3.569150000	0.718818000
C	2.907879000	2.904672000	3.592007000	C	4.240902000	5.067828000	2.137514000
H	2.253898000	2.052530000	3.457071000	H	4.253208000	4.441425000	1.245129000
C	-1.005341000	6.306125000	9.607866000	H	4.204819000	6.119483000	1.847663000
H	-1.965939000	5.880443000	9.330412000	H	3.372201000	4.826850000	2.750705000
C	0.536493000	7.085095000	11.278491000	C	6.794049000	5.339110000	0.001202000
H	0.787372000	7.272720000	12.318987000	C	1.960161000	4.169442000	4.951363000
C	6.018443000	8.769345000	0.599330000	H	1.325356000	5.020270000	5.151680000
H	5.605339000	7.783533000	0.795082000	C	6.877453000	4.621871000	4.635517000
C	1.957015000	5.432538000	1.198017000	H	7.277826000	4.597016000	5.636935000
H	2.921079000	5.002956000	1.448724000	C	9.448031000	4.446884000	0.846762000
C	-2.026934000	3.444303000	5.149731000	H	9.267299000	5.487574000	1.101778000
H	-2.740786000	3.686886000	5.932384000	C	3.834625000	6.654744000	5.042131000
C	2.975349000	11.040679000	3.771950000	C	8.615928000	2.243390000	0.358698000
H	3.467951000	10.744798000	4.693602000	H	7.782863000	1.557807000	0.243866000
C	2.881538000	11.044346000	1.363899000	C	10.750530000	4.011614000	0.622294000
H	3.267008000	10.710895000	0.404793000	H	11.576281000	4.711014000	0.721798000
C	-0.939795000	4.290872000	4.923223000	C	9.674671000	1.259498000	5.537578000
H	-0.841499000	5.191073000	5.522477000	C	4.395799000	4.182269000	7.580147000
C	7.007065000	11.310463000	0.034295000	H	3.682819000	3.447842000	7.219978000
H	7.388541000	12.304708000	-0.182452000	C	6.990258000	5.203218000	-1.381261000
C	-0.522346000	6.515379000	0.538078000	H	7.214269000	4.224369000	-1.792660000
H	-1.495385000	6.930262000	0.288727000	C	7.888380000	0.468423000	7.197191000
C	4.322508000	2.863504000	3.692892000	C	5.172112000	2.767689000	-0.610179000
H	4.950129000	1.983121000	3.642955000	H	5.187391000	3.348059000	-1.521217000
C	0.487879000	6.468670000	-0.423196000	C	5.778244000	6.110732000	7.188593000
H	0.308617000	6.849231000	-1.425016000	H	6.138740000	6.893769000	6.526822000
C	1.876802000	11.896723000	3.817329000	C	1.525274000	2.863173000	4.616251000
H	1.507409000	12.241731000	4.779495000	H	0.501838000	2.523129000	4.523583000
C	9.456925000	9.760168000	3.388791000	C	6.200943000	6.085114000	8.514386000
H	10.068617000	8.897461000	3.103890000	H	6.900994000	6.836326000	8.870424000
H	10.105735000	10.467909000	3.915902000	C	6.600849000	6.626324000	0.509265000
H	9.103473000	10.241246000	2.471286000	H	6.508710000	6.777605000	1.580670000
C	-0.212296000	2.880249000	3.124821000	C	10.992843000	2.688440000	0.250315000
H	0.462811000	2.681560000	2.298909000	H	12.007255000	2.352400000	0.052114000
C	7.391434000	10.225914000	-0.756525000	C	2.666109000	2.115001000	4.409819000
H	8.070921000	10.371241000	-1.591661000	H	2.746074000	1.081652000	4.097508000
C	1.723574000	5.922480000	-0.088606000	C	10.085295000	1.264411000	4.198426000
H	2.515583000	5.871461000	-0.831027000	H	9.336684000	1.136109000	3.421758000
C	6.961937000	10.734658000	4.975694000	C	2.757961000	7.081157000	5.833926000
H	6.639841000	11.309205000	4.103881000	H	2.327217000	6.398634000	6.559251000
H	7.549796000	11.395849000	5.622166000	C	10.643543000	1.450296000	6.533770000
H	6.071611000	10.428091000	5.533021000	H	10.342585000	1.463799000	7.577264000
C	6.887865000	8.957585000	-0.473839000	C	6.932231000	6.306057000	-2.226750000
H	7.166009000	8.109904000	-1.094411000	H	7.080765000	6.170104000	-3.294639000
C	1.786268000	11.901173000	1.410018000	C	4.426901000	7.589619000	4.189054000
H	1.324949000	12.232417000	0.483301000	H	5.302416000	7.313878000	3.608787000
C	-2.200085000	2.303244000	4.373621000	C	5.714352000	5.110602000	9.386401000
H	-3.043736000	1.641749000	4.549076000	H	6.034356000	5.095209000	10.424607000
C	1.275081000	12.329063000	2.636249000	C	9.921831000	1.807790000	0.122676000
H	0.423169000	13.002670000	2.669419000	H	10.096255000	0.776820000	-0.174357000
C	8.664245000	8.411410000	6.058584000	C	4.378157000	1.620981000	-0.361554000
H	7.849715000	8.087696000	6.714200000	H	3.681422000	1.152826000	-1.045135000
H	9.287851000	9.113866000	6.622509000	C	4.648112000	1.233751000	0.935245000
H	9.280128000	7.536133000	5.824891000	H	4.204324000	0.428897000	1.507382000
C	-1.289360000	2.030242000	3.352300000	C	4.806731000	4.166530000	8.915049000
H	-1.425698000	1.157687000	2.719172000	H	4.406249000	3.413004000	9.588251000
				C	4.822330000	-0.642773000	4.980251000
				H	3.740568000	-0.775737000	4.883542000
				H	5.040427000	0.031604000	5.811471000
				C	3.930477000	8.890513000	4.084677000
				H	4.411108000	9.594602000	3.410664000
				C	2.255399000	8.373665000	5.727327000
				H	1.416072000	8.674302000	6.348673000
				C	11.983107000	1.640928000	6.198876000
4a'							
Lu	5.820103000	2.300899000	3.774521000				
O	5.291014000	-0.013136000	3.749767000				
N	5.454540000	4.801418000	2.916105000				
N	5.575802000	2.071901000	1.514154000				
N	3.794034000	2.879107000	4.602697000				
C	4.386736000	5.226753000	5.228635000				

H	12.717416000	1.801091000	6.984074000	H	6.482580000	-1.849023000	5.656374000
C	2.834046000	9.285267000	4.843763000	C	6.550200000	7.737240000	-0.335230000
H	2.444102000	10.296008000	4.762919000	H	6.396769000	8.725839000	0.089220000
C	8.584757000	-0.669584000	7.630226000	C	12.379059000	1.626476000	4.862925000
H	9.417762000	-1.043135000	7.040717000	H	13.424610000	1.765944000	4.601092000
C	6.702997000	7.581160000	-1.708685000	C	6.820400000	0.937508000	7.972780000
H	6.661277000	8.443290000	-2.368374000	H	6.281789000	1.819848000	7.639042000
C	6.218107000	-0.904562000	3.072650000	C	11.424350000	1.436019000	3.862635000
H	7.239936000	-0.606819000	3.336877000	H	11.719350000	1.429593000	2.817611000
H	6.064011000	-0.777433000	1.999949000	C	8.212949000	-1.329864000	8.800865000
C	5.887719000	-2.283783000	3.613944000	H	8.753723000	-2.219160000	9.114302000
H	6.720495000	-2.982116000	3.496448000	C	7.155039000	-0.847411000	9.569362000
H	5.014838000	-2.698812000	3.097758000	H	6.871577000	-1.353715000	10.488231000
C	5.562937000	-1.971337000	5.076321000	C	6.464225000	0.292287000	9.153684000
H	4.955579000	-2.741378000	5.559051000	H	5.645341000	0.679874000	9.754096000

8. References

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