Alkyl Complexes of La and Sm Supported by Chiral Binaphthylamido Ligand. Syntheses, Structures and Catalytic Activity in Hydroamination of Amino-1,3-dienes

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Table 1. Crystallographic data for complexes 1-2.

	RX793 (1)	**RX794 (2)**
formula	C_{45} H_{54} Li_2 N_2 O_3 Sm_1	2(C_{46} H_{54} La_1 Li_3 N_2 O_3), C_4 H_8 O
Fw	835.14	1757.39
crystal system	monoclinic	monoclinic
space group	*P* 2_1	*P* 2_1
a [Å]	16.6559(4)	19.1789(13)
b [Å]	13.5871(3)	10.6715(6)
c [Å]	18.4721(4)	22.0313(14)
α [°]	90	90
β [°]	90.9210(10)	96.469(4)
γ [°]	90	90
V [Å^3]	4179.80(16)	4480.4(5)
Z	2	2
F(000)	1720	1816
λ[Å]	0.71075	0.71075
T [K]	100(1)	100(1)
ρ_{calcd} [Mg m^{-3}]	1.327	1.303
μ($Mo_{K\alpha}$) [mm^{-1}]	1.444	0.995
θrange [° min-max]	1.63 - 45.33	0.93 - 30.58
no. of data collected	138 035	101 214
no. of unique data	60 991	26 335
R(int)	0.0234	
no. of variable parameters/ restraints	955 / 0	1001 / 259
no. of obsd. refl.[a]	54 060	24 407
R[b] obsd., all	0.0332, 0.0426	0.0980, 0.1052
*R*w[c] obsd., all	0.0735, 0.0776	0.2427, 0.2463
Flack parameter	0.006(3)	0.11(2)
S	1.033	1.264
$(\Delta/\sigma)_{max}$	0.014	0.015
$(\Delta/\rho)_{max, min}$ [e Å^{-3}]	0.876, -0.793	0.914, -0.855

[a] Data with $F_o>4\sigma(F_o)$. [b] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [c] $Rw = [\Sigma w(|F_o^2|-|F_c^2|)^2/\Sigma w|F_o^2|^2]^{1/2}$.

(1) RX793

d(Å)	X=A	X=B
C1X–SmX	2.7756(13)	2.8046(14)
C2X–SmX	2.8560(13)	2.8770(13)
C3X–SmX	2.9533(15)	2.9430(14)
C4X–SmX	2.8649(14)	2.8575(13)
N1X–SmX	2.4558(12)	2.4641(12)
N2X–SmX	2.3411(12)	2.3441(12)
C50X–SmX	2.5879(14)	2.5978(14)
C50X–Li2X	2.186(3)	2.185(3)
C60X–SmX	2.5893(15)	2.5791(17)
C60X–Li1X	2.161(4)	2.166(4)
C70X–SmX	2.5703(17)	2.5608(17)
C70X–Li1X	2.214(4)	2.207(4)
Li1X–O80X	1.933(4)	1.951(4)
Li2X–O40X	1.916(3)	1.933(3)
Li2X–N1X	2.053(3)	2.050(3)
Li1X–O90X	1.937(4)	1.946(4)

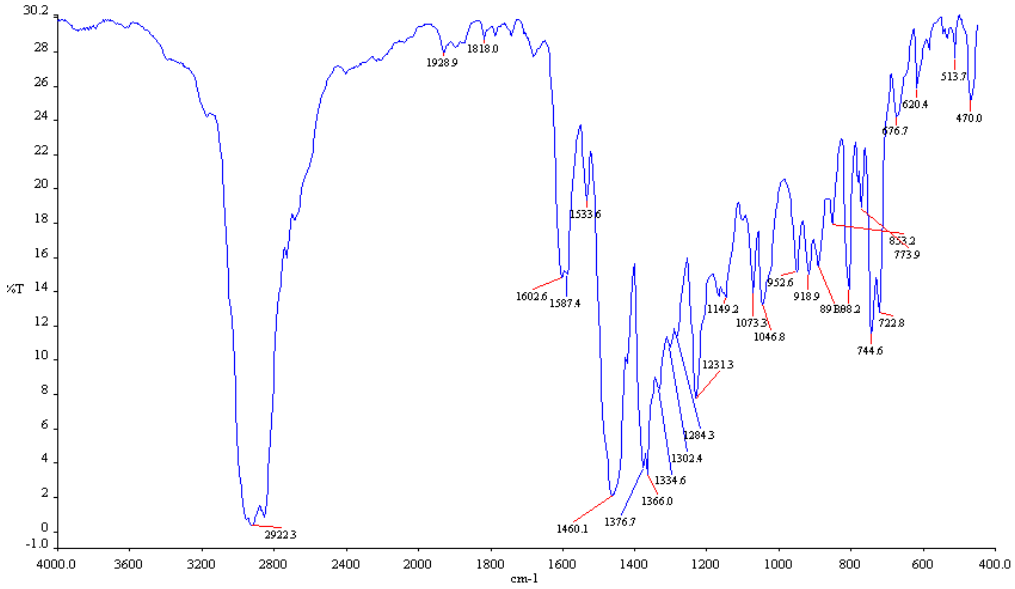
All esds are estimated using the full covariance matrix.

(2) RX794

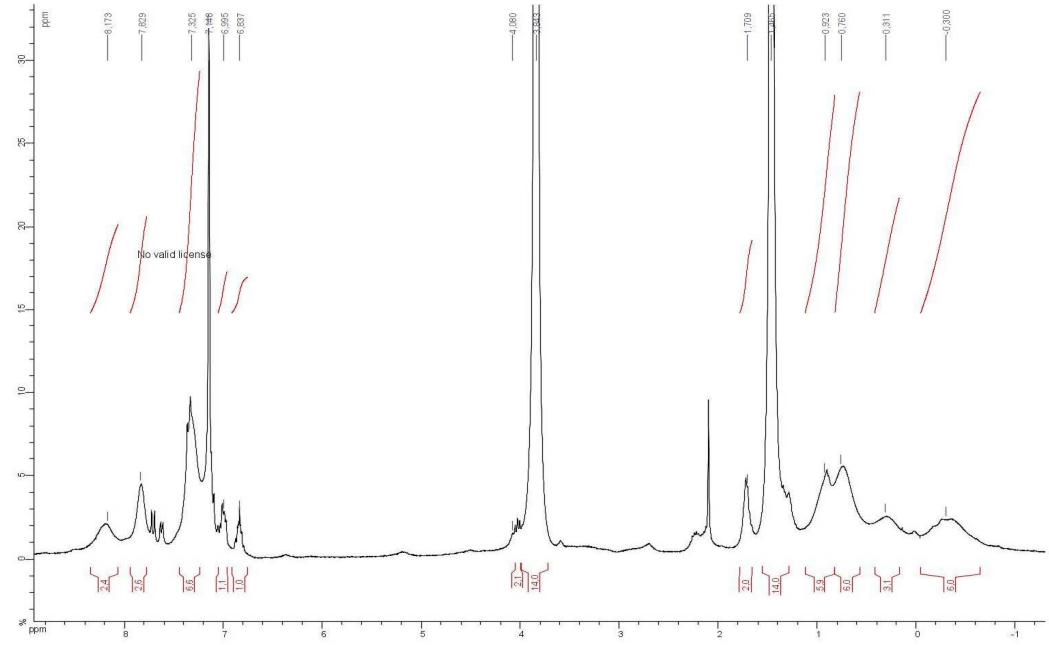
d(Å)	X=A	X=B
C1X–LaX	2.996(7)	3.149(11)
C2X–LaX	3.189(9)	3.301(10)
C3X–LaX	3.173(8)	3.083(12)
C4X–LaX	3.079(9)	2.898(11)
N1X–LaX	2.626(7)	2.647(10
N2X–LaX	2.677(8)	2.612(8)
C50X–LaX	2.832(11)	2.691(14)
C50X–Li2X	2.23(2)	2.18(3)
C60X–LaX	2.704(10)	2.749(12)
C60X–Li1X	2.21(2)	2.08(3)
C70X–LaX	2.704(8)	2.731(12)
C70X–Li1X	2.18(2)	2.11(3)
Li1X–O80X	1.946(19)	1.86(3)
Li2X–O40X	1.993(19)	1.96(2)
Li2X–N1X	2.017(19)	2.08(2)
Li3X–N2X	2.068(19)	2.01(3)
LaX–C55X	2.716(16)	2.715(15)
C55X–Li3X	2.12(2)	2.08(4)
Li3X–O50X	1.968(19)	2.06(3)

All esds are estimated using the full covariance matrix.

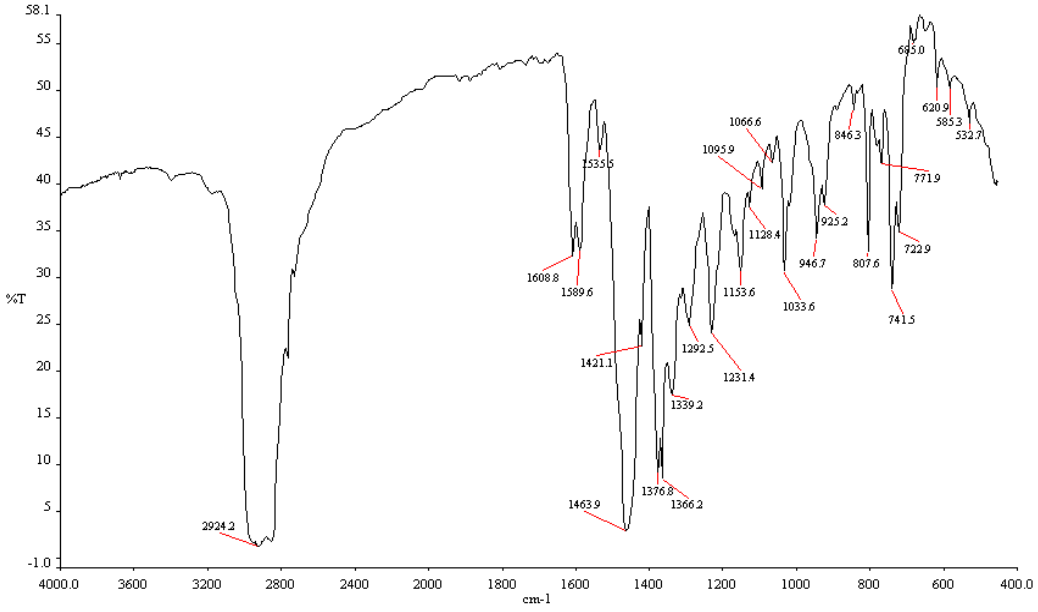
IR of complex **[(*R*)-$C_{20}H_{12}(NC_5H_9)_2$]Sm[(μ-Me)$_2$Li(THF)$_2$(μ-Me)Li(THF)] (1)**



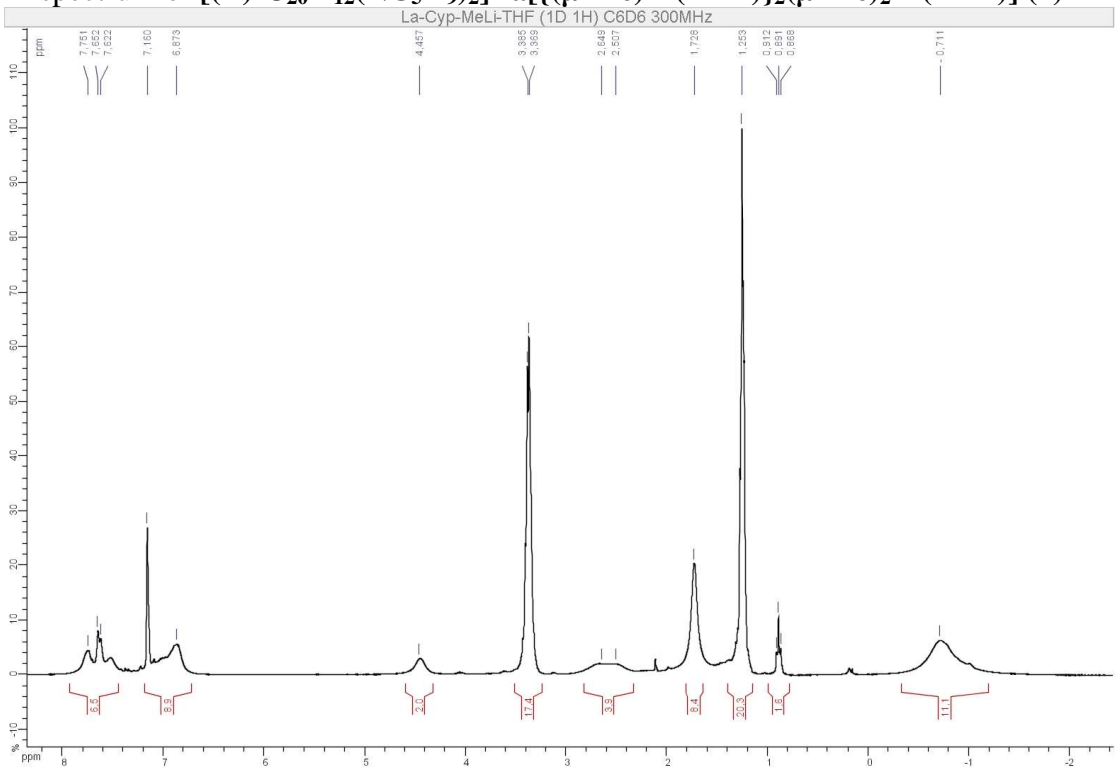
^{1}H NMR spectrum of **[(*R*)-$C_{20}H_{12}(NC_5H_9)_2$]Sm[(μ-Me)$_2$Li(THF)$_2$(μ-Me)Li(THF)] (1)**



IR spectrum of complex **[(*R*)-$C_{20}H_{12}(NC_5H_9)_2$]La[{(μ-Me)Li(THF)}$_2$(μ-Me)$_2$Li(THF)] (2)**



^{1}H NMR spectrum of **[(*R*)-$C_{20}H_{12}(NC_5H_9)_2$]La[{(μ-Me)Li(THF)}$_2$(μ-Me)$_2$Li(THF)] (2)**



^{13}C NMR spectrum of **[(*R*)-$C_{20}H_{12}(NC_5H_9)_2$]La[{(μ-Me)Li(THF)}$_2$(μ-Me)$_2$Li(THF)] (2)**