Electron Supporting Information

Metallacyclic Yttrium Alkyl and Hydrido complexes: synthesis, structures and catalytic activity in intermolecular olefin hydrophosphination and hydroamination

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Table 1. Crystallographic data and structure refinement details for complexes **2**, **3**, **5**, **6**.

	2	**3**	**5**	**6**
Formula	$C_{40}H_{67}N_2O_2SiY\cdot(C_7H_8)_2$	$C_{52}H_{94}LiN_2O_4Si_2Y$	$C_{68}H_{106}N_4O_3Y_2\cdot(C_6H_{14})_{0.5}$	$C_{111}H_{189}Li_2N_6O_{16}Y_3$
M_r	909.22	963.32	1248.47	2144.29
Crystal system	Orthorhombic	Triclinic	Monoclinic	Trigonal
Space group	$P2_12_12_1$	P-1	C2	R3c
a [Å]	9.965(1)	12.6489(7)	23.6249(6)	16.5905(7)
b [Å]	19.492(2)	20.352(1)	13.2778(4)	16.5905(7)
c [Å]	26.587(3)	24.592(1)	12.4270(3)	74.717(3)
α [°]	90	68.123(1)	90	90
β [°]	90	81.393(1)	112.176(3)	90
γ [°]	90	76.144(1)	90	120
V [Å^3]	5164.0(9)	5691.1(5)	3609.8(2)	17810(1)
Z	4	4	2	6
ρ_{calcd} [g cm^{-3}]	1.169	1.125	1.149	1.200
μ [mm^{-1}]	1.192	1.107	1.643	1.514
F(000)	1960	2092	1338	6888
Crystal size [mm^3]	0.43×0.17×0.16	0.45×0.30×0.28	0.80×0.40×0.25	0.58×0.35×0.30
θ range [°]	2.42−26.00	1.83−26.00	3.54−27.00	2.46−27.00
Index ranges	−12≤h≤12	−15≤h≤15	−30≤h≤30	−21≤h≤21
	−24≤k≤24	−25≤k≤25	−16≤k≤16	−21≤k≤21
	−32≤l≤32	−30≤l≤30	−15≤l≤15	−95≤l≤95
Reflns collected	55461	47751	29422	52002
Independent reflns[R_{int}]	10068 [0.0358]	22115 [0.0896]	7829 [0.0534]	8606 [0.0707]
Completeness to θ	99.2	98.8	99.4	99.5
Data / restraints / parameters	10068 / 17 / 556	22115 / 122 / 1180	7829 / 122 / 466	8606 / 34 / 326
goodness-of-fit on F^2	1.038	0.831	1.054	1.057
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0341	R_1 = 0.0539	R_1 = 0.0506	R_1 = 0.0657
	wR_2 = 0.0811	wR_2 = 0.0846	wR_2 = 0.1179	wR_2 = 0.1670
R indies (all data)	R_1 = 0.0369	R_1 = 0.1402	R_1 = 0.0690	R_1 = 0.0810
	wR_2 = 0.0822	wR_2 = 0.0976	wR_2 = 0.1264	wR_2 = 0.1766
Largest diff. peak/hole [e/Å^3]	0.846 / −0.264	0.787 / −0.632	0.925 / −0.676	1.182 / −0.746

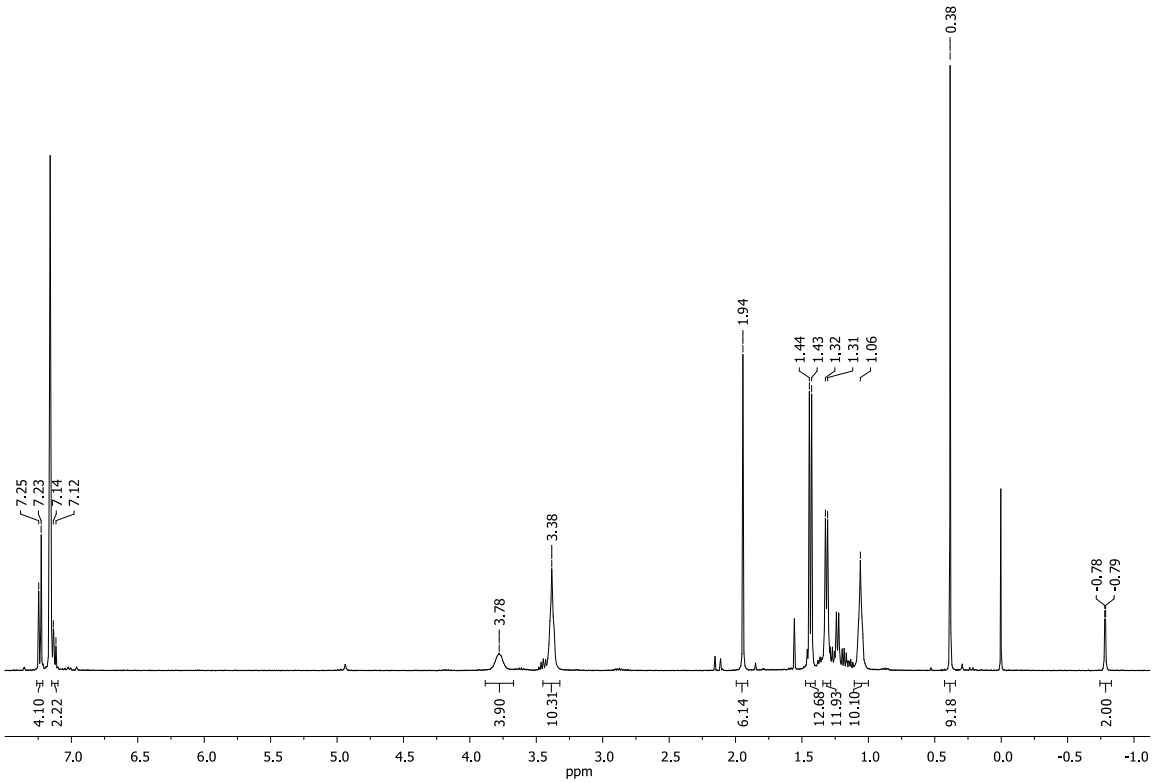

Fig 1. ^{1}H NMR spectra of complex [L^{1}]Y(CH$_2$SiMe$_3$)(THF)$_2$ (**2**) (400 MHz, C$_6$D$_6$, 293 K).

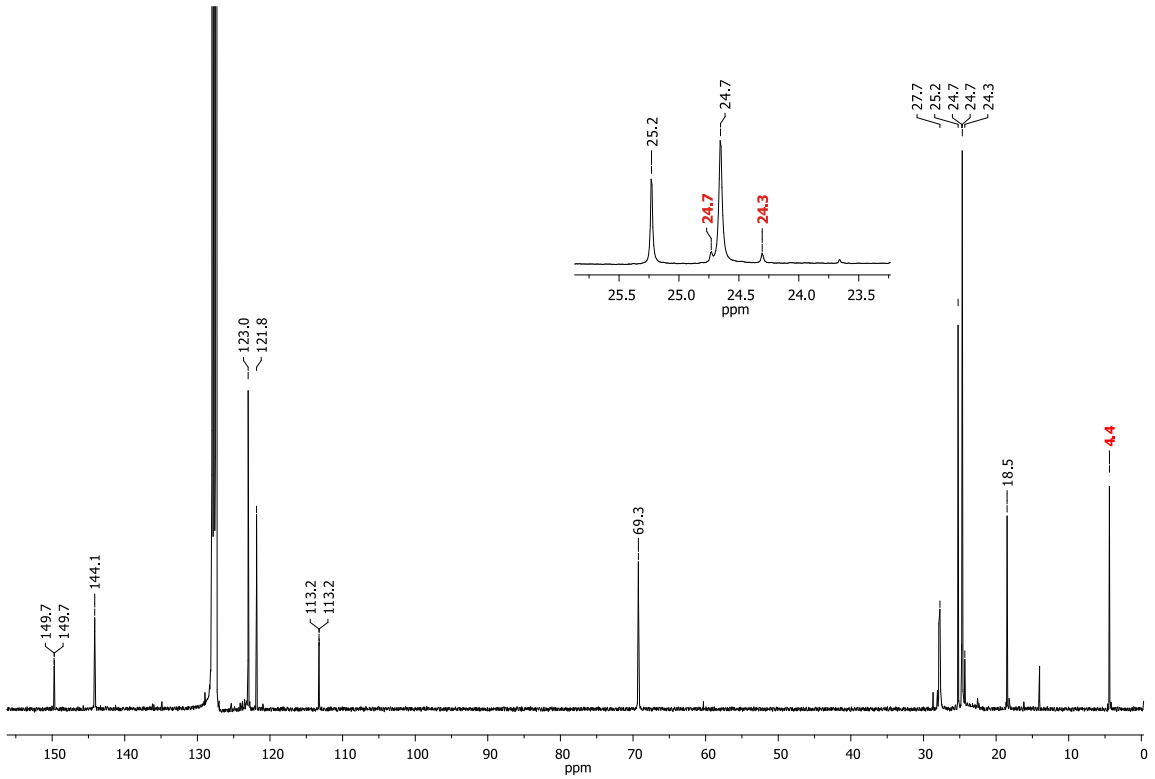

Fig 2. ^{13}C{^{1}H} NMR spectra of complex [L^{1}]Y(CH$_2$SiMe$_3$)(THF)$_2$] (**2**) (100 MHz, C$_6$D$_6$, 293 K).

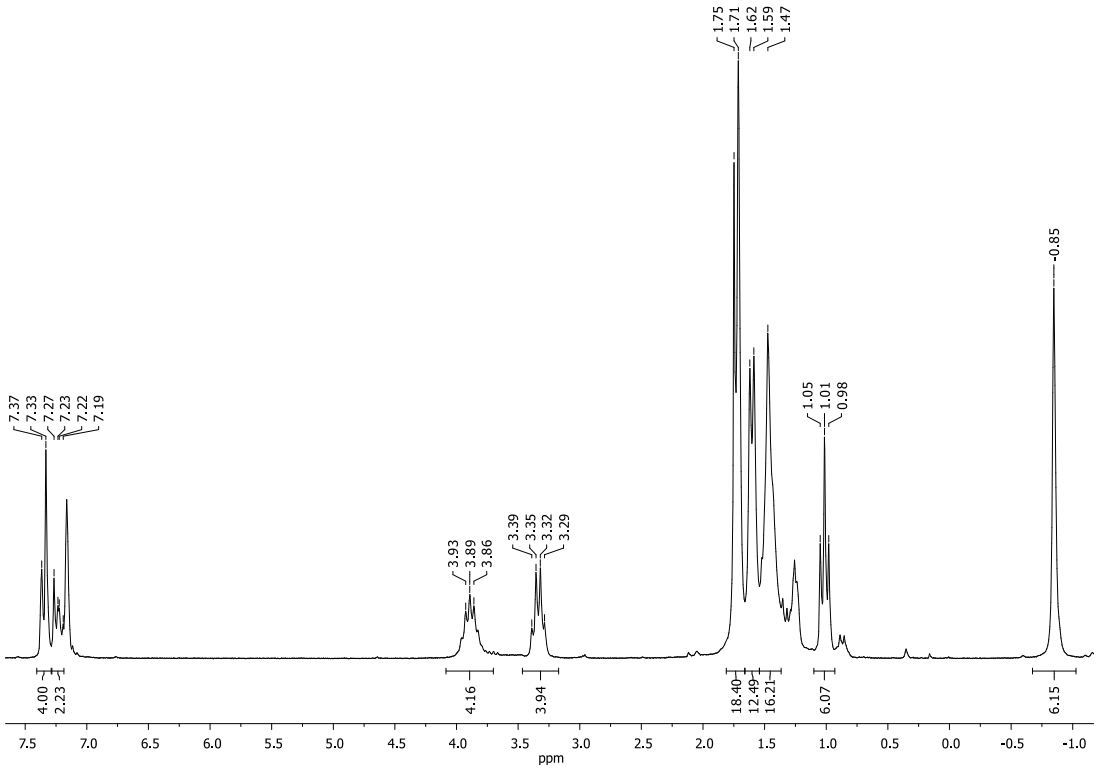

Fig 3. ^{1}H NMR spectra of complex [L^{1}]Y(OEt$_2$)(μ-Me)$_2$Li(TMEDA)] (**4**) (200 MHz, C_6D_6, 293 K).

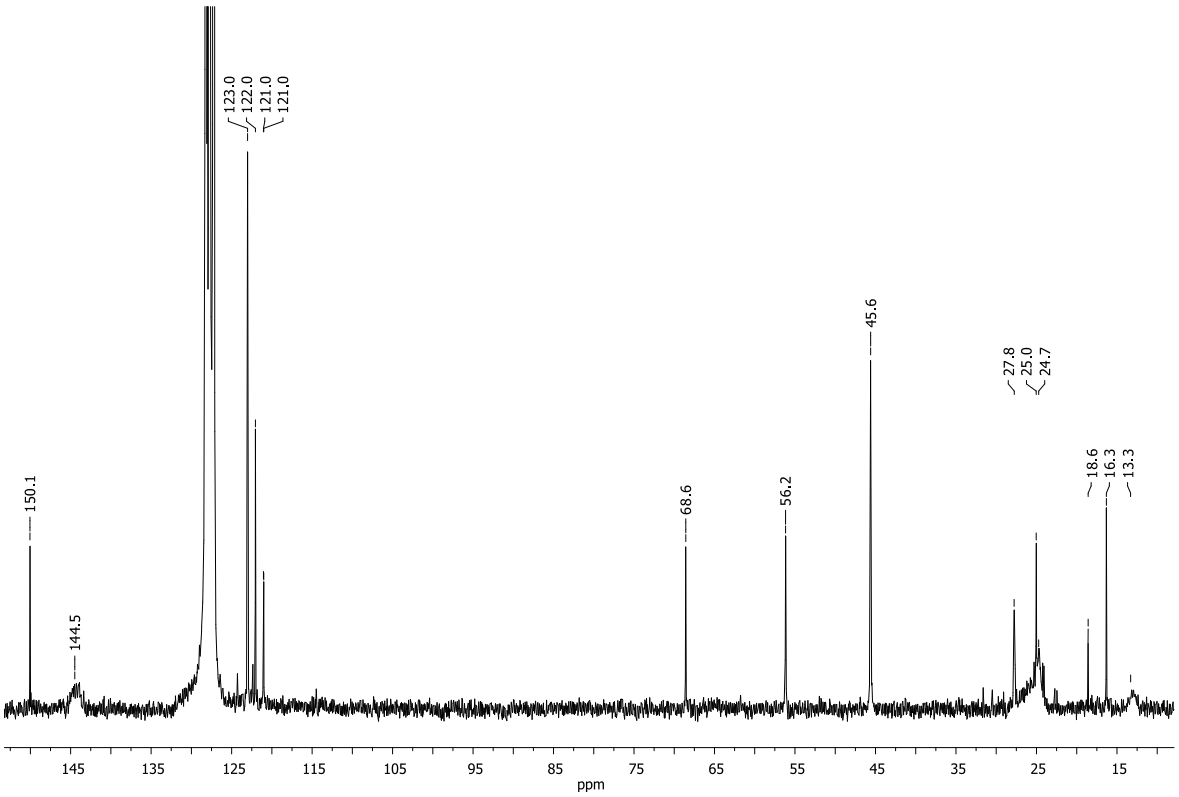

Fig 4. ^{13}C{^{1}H} NMR spectra of complex [L^{1}]Y(OEt$_2$)(μ-Me)$_2$Li(TMEDA)] (**4**) (50 MHz, C_6D_6, 293 K).

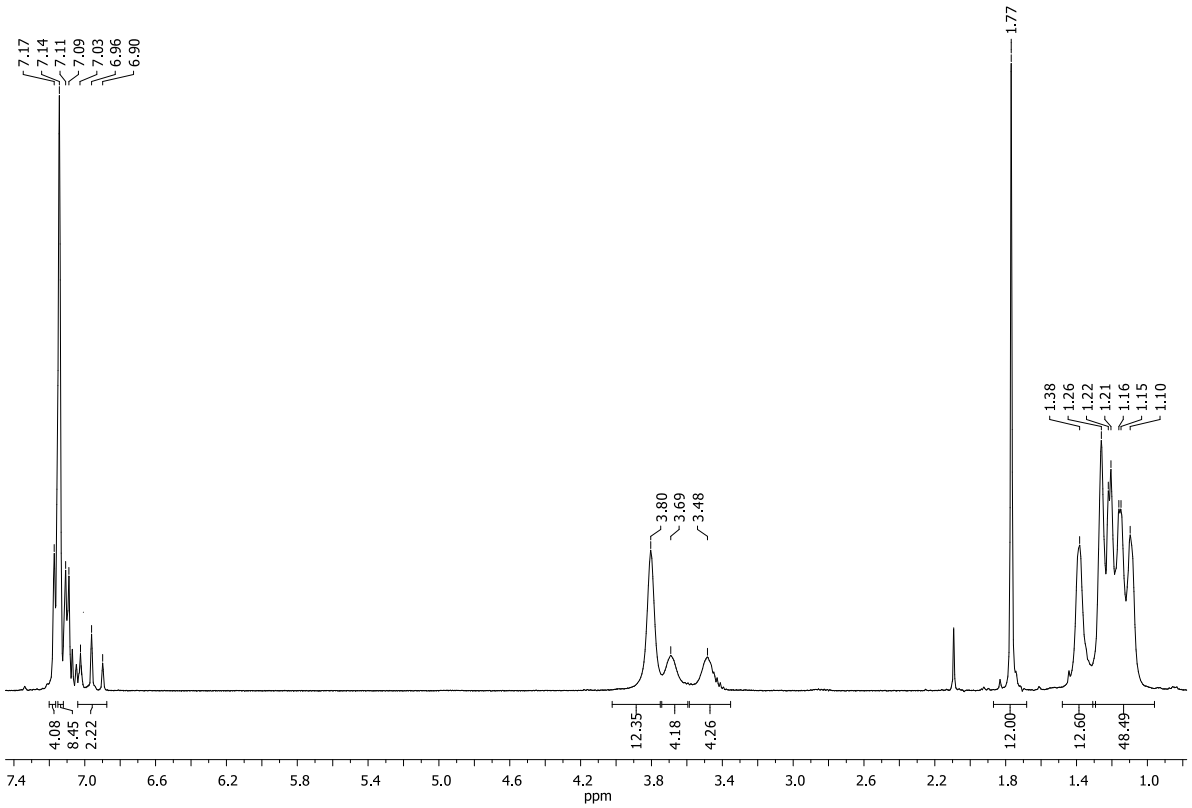

Fig 5. ^{1}H NMR spectra of complex {[L^{1}]Y(THF)(μ-H)]}$_2$(μ-THF) (**5**) (400 MHz, C_6D_6, 293 K).

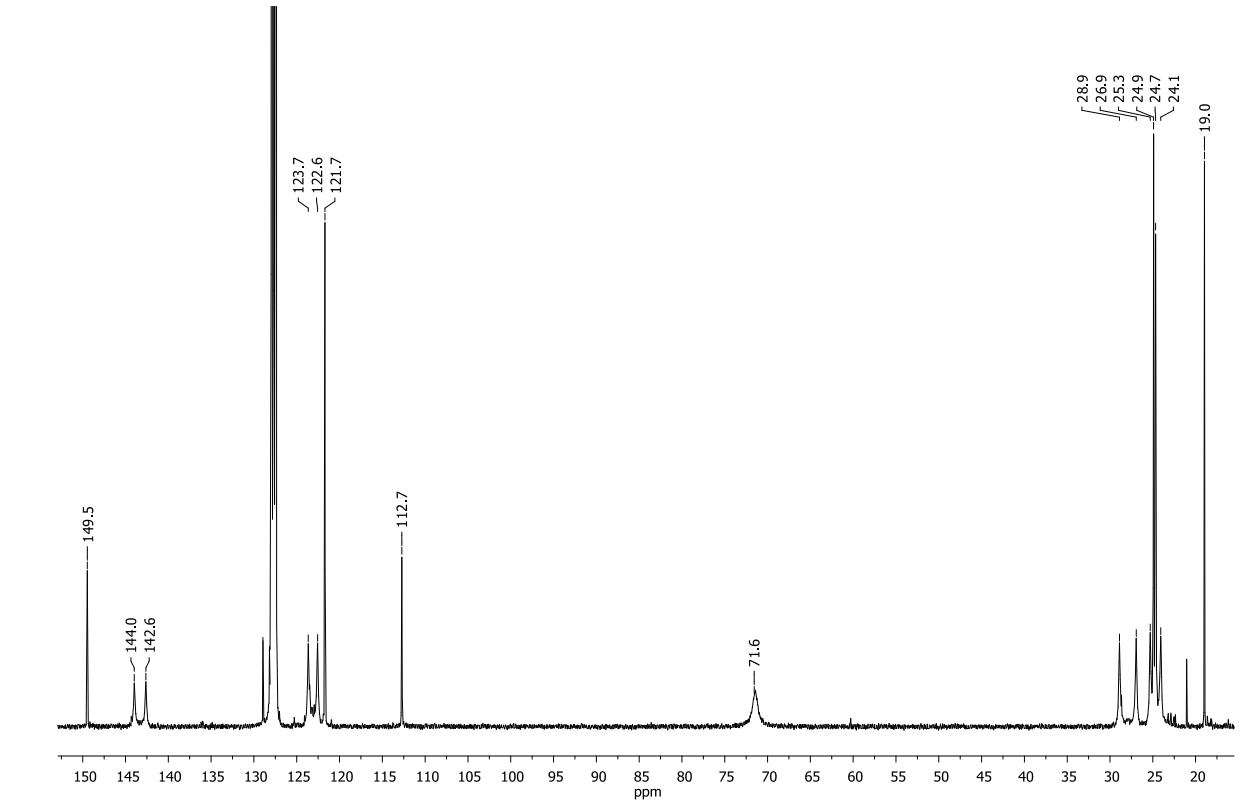

Fig 6. ^{13}C{^{1}H} NMR spectra of complex {[L^{1}]Y(THF)(μ-H)]}$_2$(μ-THF) (**5**) (100 MHz, C_6D_6, 293 K).

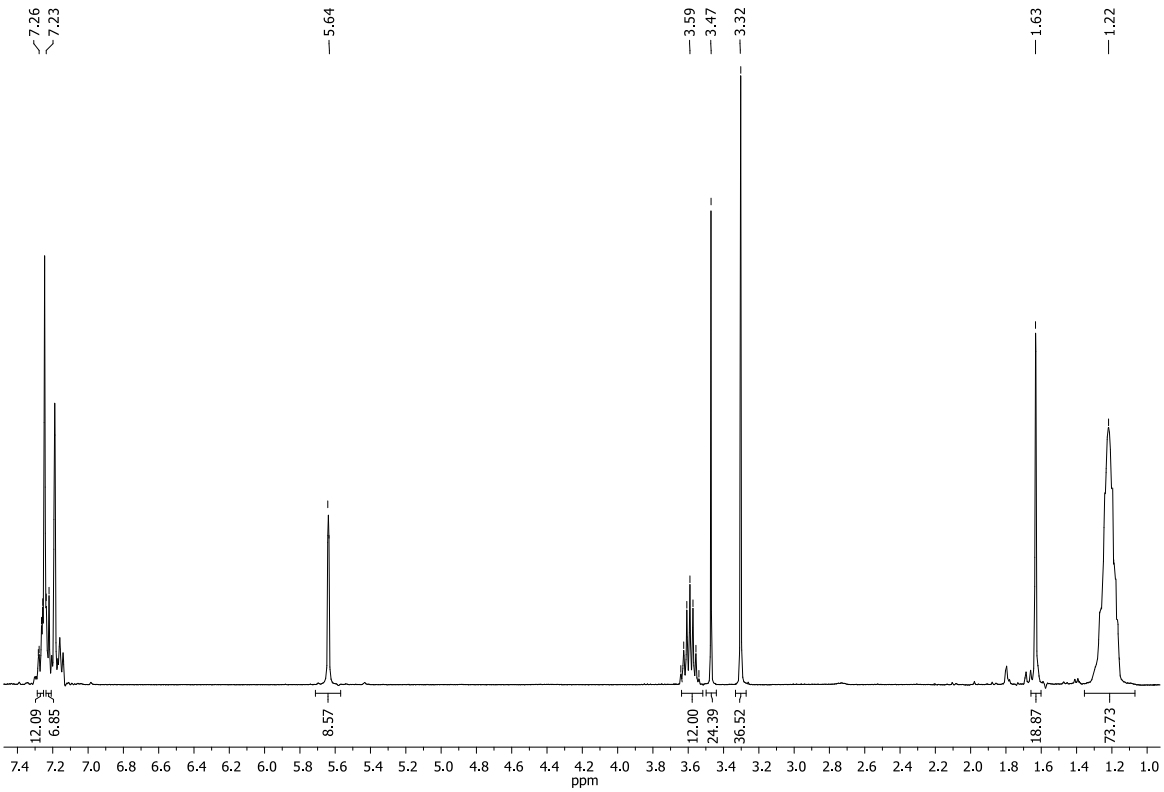

Fig 7. ^{1}H NMR spectra of complex {[L^{1}]Y}$_{3}$(μ^{2}-OMe)$_{3}$(μ^{3}-O)}{Li(DME)$_{3}$}$_{2}$ (**6**) (200 MHz, C_6D_6, 293 K).

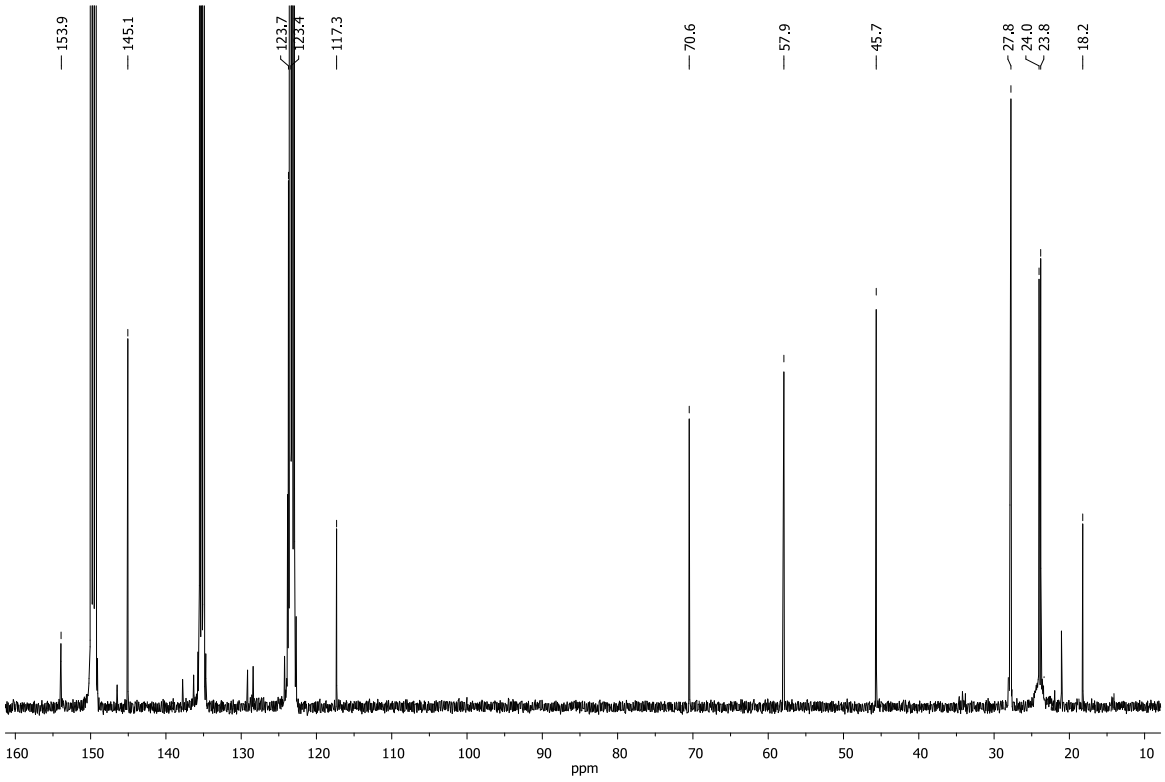

Fig 8. ^{13}C{^{1}H} NMR spectra of complex {[L^{1}]Y}$_{3}$(μ^{2}-OMe)$_{3}$(μ^{3}-O)}{Li(DME)$_{3}$}$_{2}$ (**6**) (50 MHz, C_6D_6, 293 K).

Computational details

In view of the good performance of density functional theory (DFT), we performed DFT calculations at the B3PW91 level of theory on all stationary points of the potential energy surfaces (PES) we studied using the GAUSSIAN09 program suite.[i] The equilibrium structures were fully optimized at the Becke's 3-parameter hybrid functional[ii] combined with the non-local correlation functional provided by Perdew/Wang.[iii] RECP (augmented by a *f* polarization function, α = 1.0) was used to represent the yttrium, chlorine and silicon.[iv] For the rest of non-metal atoms the 6-31G(d,p) basis set was used.[v] In all computations no symmetry constraints were imposed on the geometry. Full geometry optimization was performed for each structure using Schlegel's analytical gradient method[vi] and the attainment of the energy minimum was verified by calculating the vibrational frequencies that result in absence of imaginary eigenvalues. The nature of the stationary points (local minima, transition states) were identified by the number of imaginary frequencies

Cartesian coordinates:

[2,6-iPr$_2$C$_6$H$_3$NC(Me)=C(Me)NC$_6$H$_3$iPr$_2$-2,6]Y(OtBu)(THF)(DME)

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scf done: -2012.840109

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N	1.722990	1.249470	5.275703
N	4.577441	1.848568	5.246433
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Complex 1

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scf done: -2205.999533

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H -2.780599 12.225866 9.249049

Complex 2

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scf done: -1866.335290

Y 1.266553 18.921618 6.577420

Si 3.456786 22.245440 6.398910

O	-0.898910	18.327090	5.534426
O	-0.582618	19.577147	8.178069
N	2.175278	17.582918	5.082095
N	2.172311	17.495572	7.978947
C	3.363123	17.412235	5.838821
C	3.362493	17.351722	7.228048
C	4.680056	17.511316	5.091891
H	5.398090	16.742521	5.394597
H	5.169777	18.482741	5.242347
H	4.509743	17.393499	4.018964
C	4.678111	17.285348	7.971781
H	5.398310	16.636335	7.467451
H	4.518815	16.881499	8.975075
H	5.154186	18.268179	8.087689
C	2.074735	17.060865	3.776842
C	1.873009	17.934210	2.668347
C	1.626761	17.398716	1.399316
H	1.460280	18.077090	0.565410
C	1.624294	16.029506	1.169985
H	1.441192	15.634202	0.174323
C	1.882425	15.176012	2.235275
H	1.904199	14.102355	2.062349
C	2.099744	15.657028	3.529304
C	1.983389	19.446003	2.786807
H	2.300650	19.670710	3.811529
C	0.643549	20.153562	2.544757
H	-0.123560	19.791975	3.236549
H	0.278603	19.975781	1.526146
H	0.743637	21.236831	2.679108
C	3.056134	20.000433	1.837557
H	4.022393	19.516331	2.008786
H	3.186058	21.076761	1.987121
H	2.787667	19.841302	0.787231

C	2.336702	14.641802	4.636595
H	2.395757	15.191261	5.579391
C	1.183291	13.633172	4.742586
H	0.225777	14.132519	4.922493
H	1.357085	12.933619	5.566975
H	1.078753	13.038317	3.828516
C	3.670077	13.903212	4.445116
H	3.856869	13.217901	5.279611
H	4.507948	14.603508	4.387272
H	3.667667	13.311485	3.522205
C	2.064418	17.048937	9.317447
C	2.368196	17.903645	10.414696
C	2.110935	17.467242	11.719234
H	2.339061	18.128906	12.551906
C	1.582455	16.209043	11.978166
H	1.391554	15.890065	12.999564
C	1.318850	15.358777	10.911534
H	0.923922	14.364162	11.107136
C	1.555290	15.750074	9.590220
C	2.979978	19.283614	10.232899
H	3.161376	19.425402	9.162532
C	2.026598	20.395103	10.691666
H	1.074756	20.335377	10.157064
H	2.461745	21.383253	10.504602
H	1.816070	20.321634	11.765016
C	4.327255	19.411450	10.959223
H	5.026667	18.630773	10.648249
H	4.206344	19.335595	12.045727
H	4.787790	20.382123	10.746114
C	1.281627	14.756980	8.475752
H	1.462764	15.282525	7.533787
C	-0.174531	14.272332	8.470440
H	-0.872120	15.112886	8.385100

H	-0.427204	13.727179	9.386964
H	-0.353110	13.596315	7.626992
C	2.252261	13.569837	8.560459
H	3.291614	13.908284	8.512277
H	2.085433	12.866060	7.737859
H	2.125027	13.017687	9.498822
C	1.856492	21.276495	6.558158
H	1.166094	21.714676	5.808432
H	1.442097	21.585102	7.537740
C	4.801984	21.587135	7.580249
H	5.020452	20.535108	7.370759
H	4.482738	21.664114	8.624817
H	5.732427	22.155683	7.472969
C	4.160232	22.172771	4.630380
H	4.382572	21.142511	4.336448
H	5.085398	22.754420	4.552681
H	3.446132	22.584271	3.908852
C	3.223456	24.100482	6.820666
H	2.490648	24.563251	6.149802
H	4.161871	24.659644	6.729407
H	2.858460	24.225259	7.846700
C	-2.062860	19.159866	5.331473
H	-1.719863	20.101857	4.891895
H	-2.521165	19.371015	6.302775
C	-2.999592	18.379372	4.397654
H	-3.426482	19.019030	3.621119
H	-3.829391	17.946260	4.965830
C	-2.102957	17.270969	3.833251
H	-2.663034	16.378794	3.541620
H	-1.534965	17.620638	2.966193
C	-1.157559	17.010167	4.990169
H	-1.624698	16.391231	5.768638
H	-0.195011	16.585100	4.707717

C -1.228021 18.579864 9.010178

H -0.451137 17.951741 9.452442

H -1.871245 17.962474 8.369396

C -2.040939 19.368135 10.027217

H -2.900800 18.803134 10.396153

H -1.416859 19.638531 10.885079

C -2.429763 20.615601 9.229942

H -3.281575 20.401694 8.573678

H -2.696251 21.468224 9.859898

C -1.169841 20.879036 8.415142

H -1.354466 21.355539 7.448691

H -0.448526 21.489401 8.968764

Complex 3

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scf done: -1564.548103

Y 12.127311 23.583205 21.199022

Si 14.987942 20.907349 20.566729

Si 11.656529 27.401176 20.196202

N 10.207789 22.498604 21.114973

N 11.748779 23.397665 23.402876

C 10.424664 21.678910 22.247907

C 11.173697 22.102444 23.334446

C 9.998866 20.232119 22.127074

H 9.894415 19.738015 23.095239

H 10.712911 19.644864 21.531076

H 9.035072 20.168617 21.611583

C 11.611388 21.092679 24.383240

H 10.768486 20.555780 24.832398

H 12.140613 21.599084 25.193729

H 12.289744 20.335608 23.967414

C 9.080422 22.317944 20.295871

C 9.220682 21.810973 18.972485

C 8.093871 21.693154 18.153167

H	8.214901	21.312469	17.140788
C	6.824388	22.035736	18.601998
H	5.959300	21.926955	17.951912
C	6.682362	22.528237	19.894003
H	5.694569	22.814692	20.250451
C	7.781568	22.689306	20.740959
C	10.568556	21.387729	18.412943
H	11.281255	21.409710	19.245065
C	10.549881	19.953658	17.867683
H	10.210682	19.245164	18.629924
H	11.553905	19.652818	17.547248
H	9.886370	19.854390	17.000174
C	11.067695	22.369844	17.343288
H	11.136462	23.388016	17.739184
H	10.386066	22.394529	16.484116
H	12.060059	22.078911	16.978455
C	7.563988	23.309430	22.110352
H	8.551513	23.435566	22.563219
C	6.924899	24.701163	21.996700
H	7.527767	25.355523	21.359452
H	6.841207	25.170464	22.983025
H	5.917376	24.652689	21.566175
C	6.731436	22.396199	23.020241
H	7.212679	21.421584	23.145501
H	5.730695	22.224954	22.604138
H	6.605507	22.841839	24.013920
C	12.038721	23.992391	24.633539
C	11.076444	24.138312	25.676717
C	11.434706	24.768583	26.871318
H	10.682713	24.877619	27.650667
C	12.706204	25.286420	27.080287
H	12.958964	25.783428	28.013731
C	13.648648	25.156811	26.066486

H	14.649695	25.551098	26.222960
C	13.351699	24.513099	24.863981
C	9.621779	23.723749	25.509032
H	9.528370	23.197542	24.555728
C	8.719780	24.965863	25.448619
H	7.672030	24.682462	25.292599
H	9.020597	25.627426	24.630962
H	8.773773	25.540932	26.380959
C	9.145856	22.767284	26.611714
H	9.786060	21.882387	26.675202
H	8.120973	22.431668	26.414059
H	9.147856	23.249207	27.596929
C	14.438928	24.376027	23.813054
H	14.183710	23.492438	23.210972
C	14.472549	25.594793	22.879972
H	13.497869	25.797478	22.419723
H	15.205209	25.462924	22.074738
H	14.740337	26.498127	23.441309
C	15.836604	24.128424	24.392121
H	15.834650	23.289760	25.095045
H	16.228685	25.008373	24.915774
H	16.540341	23.895794	23.585530
C	14.112129	22.516010	20.221447
H	13.859740	22.516434	19.143747
H	14.861997	23.323844	20.335392
C	16.554319	20.628157	19.483757
H	17.279960	21.435247	19.638396
H	16.292217	20.620541	18.419305
H	17.051544	19.678246	19.715752
C	13.858814	19.399029	20.242233
H	12.978746	19.431433	20.892197
H	14.388076	18.457585	20.430342
H	13.507467	19.386159	19.204926

C	15.588713	20.776652	22.377908
H	14.751258	20.866881	23.077477
H	16.306462	21.569901	22.612945
H	16.083191	19.815175	22.559998
C	11.726926	25.570316	19.853141
H	12.371572	25.432343	18.965015
H	10.709793	25.271811	19.529232
C	13.404613	28.181037	20.146029
H	14.066294	27.728609	20.890941
H	13.365761	29.259747	20.336708
H	13.859176	28.029229	19.160241
C	10.613179	28.383101	18.914232
H	9.581059	28.014164	18.895926
H	11.024349	28.260970	17.905546
H	10.583551	29.455968	19.141051
C	10.876591	27.791388	21.898735
H	11.457226	27.347508	22.714040
H	9.863009	27.378453	21.954400
H	10.810193	28.871411	22.075402

[i] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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