

## Electron Supporting Information

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

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

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

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

**Fig 3.**  $^1\text{H}$  NMR spectra of complex  $[\text{L}^1]\text{Y}(\text{OEt}_2)(\mu\text{-Me})_2\text{Li}(\text{TMEDA})$  (**4**) (200 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

**Fig 4.**  $^{13}\text{C}\{\text{H}\}$  NMR spectra of complex  $[\text{L}^1]\text{Y}(\text{OEt}_2)(\mu\text{-Me})_2\text{Li}(\text{TMEDA})$  (**4**) (50 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

**Fig 5.**  $^1\text{H}$  NMR spectra of complex  $\{[\text{L}^1]\text{Y}(\text{THF})(\mu\text{-H})\}_2(\mu\text{-THF})$  (**5**) (400 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

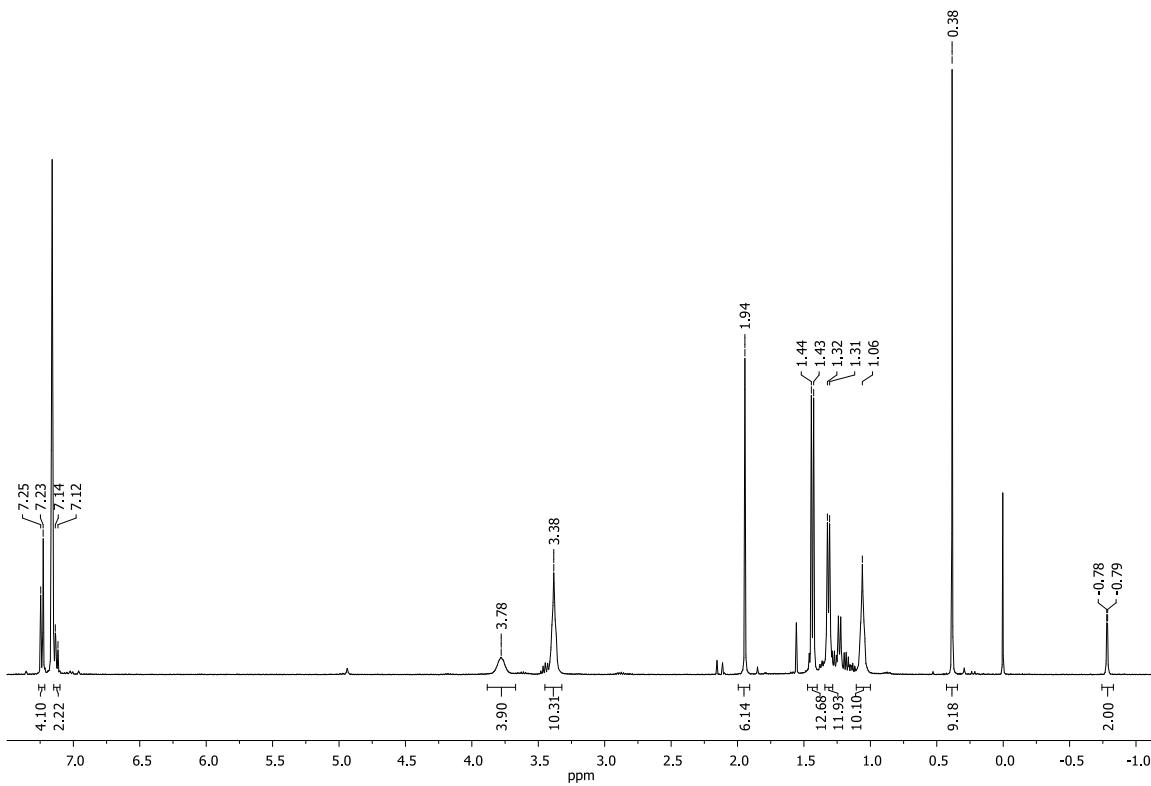
**Fig 6.**  $^{13}\text{C}\{\text{H}\}$  NMR spectra of complex  $\{[\text{L}^1]\text{Y}(\text{THF})(\mu\text{-H})\}_2(\mu\text{-THF})$  (**5**) (100 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

**Fig 7.**  $^1\text{H}$  NMR spectra of complex  $\{[\text{L}^1]\text{Y}\}_3(\mu^2\text{-OMe})_3(\mu^3\text{-O})\}[\text{Li}(\text{DME})_3]_2$  (**6**) (200 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

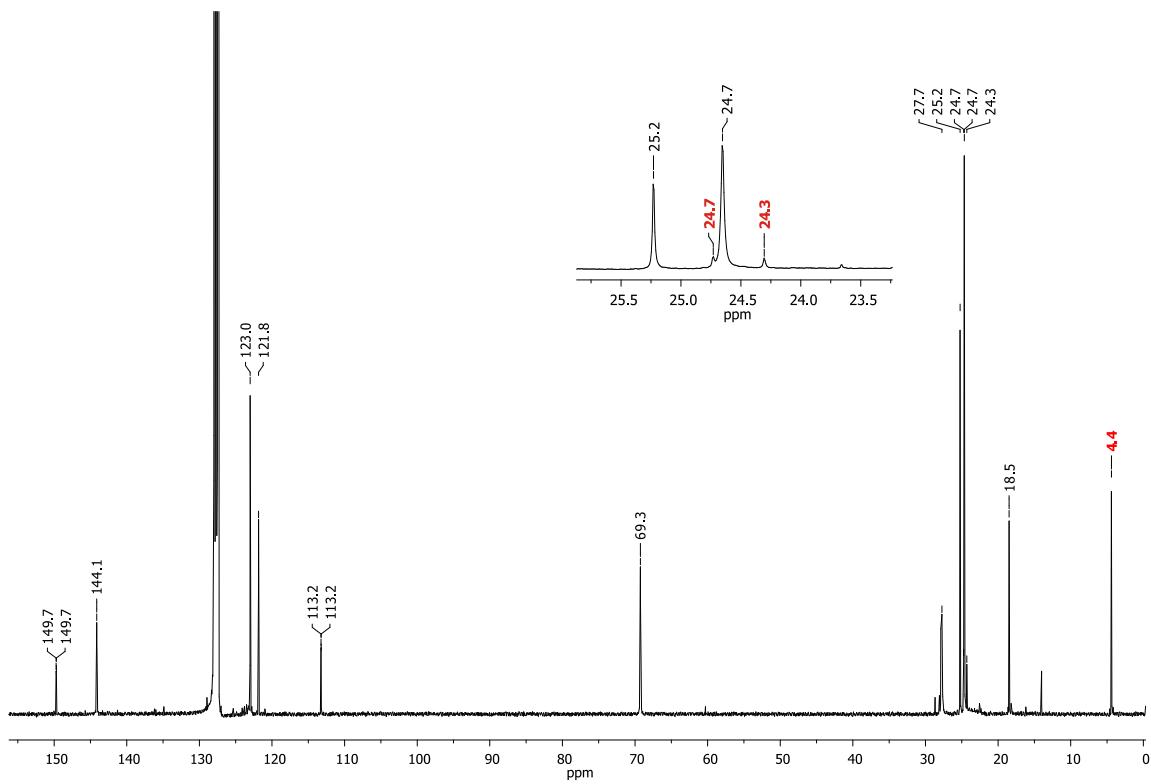
**Fig 8.**  $^{13}\text{C}\{\text{H}\}$  NMR spectra of complex  $\{[\text{L}^1]\text{Y}\}_3(\mu^2\text{-OMe})_3(\mu^3\text{-O})\}[\text{Li}(\text{DME})_3]_2$  (**6**) (50 MHz,  $\text{C}_6\text{D}_6$ , 293 K).

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

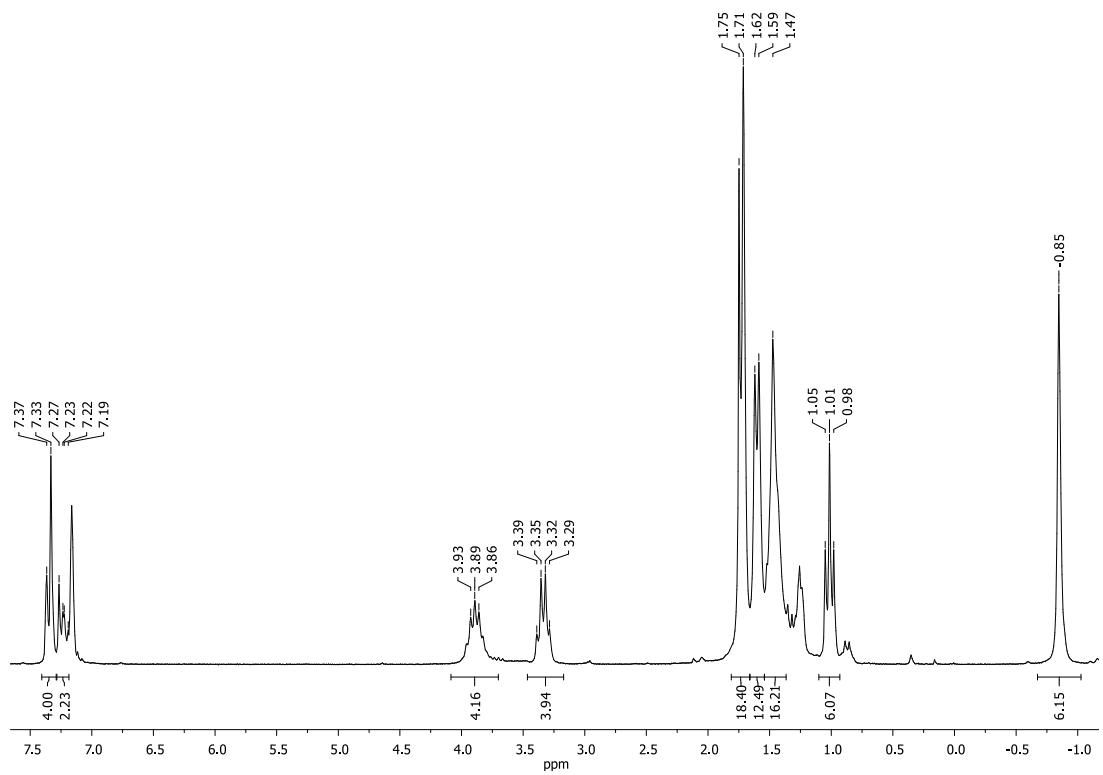
	<b>2</b>	<b>3</b>	<b>5</b>	<b>6</b>
Formula	C <sub>40</sub> H <sub>67</sub> N <sub>2</sub> O <sub>2</sub> SiY·(C <sub>7</sub> H <sub>8</sub> ) <sub>2</sub>	C <sub>52</sub> H <sub>94</sub> LiN <sub>2</sub> O <sub>4</sub> Si <sub>2</sub> Y	C <sub>68</sub> H <sub>106</sub> N <sub>4</sub> O <sub>3</sub> Y <sub>2</sub> ·(C <sub>6</sub> H <sub>14</sub> ) <sub>0.5</sub>	C <sub>111</sub> H <sub>189</sub> Li <sub>2</sub> N <sub>6</sub> O <sub>16</sub> Y <sub>3</sub>
M <sub>r</sub>	909.22	963.32	1248.47	2144.29
Crystal system	Orthorhombic	Triclinic	Monoclinic	Trigonal
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	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 <sup>3</sup> ]	5164.0(9)	5691.1(5)	3609.8(2)	17810(1)
Z	4	4	2	6
ρ <sub>calcd</sub> [g cm <sup>-3</sup> ]	1.169	1.125	1.149	1.200
μ [mm <sup>-1</sup> ]	1.192	1.107	1.643	1.514
F(000)	1960	2092	1338	6888
Crystal size [mm <sup>3</sup> ]	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 -24≤k≤24 -32≤l≤32	-15≤h≤15 -25≤k≤25 -30≤l≤30	-30≤h≤30 -16≤k≤16 -15≤l≤15	-21≤h≤21 -21≤k≤21 -95≤l≤95
Reflns collected	55461	47751	29422	52002
Independent reflns[R <sub>int</sub> ]	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
Final R indices [ $\bar{R} > 2\sigma(I)$ ]	$R_1 = 0.0341$ $wR_2 = 0.0811$	$R_1 = 0.0539$ $wR_2 = 0.0846$	$R_1 = 0.0506$ $wR_2 = 0.1179$	$R_1 = 0.0657$ $wR_2 = 0.1670$
R indies (all data)	$R_1 = 0.0369$ $wR_2 = 0.0822$	$R_1 = 0.1402$ $wR_2 = 0.0976$	$R_1 = 0.0690$ $wR_2 = 0.1264$	$R_1 = 0.0810$ $wR_2 = 0.1766$
Largest diff. peak/hole [e/Å <sup>3</sup> ]	0.846 / -0.264	0.787 / -0.632	0.925 / -0.676	1.182 / -0.746



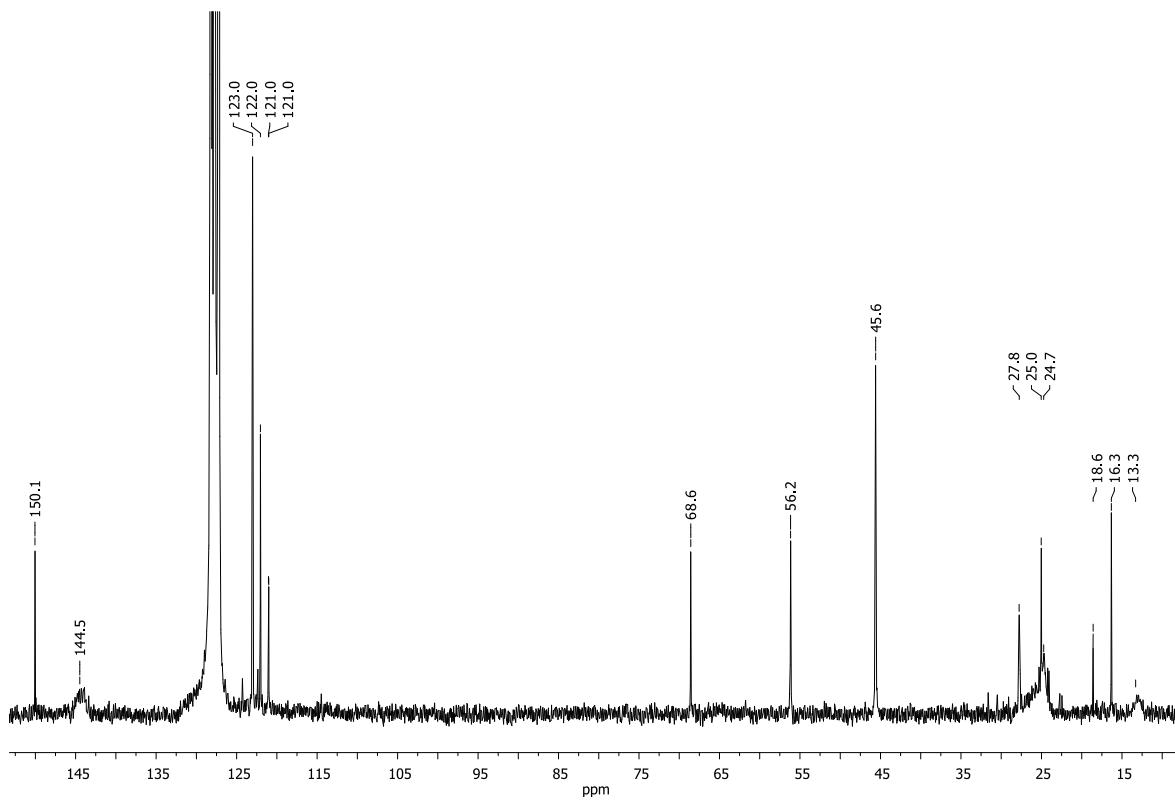
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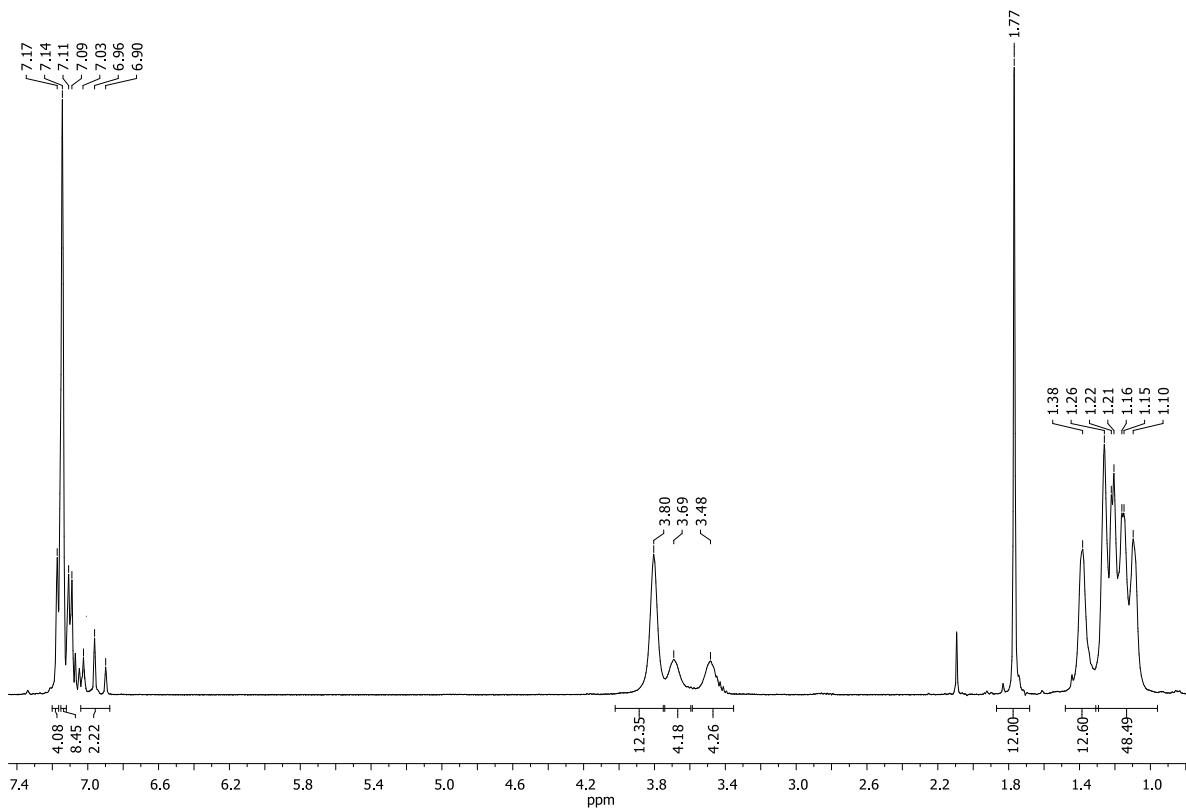
**Fig 2.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of complex  $[\text{L}^1]\text{Y}(\text{CH}_2\text{SiMe}_3)(\text{THF})_2$  (**2**) (100 MHz,  $\text{C}_6\text{D}_6$ , 293 K).



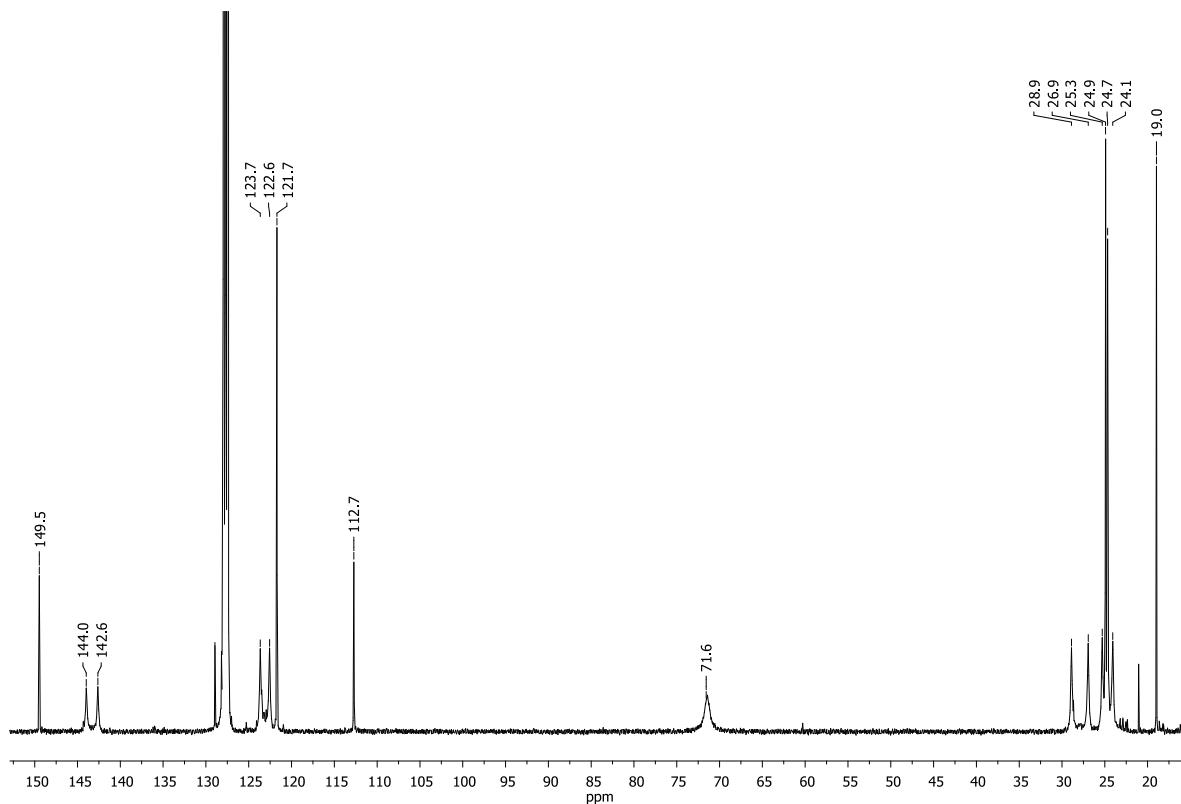
**Fig 3.**  $^1\text{H}$  NMR spectra of complex  $[\text{L}^1]\text{Y}(\text{OEt}_2)(\mu\text{-Me})_2\text{Li}(\text{TMEDA})$  (**4**) (200 MHz,  $\text{C}_6\text{D}_6$ , 293 K).



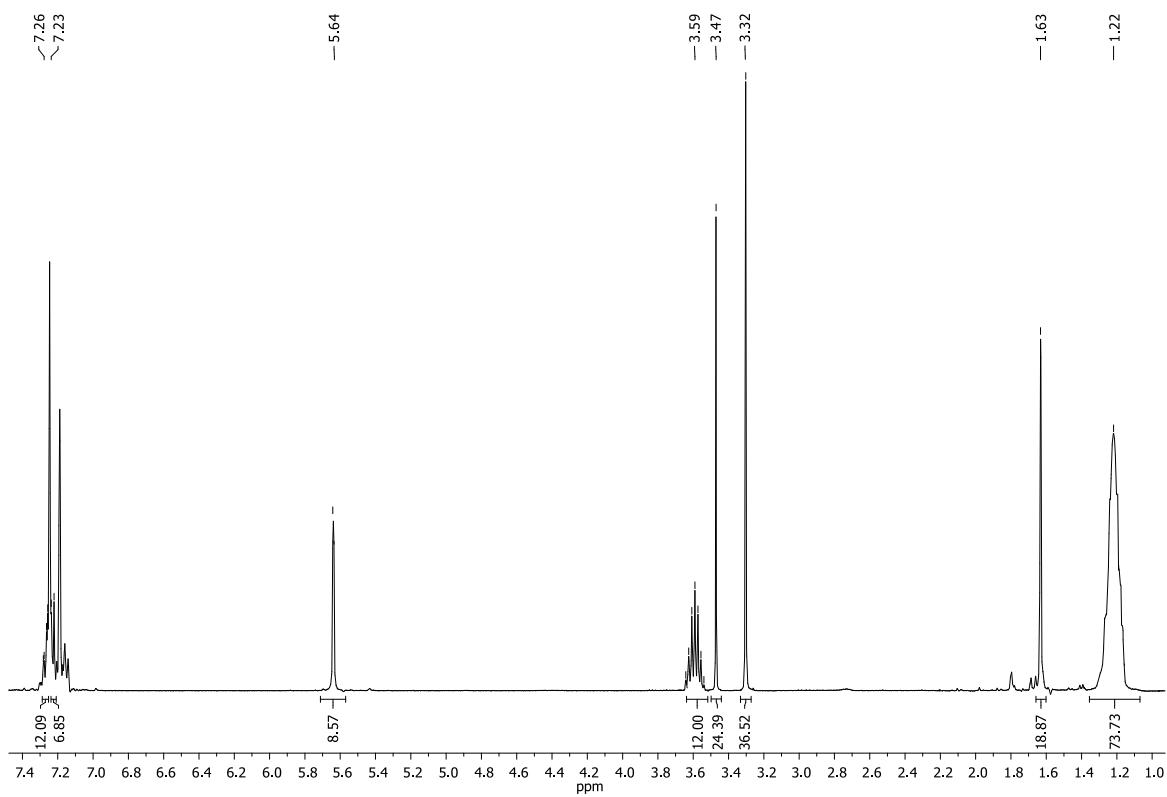
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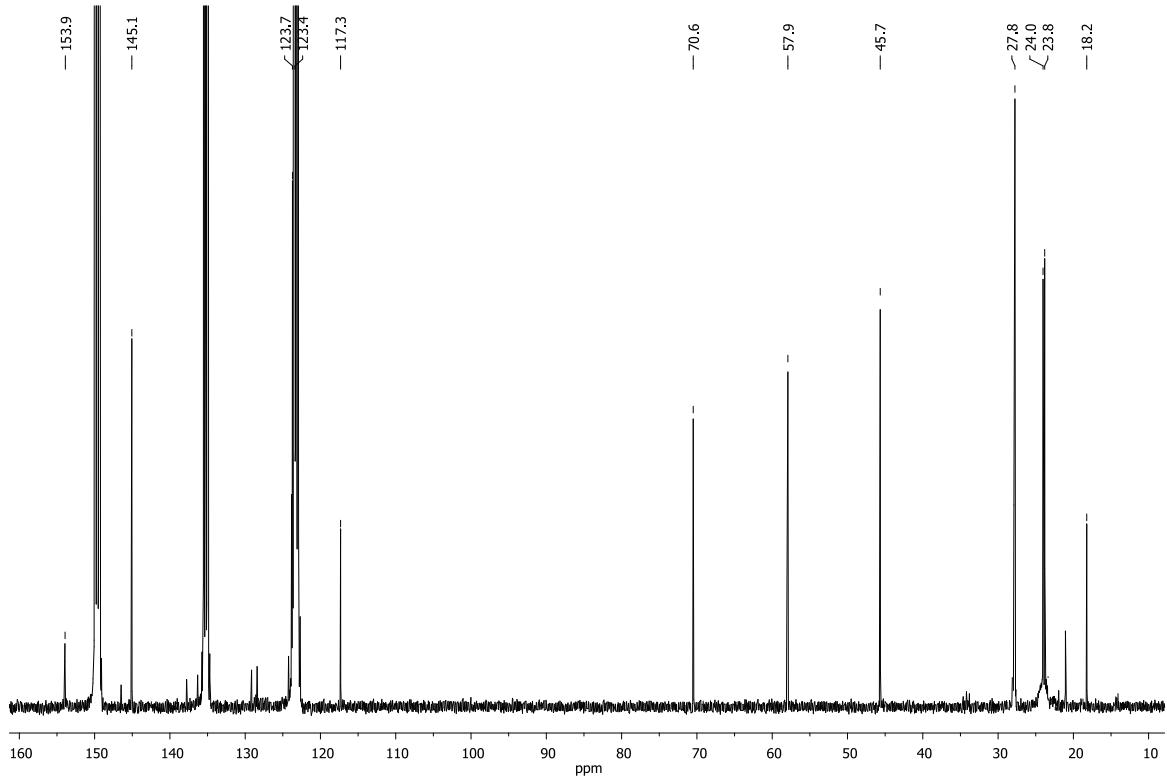
**Fig 5.**  $^1\text{H}$  NMR spectra of complex  $\{[\text{L}^1]\text{Y}(\text{THF})(\mu\text{-H})\}_2(\mu\text{-THF})$  (**5**) (400 MHz,  $\text{C}_6\text{D}_6$ , 293 K).



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**Fig 7.**  $^1\text{H}$  NMR spectra of complex  $\{\text{[L}^1\text{]Y}\}_3(\mu^2\text{-OMe})_3(\mu^3\text{-O})\{\text{Li(DME)}_3\}_2$  (**6**) (200 MHz,  $\text{C}_6\text{D}_6$ , 293 K).



**Fig 8.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of complex  $\{\text{[L}^1\text{]Y}\}_3(\mu^2\text{-OMe})_3(\mu^3\text{-O})\{\text{Li(DME)}_3\}_2$  (**6**) (50 MHz,  $\text{C}_6\text{D}_6$ , 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.<sup>i</sup> The equilibrium structures were fully optimized at the Becke's 3-parameter hybrid functional<sup>ii</sup> combined with the non-local correlation functional provided by Perdew/Wang.<sup>iii</sup> RECP (augmented by a *f* polarization function,  $\alpha = 1.0$ ) was used to represent the yttrium, chlorine and silicon.<sup>iv</sup> For the rest of non-metal atoms the 6-31G(d,p) basis set was used.<sup>v</sup> 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<sup>vi</sup> 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:



114

scf done: -2012.840109

Y	3.475478	-0.020559	4.735132
N	1.722990	1.249470	5.275703
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### ***Complex 1***

Y -5.517221 13.894040 4.014225  
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 Cl -3.075214 13.702156 5.359911  
 Cl -6.154291 15.195056 6.284469  
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 H -2.131998 10.933017 1.639698  
 H -1.611751 12.036190 0.353048  
 C -3.761626 11.533588 0.338039  
 H -3.835057 10.527970 -0.084703  
 H -3.924109 12.258044 -0.467603

C	-4.754226	11.752389	1.466956
H	-5.751039	12.073046	1.159851
H	-4.854886	10.864197	2.097722
C	-1.840081	16.563507	7.669633
H	-1.875298	16.738325	6.587112
H	-1.085742	15.797302	7.869213
C	-1.630041	17.858847	8.444018
H	-0.959653	18.551417	7.927949
H	-1.207853	17.650277	9.433541
C	-3.063797	18.380501	8.573345
H	-3.195155	19.095315	9.390022
H	-3.377818	18.867243	7.643421
C	-3.852314	17.093425	8.794285
H	-3.904477	16.829288	9.858240
H	-4.866465	17.120814	8.385951
C	-5.692360	12.729032	9.144305
H	-6.068083	12.288948	8.218449
H	-6.409660	13.478380	9.497803
C	-5.366594	11.692527	10.215429
H	-5.088420	10.743685	9.746279
H	-6.214792	11.504441	10.878598
C	-4.163698	12.314396	10.928828
H	-4.489312	13.080800	11.641765
H	-3.551530	11.585371	11.466966
C	-3.419070	12.955683	9.765550
H	-2.809527	13.819096	10.047464
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

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