Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2016

**Electronic Supplementary Information** 

## Unexpected Reactivity of Alkylaluminum Complex of Non-Innocent 1,2-bis[(2,6diisopropylphenyl)imino]acenaphthene Ligand (dpp-bian)

Mikhail V. Moskalev, Anton N. Lukoyanov, Evgenii V. Baranov, and Igor L. Fedushkin\*

G.A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences, Tropinina str. 49, 603137 Nizhny Novgorod, Russian Federation

## Contents of supplementary information:

1.	<sup>1</sup> H spectrum of compound <b>2</b>	S-2
2.	<sup>1</sup> H, <sup>13</sup> C and COSY NMR spectra of compound <b>3</b>	S-2 – S-4
3.	<sup>1</sup> H, <sup>13</sup> C and COSY NMR spectra of compound <b>4</b>	S-5 – S-7
4.	<sup>1</sup> H, <sup>13</sup> C and COSY NMR spectra of compound <b>5</b>	S-8 – S-10
5.	Table of crystallographic data of compounds <b>2</b> , <b>3</b> , and <b>5</b>	S-11



Figure 1S. <sup>1</sup>H NMR spectrum of compound 2 at 298 K in  $C_6D_6$ , 400 MHz.



Figure 2S. <sup>1</sup>H NMR spectrum of compound 3 at 298 K in  $C_6D_6$ , 400 MHz.



Figure 3S. <sup>13</sup>C NMR spectrum of compound 3 at 298 K in  $C_6D_6$ , 50 MHz.



**Figure 4S.** COSY  ${}^{1}H-{}^{1}H$  NMR spectrum of compound **3** at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 5S. COSY  $^{1}H-^{13}C$  HSQC NMR spectrum of compound **3** at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 6S. COSY  $^{1}H-^{13}C$  HMBC NMR spectrum of compound 3 at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 7S. <sup>1</sup>H NMR spectrum of compound 4 at 298 K in  $C_6D_6$ , 400 MHz.



Figure 8S.  $^{13}$ C NMR spectrum of compound 4 at 298 K in C<sub>6</sub>D<sub>6</sub>, 50 MHz.



**Figure 9S.** COSY  ${}^{1}H-{}^{1}H$  NMR spectrum of compound **4** at 298 K in C<sub>6</sub>D<sub>6</sub>.



**Figure 10S.** COSY  ${}^{1}H-{}^{13}C$  HSQC NMR spectrum of compound **4** at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 11S. COSY  ${}^{1}H-{}^{13}C$  HMBC NMR spectrum of compound 4 at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 12S. The upfiled region of the COSY  ${}^{1}H-{}^{15}N$  HSQC NMR spectrum of compound 4 at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 13S. <sup>1</sup>H NMR spectrum of compound 5 at 298 K in  $C_6D_6$ , 400 MHz.



Figure 14S. <sup>13</sup>C NMR spectrum of compound 5 at 298 K in  $C_6D_6$ , 50 MHz.



**Figure 15S.** COSY  ${}^{1}H-{}^{1}H$  NMR spectrum of compound **5** at 298 K in C<sub>6</sub>D<sub>6</sub>.



**Figure 16S.** COSY  ${}^{1}H-{}^{13}C$  HSQC NMR spectrum of compound **5** at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 175. COSY  ${}^{1}H{}^{-13}C$  HMBC NMR spectrum of compound 5 at 298 K in C<sub>6</sub>D<sub>6</sub>.



Figure 18S. The upfiled region of the COSY  ${}^{1}H-{}^{15}N$  HSQC NMR spectrum of compound 5 at 298 K in C<sub>6</sub>D<sub>6</sub>.

	2	3	5
Empirical Formula	$C_{53}H_{59}AIN_2O_3$	$C_{53}H_{69}AIN_2O$	$C_{76}H_{92}Al_2N_4O$
М	799.00	777.08	1131.49
Τ/Κ	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	<i>P</i> 2(1)/n	<i>P</i> bca	P-1
a/Å	10.6249(5)	14.8988(4)	12.1969(4)
b/Å	21.9891(11)	16.8722(5)	14.9121(5)
c/Å	19.0941(9)	36.5541(11)	19.8954(7)
lpha/deg	90	90	80.879(1)
$\beta$ /deg	94.695(1)	90	76.976(1)
γ/deg	90	90	66.171(1)
V/Å <sup>3</sup>	4446.0(4)	9188.8(5)	3215.73(19)
Ζ	4	8	2
$d_{calc}/Mg \bullet m^{-3}$	1.194	1.123	1.169
μ(Mo Kα) mm⁻¹	0.091	0.083	0.093
F(000)	1712	3376	1220
Crystal size/mm	$0.80 \times 0.63 \times 0.45$	$0.39 \times 0.28 \times 0.18$	$0.29 \times 0.14 \times 0.11$
hetarange/degree	2.12 to 27.00	1.91 to 26.00	1.764 to 25.999
	$-13 \le h \le 12$	$-18 \le h \le 18$	$-15 \le h \le 15$
h, k, l	$-28 \le k \le 14$	$-20 \le k \le 20$	$-18 \le k \le 18$
	$-24 \le l \le 24$	$-45 \le I \le 45$	$-24 \le I \le 24$
Reflections Collected	28544	75827	28185
Independent Reflections	9695	9011	12541
R <sub>int</sub>	0.0276	0.0974	0.0361
Data/Restraints/Param	9695 / 2 / 541	9011 / 1 / 534	12541 / 1 / 783
GooF	1.052	1.003	0.997
R <sub>1</sub> /wR <sub>2</sub> [I>2 σ (I)]	0.0443/0.1150	0.0456/ 0.1015	0.0472/0.1123
$R_1/wR_2$ (all data)	0.0603/0.1223	0.0846/ 0.1119	0.0740/0.1225
Larg. Diff. Peak and Hole∕e • Å⁻³	0.396 / -0.213	0.355 and -0.274	0.340 and -0.279

Table 1S. Crystal structure data for 2, 3 and 5.