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

For submission to Dalton

Transactions

Systematic molecular engineering of Zn-ketoiminates for application as precursors in atomic layer depositions of zinc oxide

Richard O´Donoghue, Daniel Peeters, Detlef Rogalla, Hans-Werner Becker, Julian Rechmann, Sebastian. Henke, Manuela Winter and Anjana Devi

Supporting information

Table S1. Selected bond lengths and angles of the 2nd enantiomer of [Zn(^{n}pki)$_2$].

Bond Lengths (Å)	[Zn(^{n}pki)$_2$]
Zn2 – O2	1.954(3)
Zn2 – N2	1.972(3)
O2 – C10	1.298(4)
N2 – C12	1.312(4)
C10 – C11	1.328(5)
C11 – C12	1.424(4)
Bond Angles (°)	
O2 – Zn2 – N2	96.76(11)
O2 – Zn2 – N2‘	118.72(11)
O2 – Zn2 – O2‘	110.62(17)
N2 – Zn2 – N2‘	116.6(2)
Torsion Angles (°)	
Zn2 – N2 – C12 – C11	0.5(5)
Zn2 – O2 – C10 – C11	6.8(5)

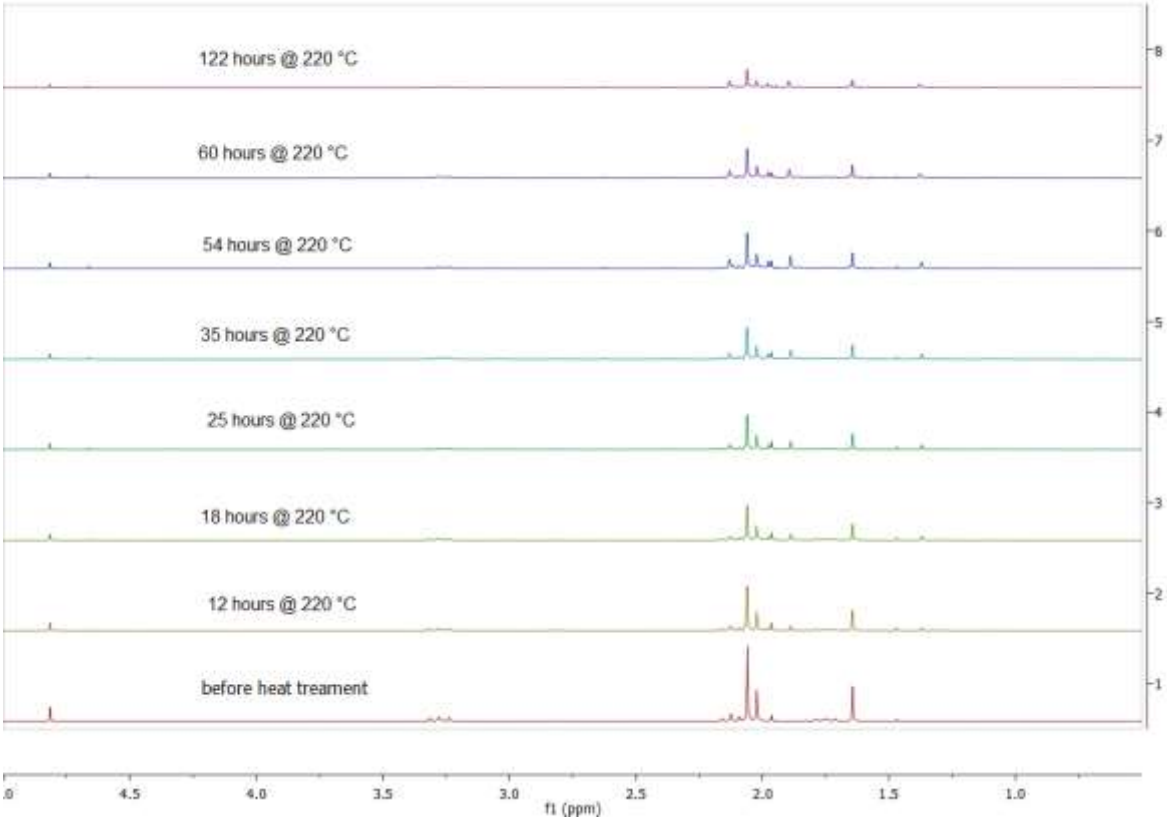

Figure S1. NMR thermal decompositional study @ 220 °C for [Zn(dapki)$_2$]

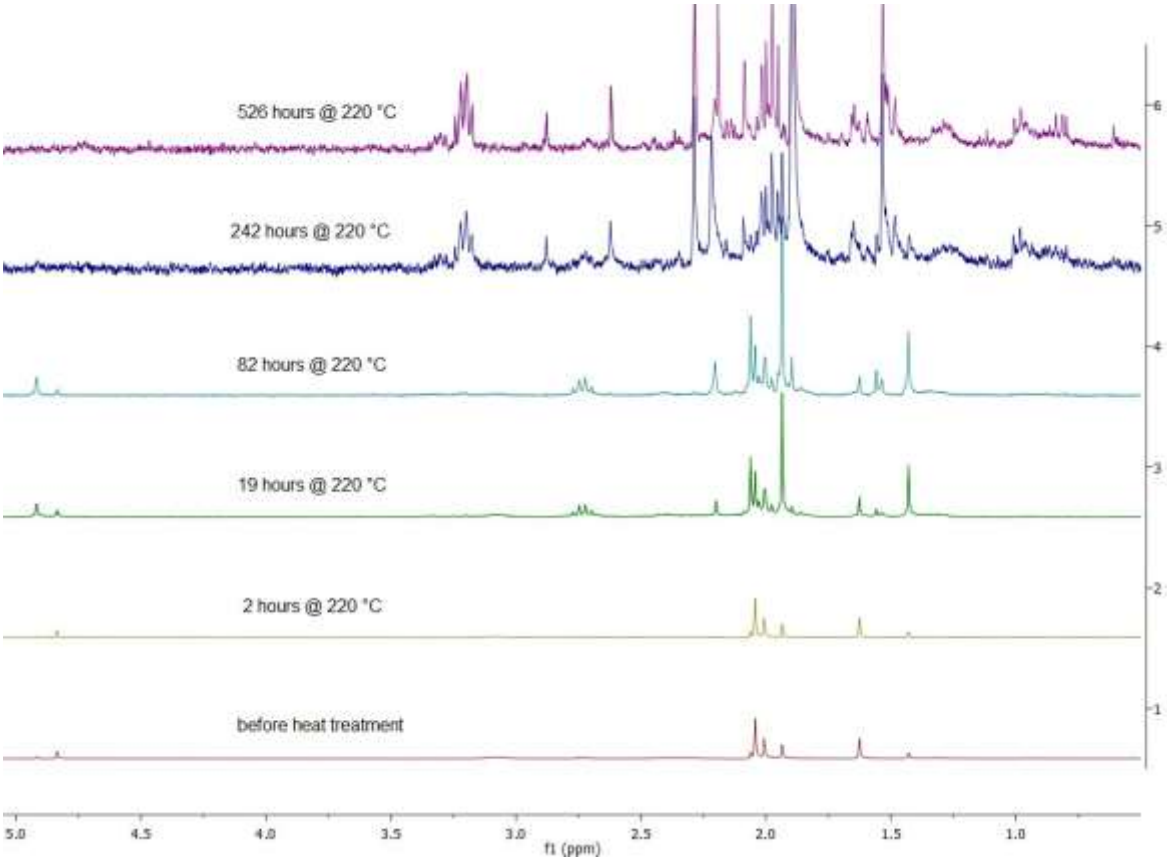

Figure S2. NMR thermal decompositional study @ 220 °C for [Zn(daeki)$_2$]

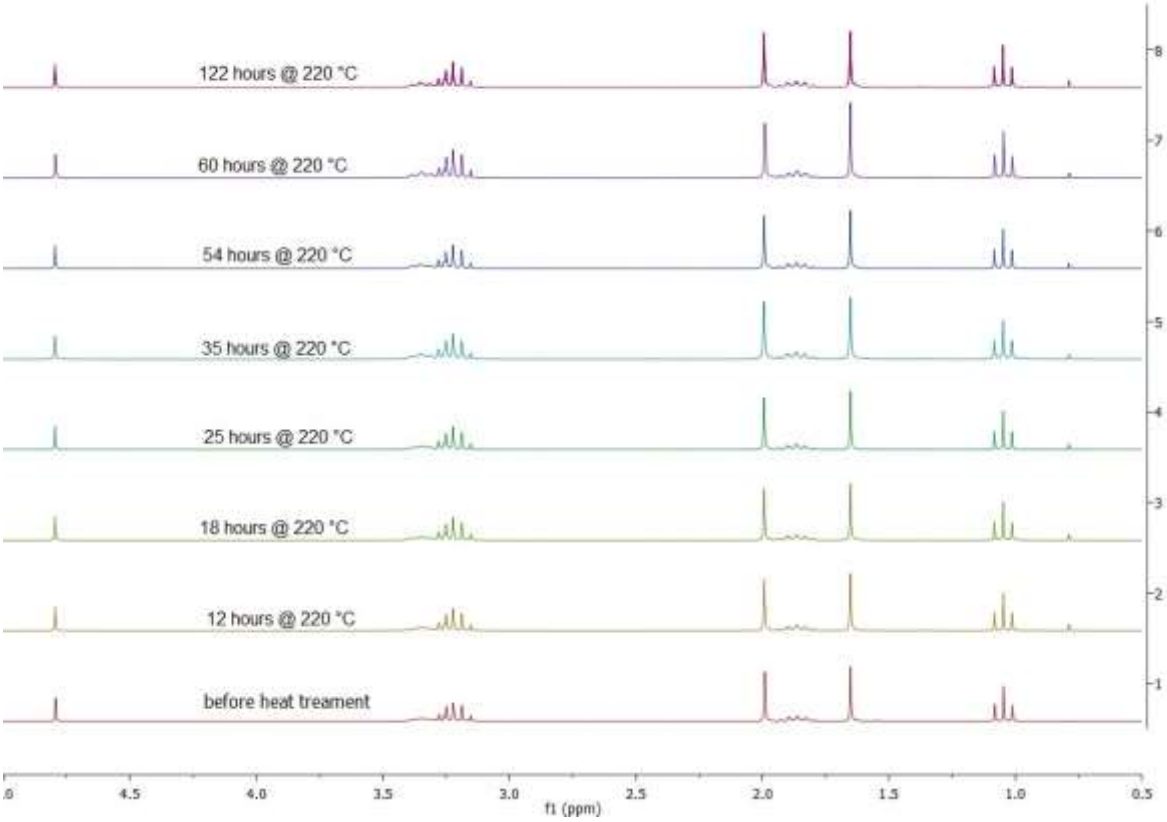

Figure S3. NMR thermal decompositional study @ 220 °C for $[Zn(epki)_2]$

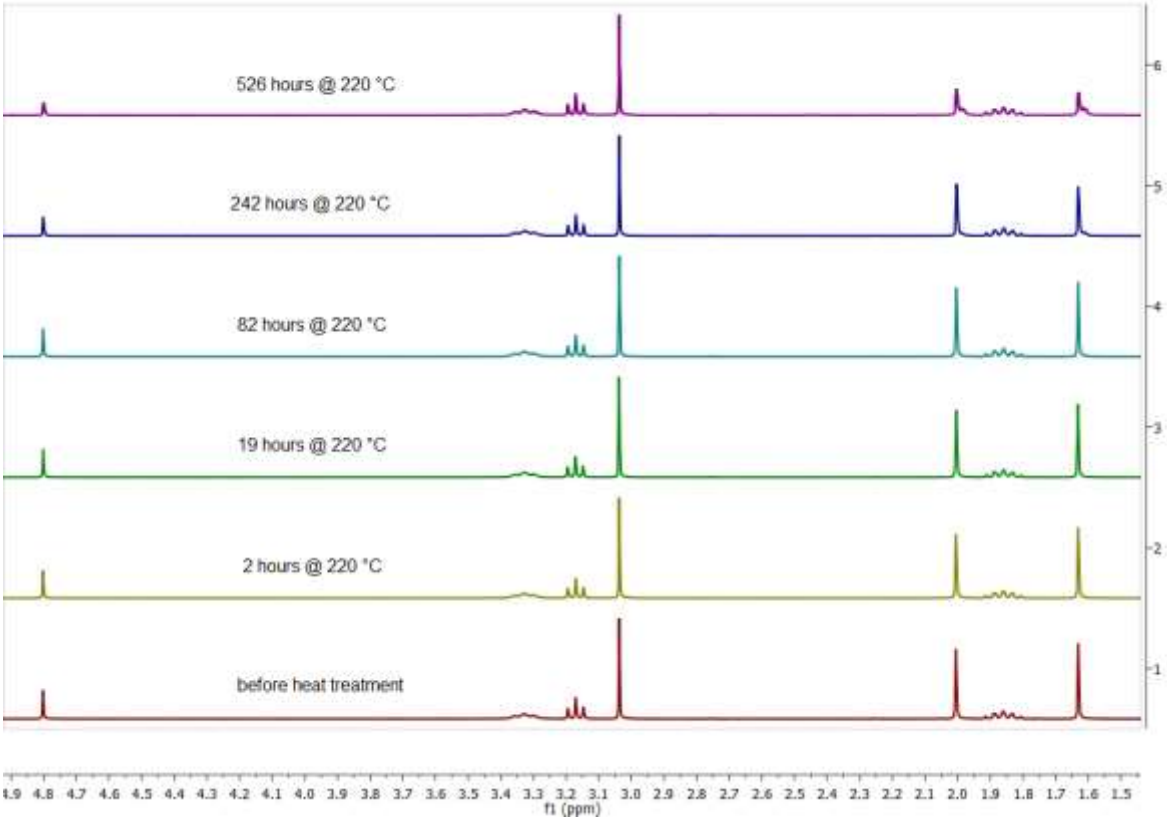

Figure S4. NMR thermal decompositional study @ 220 °C for $[Zn(mpki)_2]$

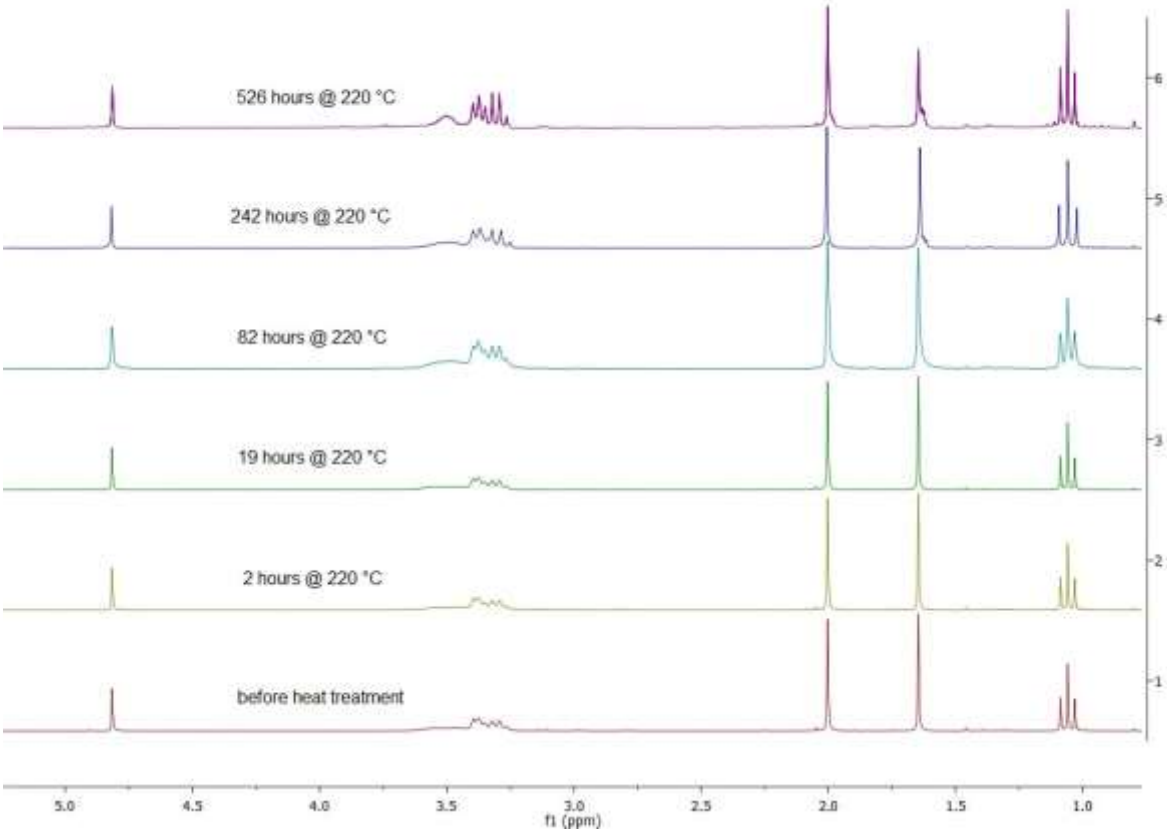

Figure S5. NMR thermal decompositional study @ 220 °C for $[Zn(eeki)_2]$

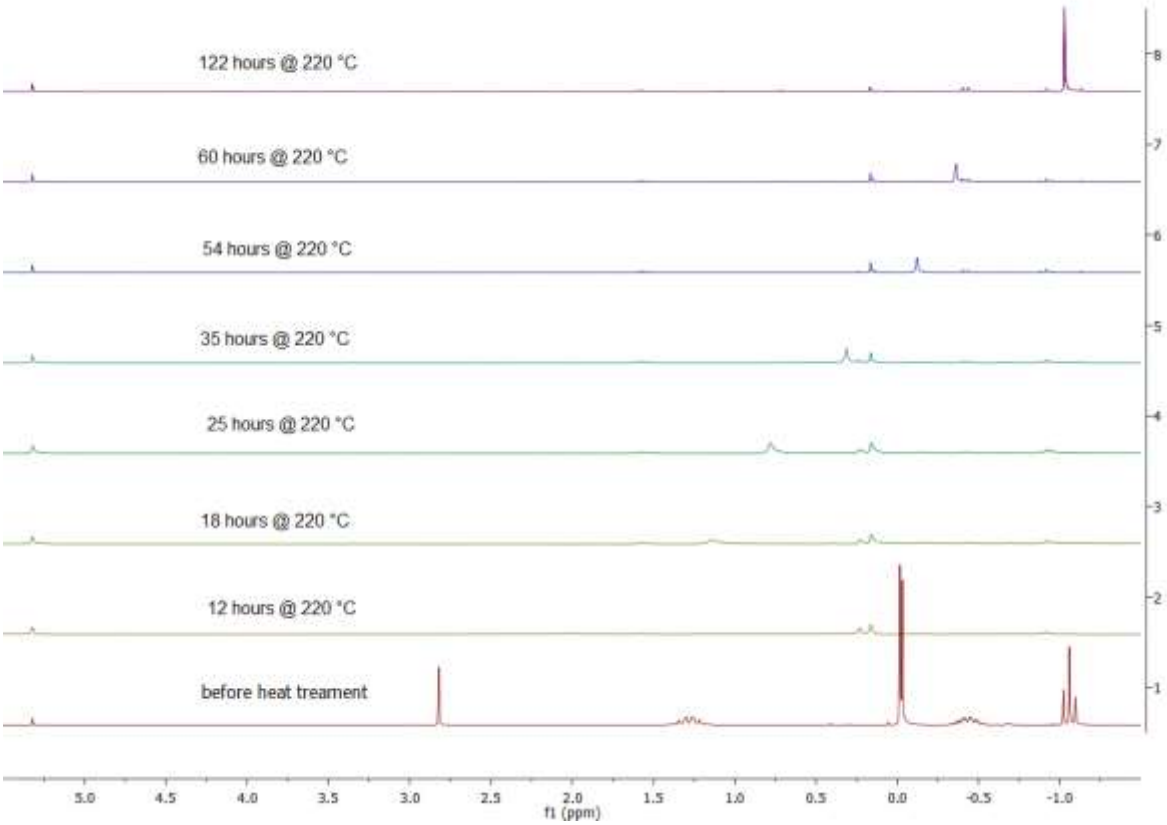

Figure S6. NMR thermal decompositional study @ 220 °C for $[Zn(^{n}pki)_2]$

Table S2. Top: Full range of RBS/NRA data from 150 – 300 °C. Bottom: XPS Zn/O ratios after sputtering and carbon impurities before sputtering. Note after sputtering the carbon signal was reduced below the detection limit of the machine.

Deposition Temperature	**150°C**	**175°C**	**200°C**	**225°C**	**250°C**	**275°C**	**300°C**
RBS							
Zn/O Ratio	1,30	0,86	0,84	0,90	0,87	0,91	0,92
C%	19,7	19,1	2,6	5,6	2,3	9,3	3,8
XPS							
Zn/O Ratio (After Sputtering)	-	1.08	-	1.08	-	1.07	-
C% (Before Sputtering)	-	18.1	-	20.1	-	25.8	-