Synthesis of cyclic carbonates catalysed by aluminium heteroscorpionate complexes Supporting Information

José A. Castro-Osma,^{a,b} Carlos Alonso-Moreno,^b Agustín Lara-Sánchez,^b Javier Martínez,^b Michael North^a* and Antonio Otero^b*

- ^a Green Chemistry Centre of Excellence, Department of Chemistry, The University of York, Heslington, York, YO10 5DD (UK). Fax: +44 1904-432-705; Tel: +44 1904 324-545; E-mail: michael.north@york.ac.uk
- ^b Departamento de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, 13071 Ciudad Real, Spain, Fax: +34 926-295-318; Tel: +34 926-295-300; E-mail: Antonio.Otero@uclm.es

Contents

NMR Spectra for ethylene carbonate 2a	2
Chemical ionization mass spectrum for ethylene carbonate 2a	3
NMR Spectra for propylene carbonate 2b	4
Chemical ionization mass spectrum for proplene carbonate 2b	5
NMR Spectra for styrene carbonate 2c	6
Electron ionization mass spectrum for styrene carbonate 2c	7
NMR Spectra for 1,2-butylene carbonate 2d	8
Chemical ionization mass spectrum for butylene carbonate 2d	9
NMR Spectra for 1,2-hexylene carbonate 2e	10
Chemical ionization mass spectrum for hexylene carbonate 2e	11
NMR Spectra for 1,2-decylene carbonate 2f	12
Chemical ionization mass spectrum for decylene carbonate 2f	13
NMR Spectra for 4-chlorostyrene carbonate 2g	14
Chemical ionization mass spectrum for 4-chlorostyrene carbonate 2g	15
NMR Spectra for 4-bromostyrene carbonate 2h	16
Electron ionization mass spectrum for 4-bromostyrene carbonate 2h	17
NMR Spectra for glycerol carbonate 2i	18
Electron ionization mass spectrum for glycerol carbonate 2i	19
NMR Spectra for 3-chloropropylene carbonate 2j	20
Chemical ionization mass spectrum for 3-chloropropylene carbonate 2j	21
NMR Spectra for 3-phenoxypropylene carbonate 2k	22
Electron ionization mass spectrum for 3-phenoxypropylene carbonate 2k	23
NMR Spectra for cyclohexyl carbonate 29	24
Electron ionization mass spectrum for cyclohexyl carbonate 29	25
Kinetic plots to determine the order with respect to complex 27	26
Plot of log(k _{obs avg}) against log[27]	27
Kinetic plots to determine the order with respect to Bu ₄ NBr	28
Plot of log(k _{obs avg}) against log[Bu ₄ NBr]	29
Plot showing that complex 27 (5 mol%) alone is not an active catalyst at 60 °C in propylene	
carbonate	30
Plot showing that Bu ₄ NBr (5 mol%) alone is not an active catalyst at 60 °C in propylene	
carbonate	30



					1			· · ·	1	' '	· ·		1 1		1			- I - I	· · ·	
00	190	180	170	160	150	140	130	120	110	100 f1 (ppm	90)	80	70	60	50	40	30	20	10	1



Chemical ionization mass spectrum for ethylene carbonate 2a



Electronic Supplementary Material (ESI) for Catalysis Science & Technology This journal is The Royal Society of Chemistry 2014

Spectrum 1A BP: 57 (4347=100%), propylene carbonate.sms 57 4347 4.542 min, Scan: 399, 40:500, Ion: 10125 us, RIC: 14112 100%-103 3557 75%-43 2014 1A 50%-25%-42 692 55 204 0% 100 Acquired Range m/z 300 400 200

Chemical ionization mass spectrum for propylene carbonate 2b





Chemical ionization mass spectrum for styrene carbonate 2c



Spectrum 1A BP: 117 (5483=100%), butylene carbonate.sms 117 5**4**83 5.840 min, Scan: 556, 40:500, Ion: 9755 us, RIC: 19053 100%-75%-1A 50%-43 2106 86 1160 42 1082 25%-116 614 0% 100 400 Acquired Range m/z 200 300

Chemical ionization mass spectrum for butylene carbonate 2d



Spectrum 1A BP: 145 (61576=100%), hexylene carb..sms 145 61\$76 7.946 min, Scan: 807, 40:500, Ion: 672 us, RIC: 199994 100%-75%-1A 50%-144 16470 25%-3 83 4761 7480 0% Acquired Range m/z 100 200 300 400

Chemical ionization mass spectrum for hexylene carbonate 2e







Chemical ionization mass spectrum for decylene carbonate 2f



Electron ionization mass spectrum for 4-chlorostyrene carbonate 2g







Chemical ionization mass spectrum for 4-bromostyrene carbonate **2h**

Electronic Supplementary Material (ESI) for Catalysis Science & Technology This journal is C The Royal Society of Chemistry 2014



Spectrum 1A BP: 119 (24056=100%), glycerol carbonate.sms 119 24**0**56 8.929 min, Scan: 924, 40:500, Ion: 4398 us, RIC: 42957 100%-75%-1A 50%-43 6524 25%-118 2146 86 1359 42 1528 0% 100 Acquired Range m/z 400 200 300

Chemical ionization mass spectrum for glycerol carbonate 2i





Chemical ionization mass spectrum for 3-chloropropylene carbonate 2j





Electron ionization mass spectrum for 3-phenoxypropylene carbonate 2k

NMR Spectra for cyclohexene carbonate 29 in CDCl₃



Chemical ionization mass spectrum for cyclohexene carbonate 29



Kinetic plots to determine the order with respect to complex 27



Electronic Supplementary Material (ESI) for Catalysis Science & Technology This journal is C The Royal Society of Chemistry 2014



Kinetic plots to determine the order with respect to Bu₄NBr



28

Electronic Supplementary Material (ESI) for Catalysis Science & Technology This journal is C The Royal Society of Chemistry 2014



Plot showing that complex 27 (5 mol%) alone is not an active catalyst at 60 $^{\circ}$ C in propylene carbonate



Plot showing that Bu₄NBr (5 mol%) alone is not an active catalyst at 60 °C in propylene carbonate

