Electronic Supplementary Information

Iron amino-bis(phenolate) complexes for the formation of organic

carbonates from CO_2 and oxiranes

Dalal Alhashmialameer,^a Julie Collins,^b Karen Hattenhauer,^a and Francesca M. Kerton^{*a}

^a Department of Chemistry, Memorial University of Newfoundland, St. John's, Newfoundland, Canada A1B 3X7. E-mail: <u>fkerton@mun.ca</u>; Tel:

^bC-CART X-ray Diffraction Laboratory, Memorial University of Newfoundland, St. John's, Newfoundland.

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Table S1.	Crystallographic	data and structure	refinement for	1 and 2.

Compound	1	2
Empirical Formula	C35H54FeClN2O3.C3H6O	$C_{29}H_{42}FeClN_2O_2 \cdot 0.5C_3H_6O_1$
CCDC no.	1452392	1452393
Formula Weight	684.18	570.98
Temperature/K	138	168
Crystal Color	Purple	Purple
Crystal System	Monoclinic	Monoclinic
Crystal Dimensions	0.3 X 0.3 X 0.17 mm	$0.29 \times 0.2 \times 0.2 \text{ mm}$
Lattice Parameters	a = 12.492(3) Å	a = 27.898(9) Å
	b = 9.7027(19) Å	b = 9.683(3) Å
	c = 31.799(6) Å	c = 23.472(8) Å
	$\alpha = 90^{\circ}$	$\alpha = 90^{\circ}$
	$\beta = 94.843(3)^{\circ}$	$\beta = 110.032(4)^{\circ}$
	$V = 3840.6(13) \text{ Å}^3$	V = 5957(3) Å
Space Group	P21/n	C2/c
Z value	4	8
D _{calc}	1.183 g/mm ³	1.273 g/cm^3
F000	1476.0	2440.0
μ(ΜοΚα)	0.498 mm ⁻¹	0.627 cm^{-1}
Reflections collected	34918	27235
Independent reflections	8486	6525
R _{int}	0.0417	0.0380
R, wR ₂ (all) ^{a}	0.0417, 0.1025	0.0392, 0.1006
$R, wR_2 \left[I \!\!> \!\!\!= \!\! 2\sigma\left(I\right)\right]^a$	0.0400, 0.1039	0.0375, 0.0988
GOF-fit on F^2	1.051	1.051

$${}^{a}R_{1} = \Sigma(|F_{o}) - |F_{c}|) / \Sigma|F_{o}|; wR_{2} = [\Sigma(w(F_{o}^{2} - F_{c}^{2})^{2}) / \Sigma w(F_{o}^{2})^{2}]^{1/2}$$

	1	2
Fe-O(1)	1.8696(12)	1.8805(12)
Fe-O(2)	1.8734(11)	1.8690(12)
Fe-N(1)	2.1864(13)	2.1826(14)
Fe-N(2)	2.1681(13)	2.1902(14)
Fe-Cl	2.2466(6)	2.2488(8)
O(1)-Fe-O(2)	97.34(5)	98.85(5)
O(1)-Fe-Cl	111.90(4)	109.07(4)
O(2)-Fe-Cl	110.54(4)	110.41(4)
N(1)-Fe-Cl	97.84(4)	99.25(4)
N(2)-Fe-Cl	98.54(4)	96.29(4)
O(1)-Fe- N(1)	86.06(5)	87.84(5)
O(1)-Fe- N(2)	145.15(5)	145.20(5)
O(2)-Fe- N(2)	87.01(5)	86.22(5)
O(2)-Fe- N(1)	147.45(5)	150.19(5)
N(1)-Fe- N(2)	72.93(5)	72.46(5)

Table S2. Selected Bond lengths (Å) and angles (°) for 1 and 2.



Figure S1. Molecular structure (ORTEP) and partial numbering scheme for **2**. Ellipsoids are shown at the 50% probability level (H-atoms omitted for clarity).



Figure S2. Electronic absorption spectrum of **2** in dichloromethane.



Figure S3. Electronic absorption spectrum of **3** in dichloromethane.



Figure S4. Electronic absorption spectrum of **4** in dichloromethane.



Figure S5. Electronic absorption spectrum of **5** in dichloromethane.



Figure S6. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of H_2L3 .



Figure S7. ¹³C NMR spectrum (300 MHz, 298 K, CDCl₃) of H_2L3 .



Figure S8. MALDI-TOF mass spectrum of H_2L3 .



Figure S9. Theoretical and Experimental isotopic distribution pattern for H_2L3 .



Figure S10. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of H_2L4 .



Figure S11. ¹³C NMR spectrum (300 MHz, 298 K, CDCl₃) of H_2L4 .



Figure S12. MALDI-TOF mass spectrum of H_2L4 .



Figure S13. Theoretical and Experimental isotopic distribution pattern for H_2L4 .



Figure S14. MALDI-TOF mass spectrum of **1**.



Figure S15. Theoretical and Experimental isotopic distribution pattern for **1** with K.



Figure S16. MALDI-TOF mass spectrum of 2.



Figure S17. Theoretical and Experimental isotopic distribution pattern for 2 with K.



Figure S18. MALDI-TOF mass spectrum of **3**.



Figure S19. Theoretical and Experimental isotopic distribution pattern for 3.



Figure S20. Theoretical and Experimental isotopic distribution pattern for **3** with K.



Figure S21. MALDI-TOF mass spectrum of 4.



Figure S22. Theoretical and Experimental isotopic distribution pattern for 4.





Figure S24. Theoretical and Experimental isotopic distribution pattern for 5.



(Table 2, entry 1).



(Table 2, entry 1).



Figure S27. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of 4-chloromethyl-1,3-dioxolan-2-one (Table 2, entry 2).



one (Table 2, entry 2).



Figure S29. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of 4-hydroxymethyl-1,3-dioxolan-2one (Table 2, entry 3).



one (Table 2, entry 3).



Figure S31. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of 4-allyloxymethyl-1,3-dioxolan-2one (Table 2, entry 4).



one (Table 2, entry 4).



Figure S33. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of 4-phenoxymethyl-1,3-dioxolan-2one (Table 2, entry 5).



one (Table 2, entry 5).



Figure S35. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of 4-phenyl-1,3-dioxolan-2-one (Table 2, entry 6).



(Table 2, entry 6).



Figure S37. ¹H NMR spectrum (300 MHz, 298 K, CDCl₃) of cis-1,2-cyclohexene carbonate (Table 2, entry 7).

