Electronic Supplementary Information

Metal β-diketonate Complexes as Highly Efficient Catalysts for Chemical Fixation of CO2 into Cyclic Carbonates in Mild Conditions

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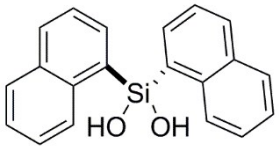
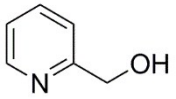
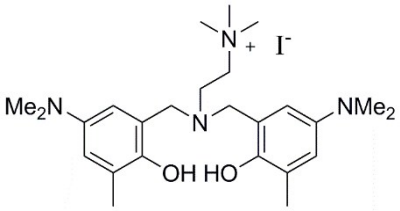
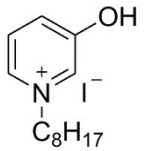
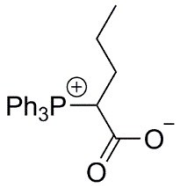
Table S1 Representative catalysts for cyclic carbonate synthesis at 1 atm of CO_2

entry	Catalyst (loading)	Cocatalyst (loading)	Substrate	Temp (^oC)	Time (h)	Yield (%)	TOF [a] (h^{-1})	Catalyst Type	Ref.
1	 (10 mol%)	TBAB (10 mol%)	Styrene Oxide (SO)	60	14	95	0.68	The hydrogen-bond donor, ammonium salt	1
2	 (8 mol%)	TBAI (8 mol%)	1, 2-Propylene Oxide (PO)	25	20	86	0.54	The hydrogen-bond donor, ammonium salt	2
3	Calix[4]pyrroles (3 mol%)	TBAI (3 mol%)	1, 2-Hexene Oxide (HO)	75	6	56	3.1	The hydrogen-bond donor, ammonium salt	3
4	 (2 mol%）	/	PO	rt	24	42	0.88	Functionalized ammonium salt	4
5		/	1, 2-Butene Oxide (BO)	50	6	92	3.1	Functionalized ammonium salt	5

	(5 mol%)								
6	Multifunctional Organocatalysts (4 mol%)	/	BO	rt	24	87	0.91	Functionalized ammonium salt	6
7	Dual-IL system [TMGH+][-O2MMIm+][Br-] (25 mol%)	/	Epichlorohydrin (ECH)	30	12	89	0.30	Functionalized ammonium salt	7
8	ChCl/urea (100mg (about 0.406 mmol) for 0.2 mmol epoxide）	/	N-benzyl spiro-epoxyoxindole	40	5	49	0.098	Functionalized ammonium salt	8
9	SO_2-supported imidazolium halides (25 mol%)	/	BO	80	1	Conv.99% Sel. 94%	3.7	Functionalized ammonium salt	9
10	MIL-101-IP (50 mg for 1 g epoxide)	/	BO	25	48	95	0.40 [b]	Functionalized ammonium salt, Porous materials	10
11	Bifunctional Metal-Free Porous Organic Framework POF-PNA-Br^- (50 mg for 30 mmol epoxide)	/	BO	40	48	91.7	0.82	Functionalized ammonium salt, Porous materials	11
12	Porous Ionic Polymers PIP-Bn-Cl (25 mg for 1 g epoxide)	/	BO	50	24	94.5	1.6 [b]	Functionalized phosphonium salt, Porous materials	12
13		/	PO	25	6	90	3	Functionalized phosphonium salt	13

	(5 mol%)								
14	Hierarchically Mesoporous o-Hydroxyazobenzene Polymers:Zn/HAzo-POP-1 (18mg for 12.5 mmol PO)	TBAB (7.2 mol%)	PO	25	48	>99	0.29 [c]	Metal Porous materials	14
15	Hierarchical Bipyridine-Constructed Framework Cu/POP-Bpy (0.5 mol%)	TBAB (7 mol%)	BO	29	48	99	4.1	Metal Porous materials	15
16	Porous iron-phosphonate nanomaterial: HPFP-1 (50 mg for 5 mmol)	TBAB (5 mol%)	PO	rt	10	87	1.7 [c]	Metal Porous materials	16
17	Mixed Ligand Zn(II) MOFs (1.8 mol%)	TBAB (1.8 mol%)	PO	40	8	99	6.9	Metal–Organic Frameworks	17
18	Amide-functionalized heterometallic helicate cages (0.125 mol%)	TBAB (3.6 mol%)	ECH	rt	24	83	27.7	Functionalized metal compound	18
19	YCl_3 (1 mol%)	TBAB (2 mol%)	BO	22	5	38	7.6	Metal salt	19
20	$Fe(O_2CNEt_2)_3$ (1 mol%)	TBAB (2 mol%)	BO	25	24	99	4.1	Fe(III) carbamates	20
21	Aluminum Porphyrin-based hyper-crosslinked polymers Al-HCP (0.25 mol%)	TBAB (2 mol%)	PO	25	5	99	79.2	Functionalized metal complex	21
22	Salen-Cu(II)@MIL-101(Cr) (6.39 mol% of Cu)	TBAB (100 mol%)	PO	25	48	82.8	0.27	Functionalized metal complex	22
	Bimetallic Aluminium–Salen	TBAB							

	Complexes (2.5 mol%)	(2.5 mol%)							
24	Dinuclear cobalt complexes (0.1 mol%)	TBAB (0.1 mol%)	ECH	120	3	73	243	Metal complex	24
25	Bifunctional aluminium catalyst (5 mol%)	/	BO	35	24	Yield 73%（conv .92%）	1.5	Functionalized metal complex	25
26	supported aluminium(salen) complexes (0.25 mol %)	/	butyl glycidyl ether	50	24	80	13.3	Functionalized metal complex	26
27	Al(III)@cage (1mol% of Al) Co(III)@cage (1mol% of Co)	TBAB (10 mol%)	PO	25	48	58	1.2	Functionalized metal complex	27
			SO		24	99	4.1		
28	$Co(acac)_2$ (0.5 mol%)	TBAI (2.5 mol%)	BO	40	8	97	24.2	Metal complex	**This work**
			PO	40	8	97	24.2		
			HO	70	4	99	49.5		
	$Co(acac)_2$ (0.1 mol%)	TBAI (0.5 mol%)	BO	40	8	41	51.2		

[a] Measured in mole of epoxide consumed/mol catalyst per hour; [b] Measured in g/(g·h); [c] Calculated by cocatalyst.

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