



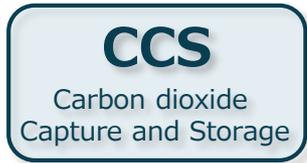
MOONSHOT
RESEARCH & DEVELOPMENT PROGRAM

December 18, 2019

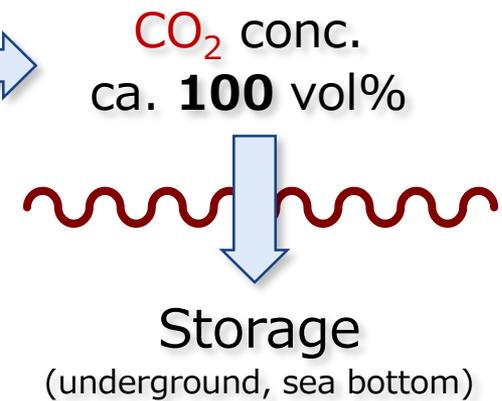
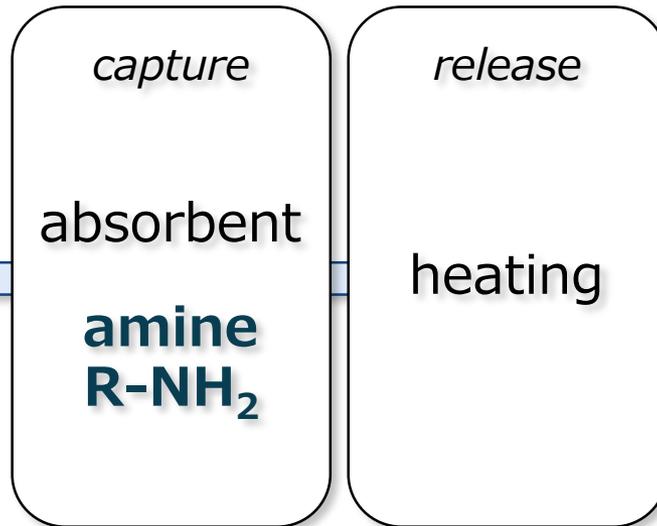
Direct Air Capture (DAC): CO₂-Selective Absorbents in Air

Kobe Gakuin University
Fuyuhiko Inagaki

CO₂ Capturing Technology



Exhaust gas
(Fire plant etc.)
CO₂ conc.
ca. **15** vol%



***Location limited**

Common Task

REDUCTION OF CO₂ SEPARATION ENERGY

CCS



Center for Low Carbon Society Strategy (LCS)
Survey on the Carbon Capture and Storage process, 2016

CO₂ separation energy

current
2.5 MJ/kg-CO₂



future
1.5 MJ/kg-CO₂

DAC



Climeworks
900 ton/year



Carbon Engineering
365 ton/year



Global Thermostat
4,000 ton/year

DAC possesses a highly potential for CO₂ reduction

Smith, P. et al. *Nature Climate Change* **2016**, 6, 42-50.

CO₂ Capturing Technology

DAC Direct Air Capture

Capturing CO₂ in air

CO₂ conc.
ca. **0.04** vol%



***Location free**

CCS
Carbon dioxide
Capture and Storage

Exhaust gas
(Fire plant etc.)

CO₂ conc.
ca. **15** vol%



capture

absorbent

amine
R-NH₂

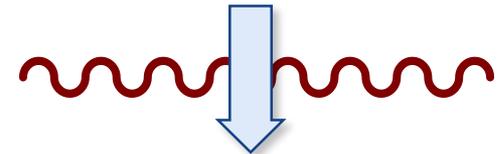
release

heating

key process



CO₂ conc.
ca. **100** vol%

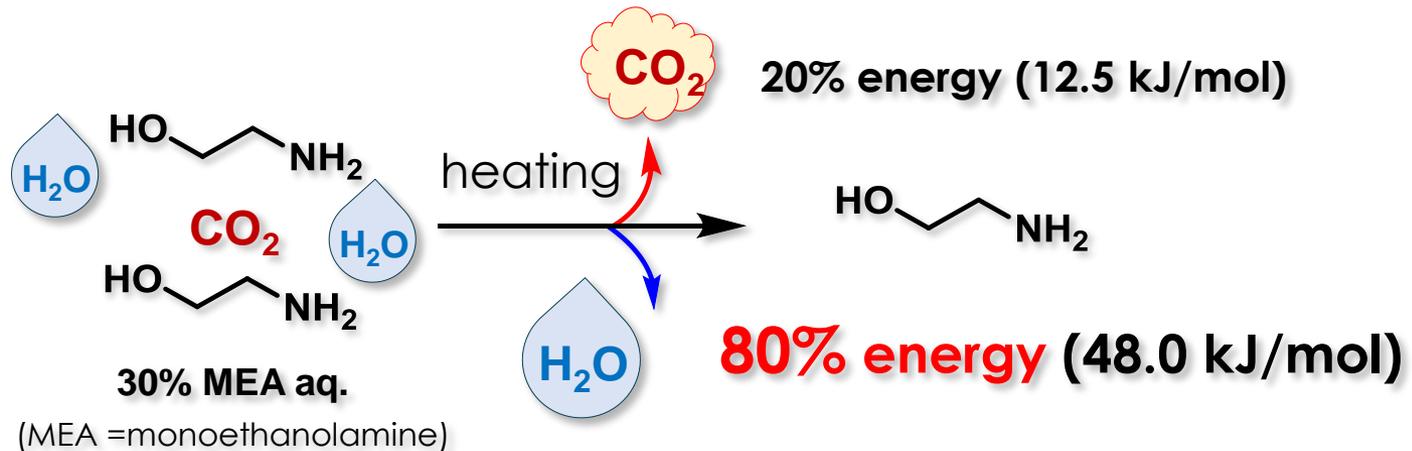


Storage

(underground, sea bottom)

***Location limited**

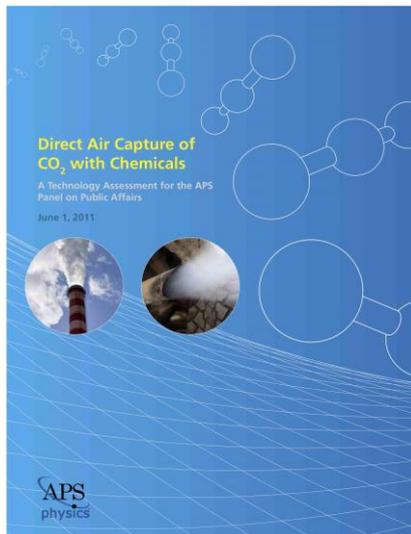
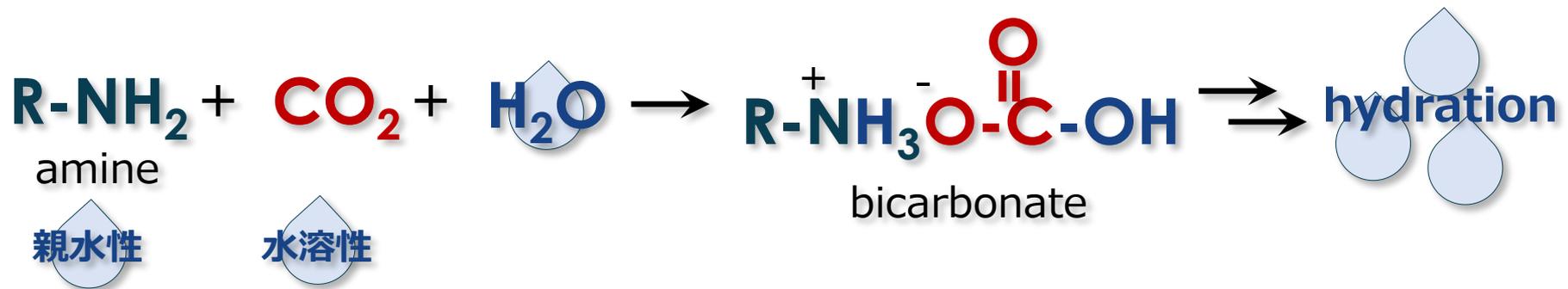
Bottleneck Issue = Water Separation?



Need for extra thermal energy of water!

Weiland, R. H. *et. al. J. Chem. Eng. Data* **1997**, 42, 1004-1006.
APS Physics, *Direct Air Capture of CO_2 with Chemicals*, **2011**, pp 59.

General : Hydration is inevitable

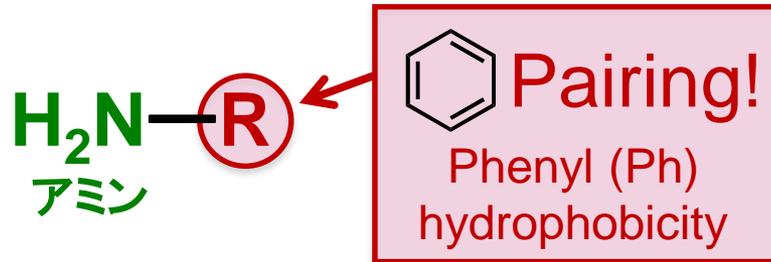


Direct Air Capture of CO₂ with Chemicals, 2011

American Physical Society (APS)

“Water vapor can compete with CO₂ for the reactive sites on sorbents, degrading capture performance. Water vapor can add to the thermal mass of a sorption system that must be heated during regeneration, adding to operating costs.”

CO₂ Selective Absorbent in Air without Hydration



※Commercial sources
(Already mass-production)

Tips

capture

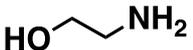
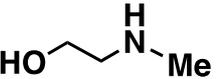
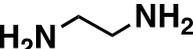
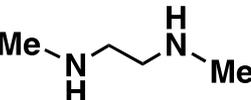
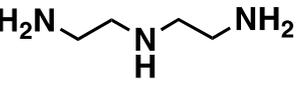
- a) CO₂ selectivity (CO₂ vs. water) up!!
※Some compounds absorb CO₂ only
- b) Similar absorption ability with MEA

release

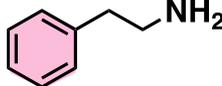
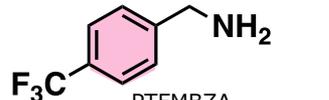
- c) Similar heating temperature with MEA (100-120 °C)
※ Some compounds under 100 °C
- d) Pure CO₂ gas production

a) CO₂ selectivity

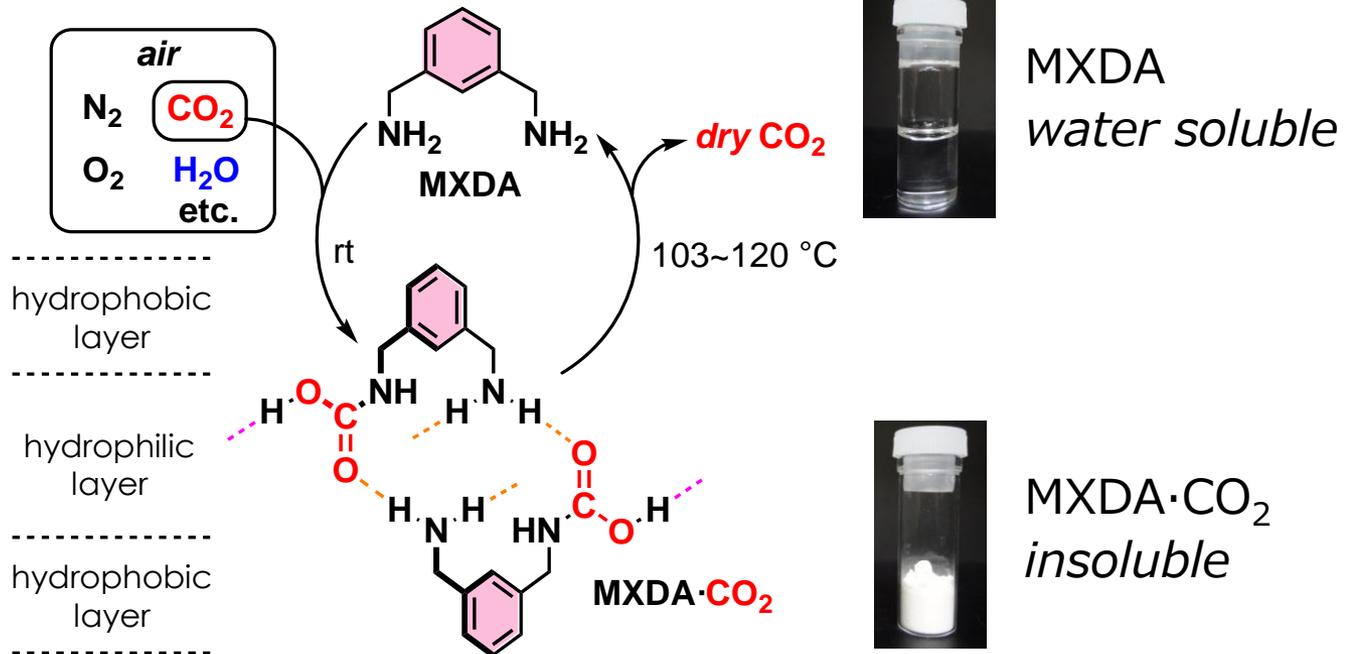
amine in air at room temperature (ca. 1 week) → elemental analysis
amine·X(CO₂)·Y(H₂O)

	CO ₂ X	H ₂ O Y	Moisture content
 MEA monoethanolamine	0.33	1	300%
 MAE 2-(methylamino)ethanol	0.34	1.8-2.7	500-800%
 EDA ethylenediamine	0.27	4.1-4.4	1,500-1,600%
 DMEDA N,N-dimethylethylenediamine	0.86	4.7-4.8	550-560%
 DETA diethylenetriamine	0.35	4.8-5	1,350-1,450%

 Phenyl pairing → CO₂ selectivity up!!

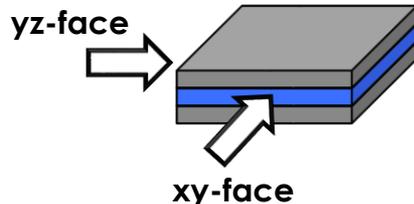
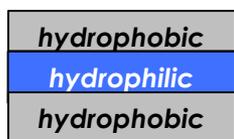
	CO ₂ X	H ₂ O Y	Moisture content
 BZA benzylamine	0.5	0.125	25%
 PEA phenethylamine	0.44	0.11	25%
 PMBZA <i>P</i> -methoxybenzylamine	0.44	0.11	25%
 PTFMBZA <i>P</i> -trifluoromethylbenzylamine	0.5	0.125	25%
 OXDA <i>o</i> -xylylenediamine	1	0	0%
 MXDA <i>m</i> -xylylenediamine	1	0	0%
 PXDA <i>p</i> -xylylenediamine	1	0	0%

Waterproof Mechanisms

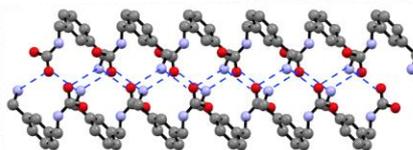


Self-assembled to form a **reverse lipid bilayer** structure with hydrophobic layers (phenyl groups) on both outer surfaces

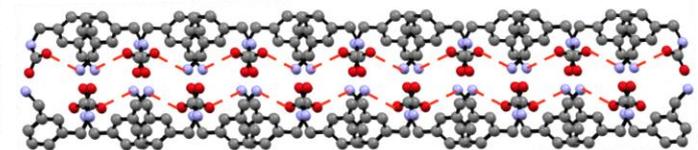
X-ray



xy-face

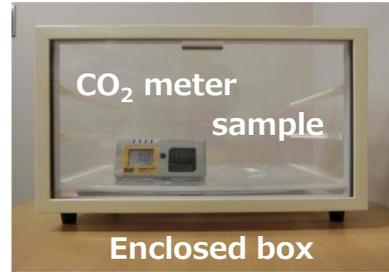


yz-face

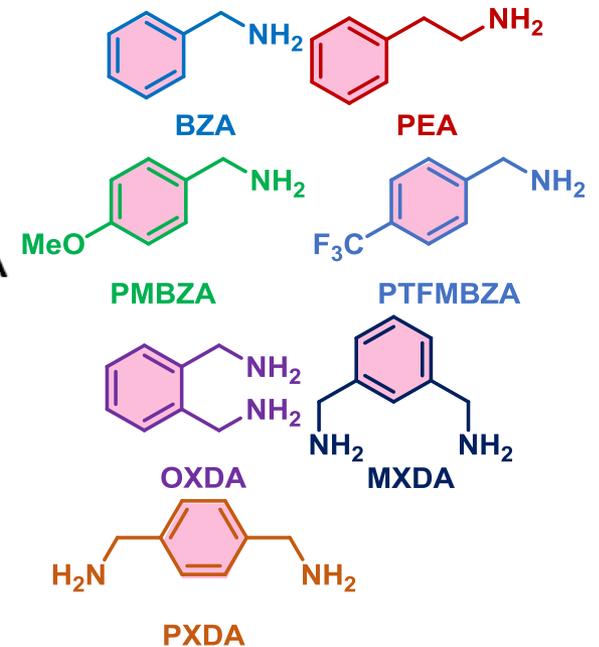
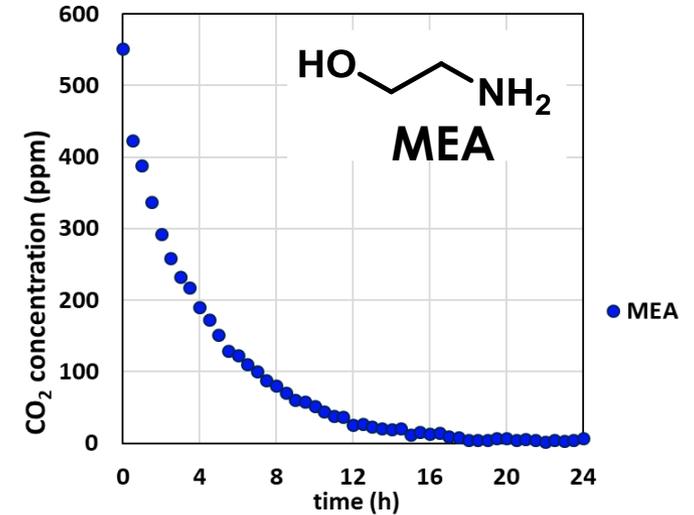
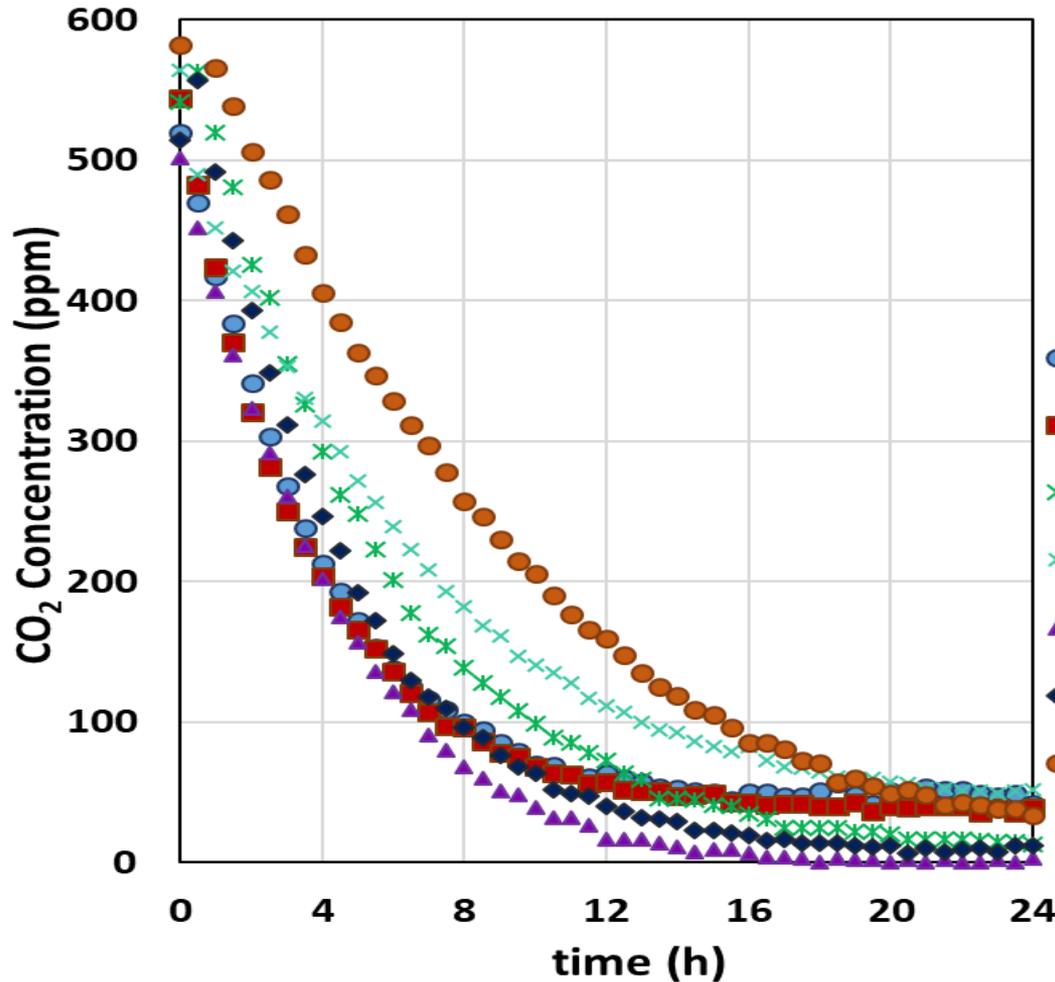


Ball color, grey : carbon, blue : nitrogen, red : oxygen

b) Absorption ability

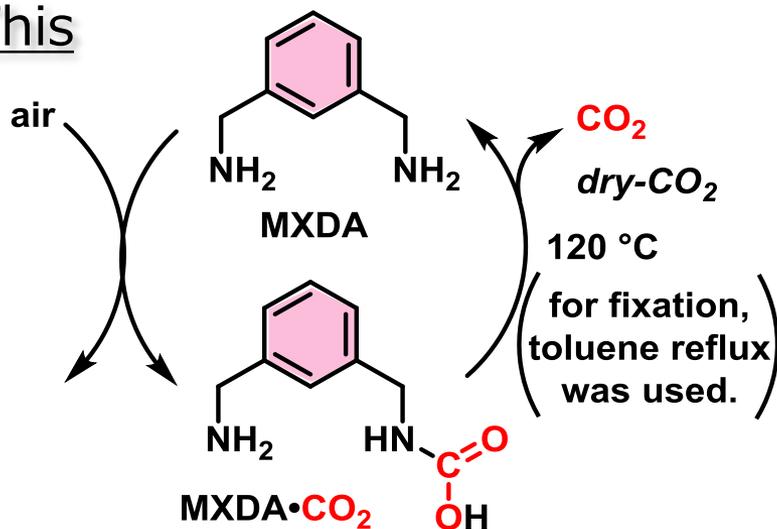


amine 5 mmol, vol. 36 L
initial CO₂ conc. ca. 600 ppm
room temperature

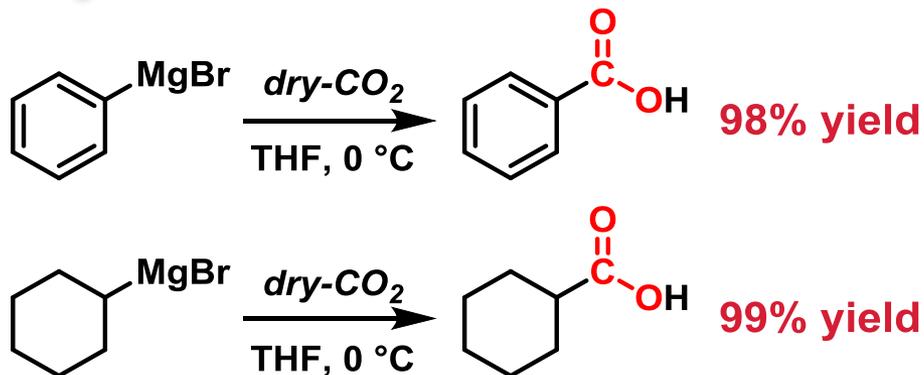


d) Utility of CO₂ gas

This

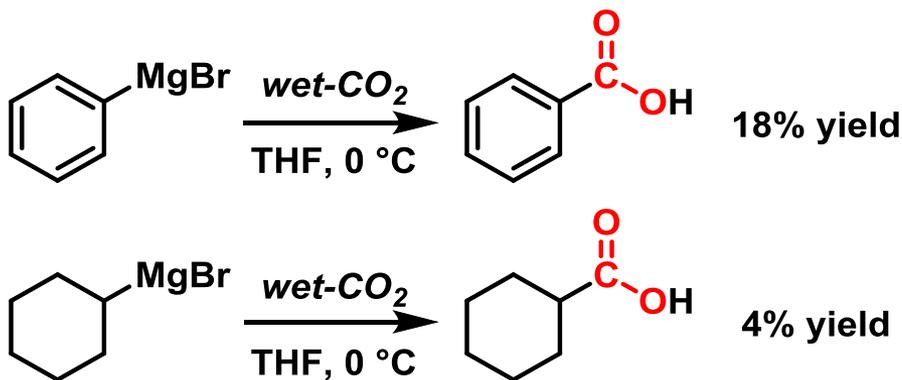
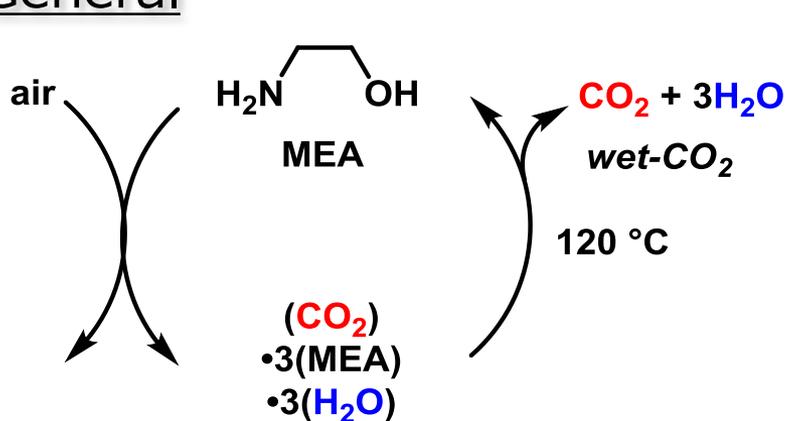


Grignard reaction



Reactive on moisture sensitive condition

General



Unreactive on moisture sensitive condition

【Paper】 CO₂-Selective Absorbents in Air: Reverse Lipid Bilayer Structure Forming Neutral Carbamic Acid in Water without Hydration

Inagaki, F.; Matsumoto, C.; Iwata, T.; Mukai, C.

J. Am. Chem. Soc. **2017**, 139, 4639-4642. DOI: [10.1021/jacs.7b01049](https://doi.org/10.1021/jacs.7b01049)

Energiless CO₂ Absorption, Generation, and Fixation Using Atmospheric CO₂

Inagaki, F.; Okada, Y.; Matsumoto, C.; Yamada, M.; Nakazawa, K.; Mukai, C.

Chem. Pharm. Bull. **2016**, 64, 8-13. DOI: [10.1248/cpb.c15-00793](https://doi.org/10.1248/cpb.c15-00793)

【Patent】 空気由来の二酸化炭素の吸収剤及び発生剤

稲垣冬彦, 向 智里, 岡田泰彦, 松本千明, 山田将之, 中澤研太

特願2015-149320, 新規国内優先権出願 特願2016-147414, 特開2017-031046

2-オキサゾリジノン誘導体の製造方法

稲垣冬彦, 向 智里, 岡田泰彦, 松本千明, 山田将之, 中澤研太

特許第6607596号

低エネルギー型の二酸化炭素発生方法、及び該方法に使用するための二酸化炭素発生剤

稲垣冬彦, 向 智里, 松本千明

特願2018-010003

【Media】 金沢大、CO₂のみ吸収・放出する新素材を開発—化学系メーカーに提案

Nikkan Kogyo Shinbun, March, 27, 2017

Carbon capture gets a boost from aromatic rings

Chemical & Engineering News, 2017, 16, 7.

CO₂-selective Absorption Using *m*-Xylylenediamine

TCI Topics 2017

**Development of an efficient atmospheric CO₂ absorber/release agent
-Challenge from medicinal chemistry-**

Gendaikagaku, November, 2017

【Address】 Fuyuhiko Inagaki

Professor

Kobe Gakuin University, Faculty of Pharmaceutical Sciences

E-mail: finagaki@pharm.kobegakuin.ac.jp