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## Bicarbonate anion coordination assisted CO<sub>2</sub> capture by using urea–morpholine hybrid receptors in water

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The development of energy-efficient sorbents for aqueous CO<sub>2</sub> capture remains a significant challenge. This work presents a new design strategy by integrating a tertiary amine (morpholine) with a urea motif into a single molecular receptor. This structure enables autonomous, base-free CO<sub>2</sub> capture in water, where the urea groups provide complementary hydrogen-bonding sites for (bi)carbonate anions, while the morpholine moiety acts as an internal proton acceptor. The resulting receptors demonstrate a rapid uptake of CO<sub>2</sub> from a simulated flue gas (10% CO<sub>2</sub>/N<sub>2</sub>), achieving a capacity of up to 1.22 mmol g<sup>-1</sup>. Spectroscopic studies (NMR, MS) and structural analysis of a model complex confirm that the capture proceeds via hydrogen-bond-stabilized bicarbonate formation. Crucially, the captured CO<sub>2</sub> can be completely released under remarkably mild conditions, either by heating at ca. 40 °C or by simple N<sub>2</sub> purging at ambient temperature. The receptors exhibit excellent recyclability over multiple capture–release cycles without capacity loss. This study highlights the potential of fine-tuning supramolecular interactions—particularly hydrogen bonding combined with a built-in base—to create low-energy, water-compatible CO<sub>2</sub> capture systems.

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### Introduction

Effective capture of carbon dioxide (CO<sub>2</sub>) is crucial for mitigating climate change, driving the search for materials that combine high adsorption capacity with low regeneration energy.<sup>1–4</sup> Conventional chemisorbents, such as inorganic bases, organic amines, and their polymeric or framework derivatives, typically rely on forming strong chemical bonds (e.g., carbonates or carbamates).<sup>5–17</sup> While effective for capture, this strong binding often necessitates substantial energy input for CO<sub>2</sub> release. The challenge is further amplified in the presence of water, a ubiquitous component in flue gas and direct air capture streams. In aqueous environments, CO<sub>2</sub> hydration readily forms carbonic acid (H<sub>2</sub>CO<sub>3</sub>), and the interaction between organic amines and CO<sub>2</sub> tends to yield (bi) carbonate salts, instead of carbamate.<sup>18</sup> Consequently, achieving both high capture efficiency and energy-favorable desorption in water-rich media remains a significant scientific and technological challenge.

Hydrogen bonding has emerged as a key secondary interaction to regulate the properties of CO<sub>2</sub> capture and release. This is exemplified by strategic modifications in organic amine systems. Introducing intramolecular hydrogen-bond donors or acceptors, such as pyridine or amide groups adjacent to the reactive amines,<sup>19–22</sup> can stabilize CO<sub>2</sub> adducts (e.g., carbamate or carbamic acid) through internal hydrogen bonding.<sup>23–26</sup> Such stabilization not only modulates binding strength but can also lower the regeneration energy by shifting the acid/zwitterion equilibrium toward more readily released neutral species, as demonstrated in aminopyridine solvents.<sup>27</sup> In these systems, the intramolecular hydrogen-bonding network is a critical descriptor for achieving low viscosity and reduced regeneration temperatures (as low as 60–80 °C).<sup>28,29</sup> Similarly, in diamide–diamine macrocycles, the carbamate product is encapsulated and stabilized by a multiple hydrogen bonding network.<sup>30</sup> In aqueous media, the design principle shifts toward employing strong, charge-assisted hydrogen bonds to capture these anions.<sup>31–33</sup> A seminal advance in this direction is the work by Custelcean *et al.* on bis-iminoguanidinium compounds.<sup>34</sup> The rigid, planar guanidine units protonate readily to form guanidinium cations that engage in complementary, strong hydrogen bonds with carbonate or bicarbonate anions, driving the spontaneous crystallization of insoluble frameworks from water and thereby removing CO<sub>2</sub> from the

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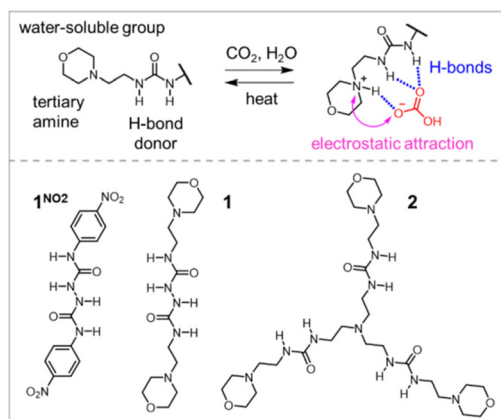
air. Notably, regeneration of these sorbents, achieved by mild heating of the solid carbonate crystals to release CO<sub>2</sub>, can occur at temperatures of 80–120 °C, underscoring how engineered hydrogen-bonding networks can enable energy-efficient capture–release cycles.<sup>34–37</sup> Collectively, these studies highlight hydrogen bonding as a versatile and powerful design element for tailoring CO<sub>2</sub> capture materials.

Like guanidium units, urea motifs can also bind oxyanions like carbonate and bicarbonate *via* anion coordination (*i.e.*, hydrogen bonding), and therefore we sought to extend this supramolecular strategy with urea-based absorbents. While conventional oligourea receptors require exogenous strong bases (*e.g.*, tetraalkylammonium hydroxides or fluorides) to activate CO<sub>2</sub> fixation,<sup>38–44</sup> we hypothesize that integrating a tertiary amine moiety directly into an oligourea scaffold may enable autonomous, base-free capture in water. In this design, the urea groups provide precise hydrogen-bonding sites to stabilize *in situ* formed HCO<sub>3</sub><sup>−</sup>/CO<sub>3</sub><sup>2−</sup> ions, while the tertiary amine serves as an intramolecular proton acceptor,<sup>45–47</sup> offering additional electrostatic stabilization and facilitating the proton-transfer processes essential for both capture and subsequent release (Fig. 2a).

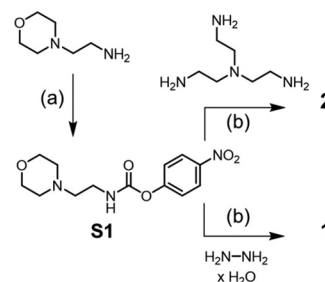
Guided by this rationale, we designed and synthesized a series of small molecules that combine morpholine (a cyclic tertiary amine, Fig. 1) with urea motifs. These morpholine-urea compounds were evaluated for CO<sub>2</sub> capture performance in water without any external organic base. Remarkably, they demonstrated rapid and efficient adsorption of CO<sub>2</sub> directly from water, achieving a capacity of up to 0.75 mol mol<sup>−1</sup> (1.22 mmol g<sup>−1</sup>) for receptor 2. More importantly, the captured CO<sub>2</sub> could be rapidly released under heating at *ca.* 40 °C, highlighting the regulation effect of anion coordination.

## Results and discussion

The designed receptors **1** and **2** were prepared in two steps from the starting material 4-(2-aminoethyl) morpholine



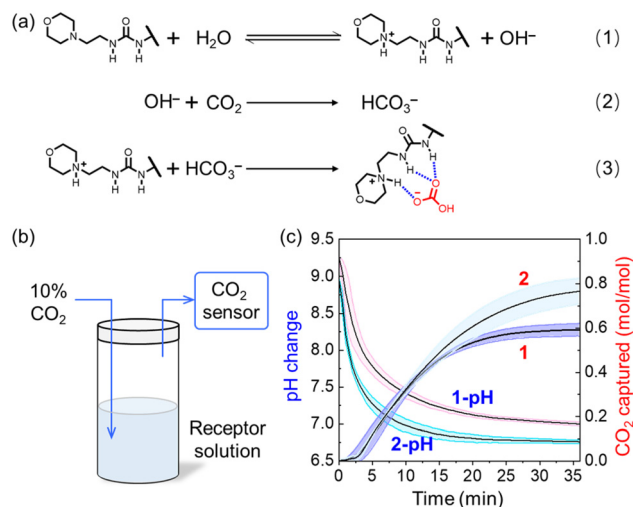
**Fig. 1** Schematic illustration of the design principles of morpholine-urea receptors and their chemical structures.



**Scheme 1** Synthetic procedure of **1** and **2**. Conditions: (a) 4-nitrophenyl chloroformate, CH<sub>2</sub>Cl<sub>2</sub>, 0 °C, 80%; (b) dry CH<sub>3</sub>CN, Et<sub>3</sub>N, 50 °C, 72% for **1**, 81% for **2**.

(Scheme 1), with the overall yields of 58% and 65%, respectively. Both receptors can be easily synthesized on the gram scale, and their structures are characterized and confirmed by NMR and MS spectroscopy (Fig. S8–S16). These two receptors display good water solubility (up to 3 M), and the control receptor **1**<sup>NO<sub>2</sub></sup> is not water soluble, which is directly synthesized from hydrazine hydrate and 4-nitrophenyl isocyanate (Fig. S1–S7).

The CO<sub>2</sub> capture performance of the two receptors was first evaluated in aqueous solution. A simulated flue gas (10% CO<sub>2</sub> in N<sub>2</sub>) was bubbled at room temperature through 15 mL of a 20 mM aqueous solution of each receptor, while the uptake process was monitored in real time using a setup equipped with a high-precision CO<sub>2</sub> sensor (Fig. 2b). The initial pH of the receptor **1** solution was 8.96, consistent with the alkalinity provided by its morpholine group (*pK<sub>a</sub>* ≈ 7.41 for *N*-methylmorpholine).<sup>48,49</sup> Upon CO<sub>2</sub> bubbling, the pH decreased to 6.77 for receptor **1** and to 6.99 for receptor **2**, confirming the existence of the HCO<sub>3</sub><sup>−</sup> anion and H<sub>2</sub>CO<sub>3</sub>. As



**Fig. 2** (a) Mechanistic scheme of the formation of HCO<sub>3</sub><sup>−</sup> and its binding with receptors in water. (b) A schematic diagram of the CO<sub>2</sub> capture experiment (gas input: 10% CO<sub>2</sub>, 90% N<sub>2</sub>; receptor solution: [receptor] = 20 mM, H<sub>2</sub>O, room temperature). (c) The pH changes and the amount of CO<sub>2</sub> captured by using receptors **1** and **2**.

recorded by the CO<sub>2</sub> sensor, the amount of captured CO<sub>2</sub> increased gradually and reached a plateau within 30 minutes (Fig. S26–S28). The determined CO<sub>2</sub> capacity reached 0.75 mol of CO<sub>2</sub> per mole of receptor for **2** (0.75 mol per mol of receptor, equivalent to 1.22 mmol g<sup>-1</sup>, Fig. 2c), which is higher than that of receptor **1** (0.58 mol mol<sup>-1</sup>). This difference can be attributed to the higher number of urea and morpholine groups present in receptor **2**, which provide additional binding sites and basicity. The observed CO<sub>2</sub> uptake trends are consistent with the pH changes of the solutions. Notably, the absorption performance of both receptors is comparable to that of monoethanolamine (MEA), a benchmark industrial absorbent, which typically captures 0.4–0.5 mol of CO<sub>2</sub> per amine.<sup>50–52</sup> Nevertheless, these receptors are not suited for direct air capture applications, as their binding affinity is insufficient for the ultra-low CO<sub>2</sub> concentrations characteristic of ambient air (Fig. S30).

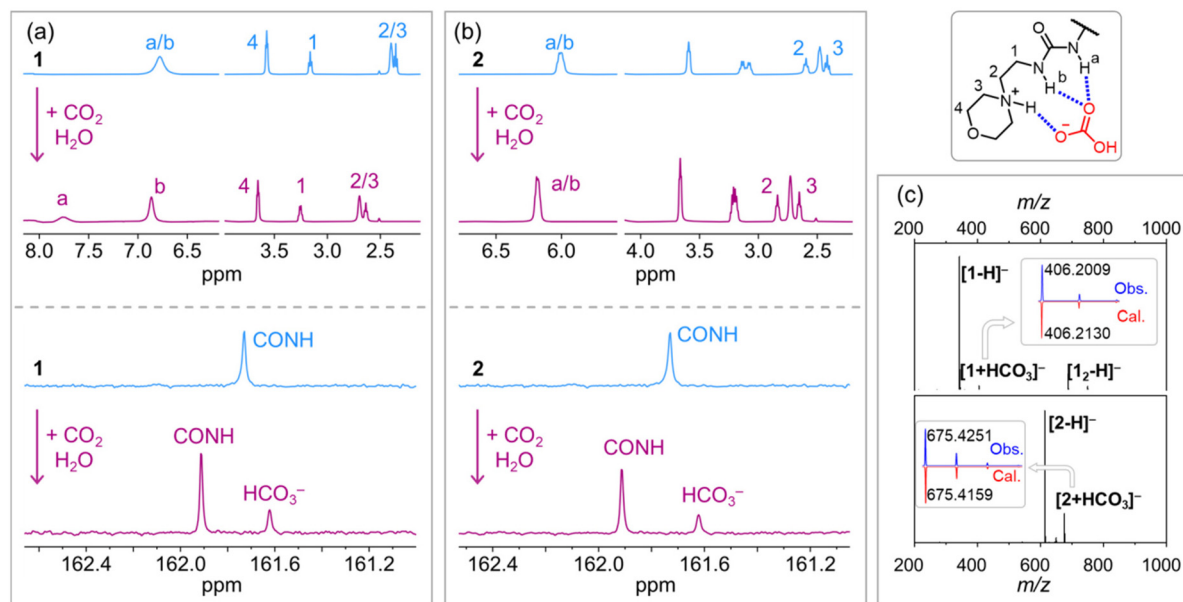
To elucidate the CO<sub>2</sub> capture mechanism, NMR and mass spectrometry (MS) experiments were performed. Following the completion of CO<sub>2</sub> uptake, as indicated by pH changes after *ca.* 30 min of CO<sub>2</sub> bubbling through a receptor-containing aqueous solution (20 mM), the resulting solutions were subjected to spectroscopic characterization.

As recorded in the <sup>1</sup>H NMR spectra, the urea NH signals (Ha and Hb) exhibited characteristic changes upon CO<sub>2</sub> capture. For receptor **1**, the original singlet at 6.78 ppm split into two doublets at 7.7 ppm and 6.8 ppm (Fig. 3a), whereas for receptor **2**, the signal shifted from 6.0 ppm to 6.2 ppm (Fig. 3b). These changes correspond to the hydrogen bonding between the urea groups and the HCO<sub>3</sub><sup>-</sup> anion produced upon CO<sub>2</sub> absorption. Additionally, protons adjacent to the morpholinyl nitrogen (H2 and H3) in both receptors showed downfield

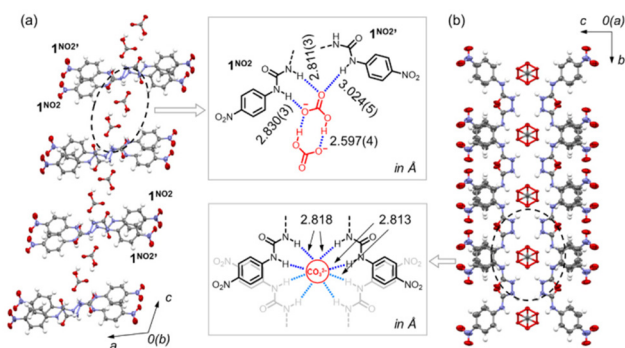
shifts, consistent with the protonation of the tertiary amine and potential hydrogen bonding with the HCO<sub>3</sub><sup>-</sup> anion. The <sup>13</sup>C NMR spectra further support the existence of the HCO<sub>3</sub><sup>-</sup> anion. After CO<sub>2</sub> exposure, new peaks appeared at 160 ppm for **1** and 161 ppm for **2**, which are assigned to the HCO<sub>3</sub><sup>-</sup> anion and consistent with reported data from the literature. Moreover, the carbonyl carbon atoms of the urea moieties exhibited clearly downfield shifts, with the most pronounced change observed for **1** ( $\Delta\delta \approx 4$  ppm). These shifts reflect the electronic perturbation induced by HCO<sub>3</sub><sup>-</sup> anion binding. In addition, the post-capture aqueous solutions of **1** and **2** were analysed by ESI-QTOF mass spectrometry. Distinct peaks were observed at 406.20 and 675.43, assigned to the adducts of [1 + HCO<sub>3</sub>]<sup>-</sup> and [2 + HCO<sub>3</sub>]<sup>-</sup>, respectively (Fig. 3c), providing direct evidence for the formation of bicarbonate complexes. The MS results combined with NMR data to support the absorption of CO<sub>2</sub> as the HCO<sub>3</sub><sup>-</sup> anion binding complexes with receptors.

To obtain structural insights into the CO<sub>2</sub> capture process, crystallization trials were conducted. Due to the high-water solubility of receptors **1** and **2**, single crystals of their HCO<sub>3</sub><sup>-</sup> complexes could not be obtained. Instead, a control receptor **1**<sup>NO<sub>2</sub></sup>, which bears terminal nitrophenyl groups and retains the bis(urea) hydrogen-bonding motif but exhibits lower water solubility, was employed. Slow vapor diffusion from acetonitrile/diethyl ether yielded single crystals of its HCO<sub>3</sub><sup>-</sup> and CO<sub>3</sub><sup>2-</sup> complexes (as tetramethylammonium salts) suitable for X-ray diffraction analysis (Fig. 4).

As shown in Fig. 4a, the HCO<sub>3</sub><sup>-</sup> complex crystallizes in the space group *C2/c*, while the CO<sub>3</sub><sup>2-</sup> complex crystallizes in the *C2/m* space group. Both structures display one-dimensional arrangements (along the *c*-axis or *b*-axis) stabilized by hydrogen bonds between the anions and the bis(urea) receptors. In



**Fig. 3** <sup>1</sup>H and <sup>13</sup>C NMR spectra of receptors (a) **1** and (b) **2** before and after CO<sub>2</sub> capture (10% DMSO-*d*<sub>6</sub>/90% H<sub>2</sub>O, 298 K). (c) ESI-QTOF spectra of receptors after CO<sub>2</sub> capture, indicating the formation of HCO<sub>3</sub><sup>-</sup> binding complexes.



**Fig. 4** Single crystal X-ray diffraction structures of (a)  $\text{HCO}_3^-$  and (b)  $\text{CO}_3^{2-}$  binding complexes of receptor  $1^{\text{NO}_2}$ . Solvent molecules and tetramethylammonium cations ( $\text{TMA}^+$ ) are omitted for clarity. Their anion binding structures with urea units are shown in the middle boxes. The  $\text{HCO}_3^-$  anion dimerizes through two complementary hydrogen bonds and interacts with urea units through three hydrogen bonds. The  $\text{CO}_3^{2-}$  anion is disordered and stabilized by eight hydrogen bonds with four urea units.

the  $\text{HCO}_3^-$  complex, a 2:2 stoichiometry between the anion and  $1^{\text{NO}_2}$  is observed. Every two  $\text{HCO}_3^-$  anions dimerize through two  $\text{O-H}\cdots\text{O}$  hydrogen bonds ( $d = 2.597 \text{ \AA}$ ), a recurring motif also reported in oligourea and guanidinium-based  $\text{CO}_2$  capture systems. Such anti-electrostatic hydrogen bonding is also widely seen for hydroxy anion dimers in the solid state.<sup>39,53–55</sup> Each bicarbonate anion is further stabilized by three  $\text{N-H}\cdots\text{O}$  hydrogen bonds from urea groups. Every two receptors adopt a parallel arrangement with an essentially linear conformation (Fig. S6).

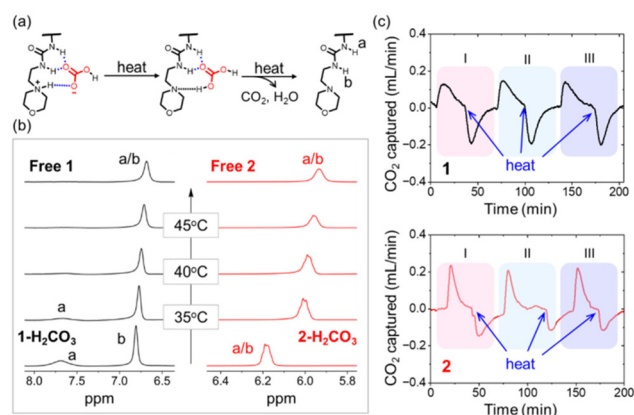
In contrast, the  $\text{CO}_3^{2-}$  complex features a V-shaped receptor conformation. Each carbonate anion is engaged in eight  $\text{N-H}\cdots\text{O}$  hydrogen bonds involving four different receptor molecules (Fig. 4b). The average  $\text{N-H}\cdots\text{O}$  distance in the  $\text{CO}_3^{2-}$  complex ( $2.82 \pm 0.01 \text{ \AA}$ ) is notably shorter than that in the  $\text{HCO}_3^-$  analogue ( $2.89 \pm 0.10 \text{ \AA}$ ), reflecting stronger binding to carbonate. Along the  $b$ -axis, adjacent  $\text{CO}_3^{2-}$  ions are linked by urea groups from different receptors, forming an infinite one-dimensional hydrogen-bonded chain that extends into a rod-like framework structure (Fig. S7).

In contrast to receptors **1** and **2**, the control receptor  $1^{\text{NO}_2}$  captures  $\text{CO}_2$  only in the presence of an external base, such as fluoride or tetramethylammonium hydroxide ( $\text{TMAOH}$ ), in acetonitrile or DMSO. This requirement is attributed to the absence of the built-in morpholine group, a feature that enables autonomous proton capture in **1** and **2**, and aligns with the behavior of other oligourea receptors reported earlier. Interestingly, once  $\text{CO}_2$  is captured, the resulting  $\text{HCO}_3^-$  complex of  $1^{\text{NO}_2}$  precipitates rapidly from acetonitrile solution within minutes, forming a hydrogen-bond-supported framework as seen in the solid state (Fig. 4). Such fast precipitation, commonly observed with guanidinium-based receptors, is seldom reported for urea-based systems. Furthermore, in the presence of  $\text{TMA}^+$  as the counteranion, the absorbed  $\text{HCO}_3^-$  anion cannot be thermally released as  $\text{CO}_2$  gas (Fig. S17–S25).

Reversible  $\text{CO}_2$  release occurs only when free protons ( $\text{H}^+$ ) are available in solution,<sup>56</sup> underscoring the crucial role of proton transfer in the regeneration step.

In the presence of  $\text{TMA}^+$  as the counteranion, the absorbed  $\text{HCO}_3^-$  anion cannot be thermally released as  $\text{CO}_2$ . This is because thermal regeneration of the absorbent necessitates the complete protonation of absorbed  $\text{HCO}_3^-$  to form labile carbonic acid ( $\text{H}_2\text{CO}_3$ ), which then dissociates to release  $\text{CO}_2$ . Nevertheless, during the heating of  $\text{TMAHCO}_3$  complexes, no labile protons are available for combination with  $\text{HCO}_3^-$ , thus precluding  $\text{CO}_2$  release and absorbent regeneration. In contrast, the receptor utilized in our work allows the absorbed  $\text{CO}_2$  to be converted into  $\text{H}^+$  and  $\text{HCO}_3^-$  during the absorption process. Specifically, the generated  $\text{H}^+$  resides on the protonated morpholine moieties, whereas  $\text{HCO}_3^-$  is connected to the urea groups *via* weak hydrogen bonds, constructing a fragile hydrogen-bonding network. This structural characteristic facilitates proton transfer from the protonated morpholine groups to  $\text{HCO}_3^-$  upon heating, which in turn promotes the formation of labile  $\text{H}_2\text{CO}_3$  (Fig. 5a).

For receptors **1** and **2**, the captured  $\text{CO}_2$  (in the form of  $\text{HCO}_3^-$ ) can be readily released under mild heating, as initially demonstrated by variable-temperature  $^1\text{H}$  NMR experiments. A solution of receptor **1** after  $\text{CO}_2$  bubbling (10 mM, 10%  $\text{DMSO-}d_6/90\% \text{ H}_2\text{O}$ ) was examined while increasing the temperature from 298 K to 308 K (35 °C). Upon heating, the urea NH signal (Ha) gradually disappeared, while the adjacent proton Hb showed a clear upfield shift (Fig. 5b). At 318 K (45 °C), the spectrum closely resembled that of the free receptor, indicating complete release of the  $\text{HCO}_3^-$  anion. A similar trend was observed for the receptor **2**. The recovery of the  $^1\text{H}$  NMR signals corresponding to the free receptors confirms that hydrogen-bonding interactions with bicarbonate are effectively disrupted upon heating, resulting in the release of  $\text{CO}_2$  gas. Such low-temperature  $\text{CO}_2$  release is rarely reported, suggesting that hydrogen-bonding interaction can serve as a tunable tool for regulating both capture and release processes.



**Fig. 5** (a) A schematic representation of the mechanism of  $\text{CO}_2$  release. (b) Variable temperature  $^1\text{H}$  NMR spectra of  $\text{CO}_2$ -binding receptors (10 mM, 10%  $\text{DMSO-}d_6/90\% \text{ H}_2\text{O}$ , 400 MHz). (c) Reversible  $\text{CO}_2$  capture and release (upon heating at 40 °C).

To assess the recyclability of the receptors, reversible CO<sub>2</sub> capture and thermal release were monitored in real time using the CO<sub>2</sub> sensor setup (Fig. 2b). An aqueous solution of receptor 1 or 2 (20 mM, 15 mL) was continuously purged with 10% CO<sub>2</sub> in N<sub>2</sub>. After uptake reached completion (~30 min), the solution was heated to 40 °C using a stir plate. The CO<sub>2</sub> sensor recorded a drop in outlet CO<sub>2</sub> concentration during the capture phase, followed by a return to the baseline level upon heating, which is consistent with the variable-temperature NMR results. This capture-release cycle was repeated multiple times without any loss in capacity (Fig. 5c), confirming excellent reversibility and stability of the receptors.

Furthermore, we found that CO<sub>2</sub> could also be liberated simply by purging the solution with pure N<sub>2</sub> gas (Fig. S31), a behavior similarly observed in other anion-based CO<sub>2</sub> capture systems where CO<sub>2</sub> is weakly bound. This result further underscores the low-energy character of CO<sub>2</sub> release in these urea-morpholine receptors. The integration of hydrogen-bonding motifs with a tertiary amine moiety enables effective capture while maintaining weak binding strength, thereby minimizing the energy penalty associated with regeneration, a feature attributed to the labile nature of the hydrogen-bonding network that stabilizes the bicarbonate anion.

## Conclusions

In summary, we have designed and synthesized new urea-morpholine receptors capable of efficient and reversible CO<sub>2</sub> capture in water without adding external bases. The synergistic function of the urea hydrogen-bond donors and the tertiary amine proton acceptor facilitates direct CO<sub>2</sub> capture, forming stable bicarbonate complexes as verified by NMR, MS, and structural analysis using a crystalline model system. A key achievement is the exceptionally mild release of CO<sub>2</sub>, achievable either by gentle heating (~40 °C) or inert gas purging, which underscores the low-energy penalty associated with disrupting the labile hydrogen-bonding network. The receptors maintain full capture capacity over multiple cycles, demonstrating robust recyclability. Compared to the control receptor 1<sup>NO<sub>2</sub></sup>, which requires added base and exhibits irreversible binding, the integrated morpholine design is essential for autonomous proton management and energy-efficient regeneration. This work establishes hydrogen-bonding donor/acceptor integration as a powerful supramolecular strategy for developing new, energy-lean carbon capture materials operable under practical, moisture-rich conditions.

## Author contributions

Data curation, investigation and methodology: Z. Sun, J. Wang, Q. Nie, N. Li, and Z. Liu. Project administration, supervision and funding acquisition: W. Zhao, X.-J. Yang, and B. Wu. Conceptualization and writing (original draft, reviewing & editing): W. Zhao and Z. Sun.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

Data supporting this article have been included as part of the supplementary information (SI). Supplementary information: details of syntheses, single crystal structures and NMR results. See DOI: <https://doi.org/10.1039/d5dt03056k>.

CCDC 2516702 (carbonate complex), 2516703 (bicarbonate complex), 2517602 (receptor 1<sup>NO<sub>2</sub></sup>) and 2517603 (receptor 1) contain the supplementary crystallographic data for this paper.<sup>57a-d</sup>

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## References

- 1 D. S. Sholl and R. P. Lively, *Nature*, 2016, **532**, 435–437.
- 2 D. M. Reiner, *Nat. Energy*, 2016, **1**, 15011.
- 3 K. S. Lackner, *Science*, 2003, **300**, 1677–1678.
- 4 S. Y. W. Chai, L. H. Ngu and B. S. How, *Greenhouse Gases: Sci. Technol.*, 2022, **12**, 394–427.
- 5 E. S. Sanz-Pérez, C. R. Murdock, S. A. Didas and C. W. Jones, *Chem. Rev.*, 2016, **116**, 11840–11876.
- 6 H. Adun, J. D. Ampah, O. Bamisile and Y. Hu, *Sustain. Prod. Consum.*, 2024, **45**, 386–407.
- 7 A. Deprez, P. Leadley, K. Dooley, P. Williamson, W. Cramer, J.-P. Gattuso, A. Rankovic, E. L. Carlson and F. Creutzig, *Science*, 2024, **383**, 484–486.
- 8 S. A. Didas, S. Choi, W. Chaikittisilp and C. W. Jones, *Acc. Chem. Res.*, 2015, **48**, 2680–2687.
- 9 F. Inagaki, C. Matsumoto, T. Iwata and C. Mukai, *J. Am. Chem. Soc.*, 2017, **139**, 4639–4642.
- 10 F. A. Chowdhury, H. Yamada, T. Higashii, K. Goto and M. Onoda, *Ind. Eng. Chem. Res.*, 2013, **52**, 8323–8331.
- 11 C. Perinu, I. M. Bernhardsen, D. D. D. Pinto, H. K. Knuutila and K.-J. Jens, *Ind. Eng. Chem. Res.*, 2018, **57**, 1337–1349.
- 12 X. Li, X. Zhao, Y. Liu, T. A. Hatton and Y. Liu, *Nat. Energy*, 2022, **7**, 1065–1075.
- 13 J. Liu, M. Yang, X. Zhou and Z. Meng, *J. Am. Chem. Soc.*, 2024, **146**, 33093–33103.
- 14 J. Singh, H. Bhunia and S. Basu, *J. Environ. Manage.*, 2019, **250**, 109457.

- 15 F. Zhao, B. Zhu, L. Wang and J. Yu, *J. Colloid Interface Sci.*, 2024, **659**, 486–494.
- 16 H. Li, M. E. Zick, T. Trisukhon, M. Signorile, X. Liu, H. Eastmond, S. Sharma, T. L. Spreng, J. Taylor, J. W. Gittins, C. Farrow, S. A. Lim, V. Crocellà, P. J. Milner and A. C. Forse, *Nature*, 2024, **630**, 654–659.
- 17 Y. Yu, Y. Shen, X. Zhou, F. Liu, S. Zhang, S. Lu, J. Ye, S. Li, J. Chen and W. Li, *Chem. Eng. J.*, 2022, **428**, 131241.
- 18 J. K. Stolaroff, D. W. Keith and G. V. Lowry, *Environ. Sci. Technol.*, 2008, **42**, 2728–2735.
- 19 J. N. Gayton, Q. Li, L. Sanders, R. R. Rodrigues, G. Hill and J. H. Delcamp, *ACS Omega*, 2020, **5**, 11687–11694.
- 20 A. F. Eftaiha, A. K. Qaroush, B. O. Al-Shami and K. I. Assaf, *Org. Biomol. Chem.*, 2021, **19**, 3873–3881.
- 21 D. Wei, R. Sang, A. Moazezbarabadi, H. Junge and M. Beller, *JACS Au*, 2022, **2**, 1020–1031.
- 22 A. Li, Y. Liu, K. Luo and Q. He, *CCS Chem.*, 2024, **6**, 2882–2894.
- 23 J. S. Derrick, M. Loipersberger, S. K. Nistanaki, A. V. Rothweiler, M. Head-Gordon, E. M. Nichols and C. J. Chang, *J. Am. Chem. Soc.*, 2022, **144**, 11656–11663.
- 24 G. Manca, F. Barzagli, J. Nagy, M. Munzarová, M. Peruzzini and A. Ienco, *Fuel*, 2024, **378**, 132859.
- 25 M. Ma, Y. Liu, Y. Chen, G. Jing, B. Lv, Z. Zhou and S. Zhang, *J. CO2 Util.*, 2023, **67**, 102277.
- 26 S. Meng, T. H. Lambert and P. J. Milner, *J. Am. Chem. Soc.*, 2025, **147**, 6786–6794.
- 27 D. Malhotra, D. C. Cantu, P. K. Koech, D. J. Heldebrant, A. Karkamkar, F. Zheng, M. D. Bearden, R. Rousseau and V.-A. Glezakou, *ACS Sustainable Chem. Eng.*, 2019, **7**, 7535–7542.
- 28 M. K. Leszczynski, D. Kornacki, M. Terlecki, I. Justyniak, G. I. Miletic, I. Halasz, P. Bernatowicz, V. Szejko and J. Lewinski, *ACS Sustainable Chem. Eng.*, 2022, **10**, 4374–4380.
- 29 A. J. Huang, A. K. Gupta, H. Z. H. Jiang, H. Zhuang, M. B. Wenny, R. A. Klein, H. Kwon, K. R. Meihaus, H. Furukawa, C. M. Brown, J. A. Reimer, W. A. de Jong and J. R. Long, *J. Am. Chem. Soc.*, 2025, **147**, 10519–10529.
- 30 Q. Q. Wang, V. W. Day and K. Bowman-James, *Org. Lett.*, 2014, **16**, 3982–3985.
- 31 S. Pawłędzio and X. Wang, *Crystals*, 2024, **14**, 77–103.
- 32 H. Cai, X. Zhang, L. Lei and C. Xiao, *ACS Omega*, 2020, **5**, 20428–20437.
- 33 G. Mezei, *Chem*, 2019, **5**, 499–501.
- 34 C. A. Seipp, N. J. Williams, M. K. Kidder and R. Custelcean, *Angew. Chem., Int. Ed.*, 2017, **56**, 1042–1045.
- 35 U. I. Premadasa, V. Bocharova, A. R. Miles, D. Stamberga, S. Belony, V. S. Bryantsev, A. Elgattar, Y. Liao, J. T. Damron, M. K. Kidder, B. Doughty, R. Custelcean and Y. Z. Ma, *Angew. Chem., Int. Ed.*, 2023, **62**, e202304957.
- 36 F. M. Brethomé, N. J. Williams, C. A. Seipp, M. K. Kidder and R. Custelcean, *Nat. Energy*, 2018, **3**, 553–559.
- 37 N. J. Williams, C. A. Seipp, F. M. Brethomé, Y.-Z. Ma, A. S. Ivanov, V. S. Bryantsev, M. K. Kidder, H. J. Martin, E. Holguin, K. A. Garrabrant and R. Custelcean, *Chem*, 2019, **5**, 719–730.
- 38 A. Pramanik, M. E. Khansari, D. R. Powell, F. R. Fronczek and M. A. Hossain, *Org. Lett.*, 2014, **16**, 366–369.
- 39 U. Manna and G. Das, *CrystEngComm*, 2019, **21**, 65–76.
- 40 I. Ravikumar and P. Ghosh, *Chem. Commun.*, 2010, **46**, 1082–1084.
- 41 R. Chutia and G. Das, *Dalton Trans.*, 2014, **43**, 15628–15637.
- 42 R. Dutta, S. Chakraborty, P. Bose and P. Ghosh, *Eur. J. Inorg. Chem.*, 2014, **2014**, 4134–4143.
- 43 U. Manna and G. Das, *CrystEngComm*, 2018, **20**, 3741–3754.
- 44 S. Kayal, U. Manna and G. Das, *Inorg. Chim. Acta*, 2019, **486**, 576–581.
- 45 G. Gao, B. Xu, X. Gao, W. Jiang, Z. Zhao, X. Li, C. Luo, F. Wu and L. Zhang, *Chem. Eng. J.*, 2023, **473**, 145277.
- 46 X. Li, J. Hou, H. Sui, L. Sun and L. Xu, *Materials*, 2018, **11**, 2431.
- 47 X. Zhou, D. Wang, C. Liu, G. Jing, B. Lv and D. Wang, *J. Environ. Sci.*, 2024, **140**, 146–156.
- 48 C. Yu, H. Ling, Z. Shen, H. Yang, D. Cao and X. Hu, *AIChE J.*, 2024, **70**, e18551.
- 49 K. Liu, K. M. Jinka, J. E. Remias and K. Liu, *Ind. Eng. Chem. Res.*, 2013, **52**, 15932–15938.
- 50 J. I. Huertas, M. D. Gomez, N. Giraldo and J. Garzón, *J. Chem.*, 2015, 965015.
- 51 M. Abdi-Khanghah, F. Hadavimoghaddam, S. Atashrouz, E. Nasirzadeh, M. A. Abuswer, M. Ostadhassan, A. Mohaddespour and A. Hemmati-Sarapardeh, *Digit. Chem. Eng.*, 2025, **15**, 100235.
- 52 M. N. Procopio, G. Urquiza, L. Castro and V. Zezatti, *Results Eng.*, 2023, **19**, 101286.
- 53 U. Manna, S. Kayal, B. Nayak and G. Das, *Dalton Trans.*, 2017, **46**, 11956–11969.
- 54 M. Giri and T. Guchhait, *ChemPlusChem*, 2024, **89**, e202400405.
- 55 U. Manna, S. Kayal, S. Samanta and G. Das, *Dalton Trans.*, 2017, **46**, 10374–10386.
- 56 B. Lv, B. Guo, Z. Zhou and G. Jing, *Environ. Sci. Technol.*, 2015, **49**, 10728–10735.
- 57 (a) CCDC 2516702: Experimental Crystal Structure Determination, 2026, DOI: [10.5517/ccdc.csd.cc2qgtzy](https://doi.org/10.5517/ccdc.csd.cc2qgtzy);  
 (b) CCDC 2516703: Experimental Crystal Structure Determination, 2026, DOI: [10.5517/ccdc.csd.cc2qgtz0](https://doi.org/10.5517/ccdc.csd.cc2qgtz0);  
 (c) CCDC 2517602: Experimental Crystal Structure Determination, 2026, DOI: [10.5517/ccdc.csd.cc2qhrzz](https://doi.org/10.5517/ccdc.csd.cc2qhrzz);  
 (d) CCDC 2517603: Experimental Crystal Structure Determination, 2026, DOI: [10.5517/ccdc.csd.cc2qhs01](https://doi.org/10.5517/ccdc.csd.cc2qhs01).