Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Supporting Information: Thermal Modulation of Reaction Equilibria Controls Mass Transfer in CO_2-Binding Organic Liquids

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Section S1: Supplementary Figures

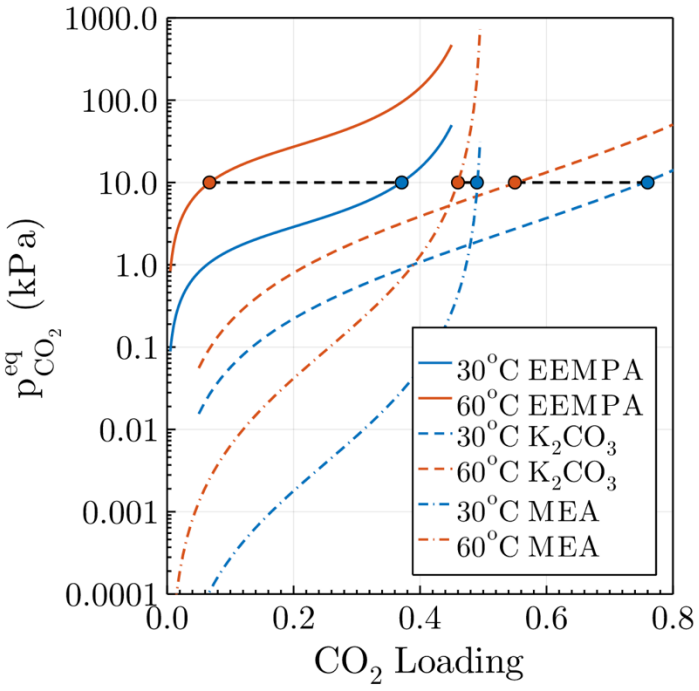


Figure S1: Vapor-Liquid Equilibria for CO_2 absorption into EEMPA, 30wt% K_2CO_3, and 30wt% MEA solutions, at 30°C and 60°C. Note that when exposed to p_{CO2} = 10kPa the equilibrium extent of the reaction with CO_2 decreases by approximately 5, 1.05 and 1.4 times for EEMPA, MEA and K_2CO_3 respectively.

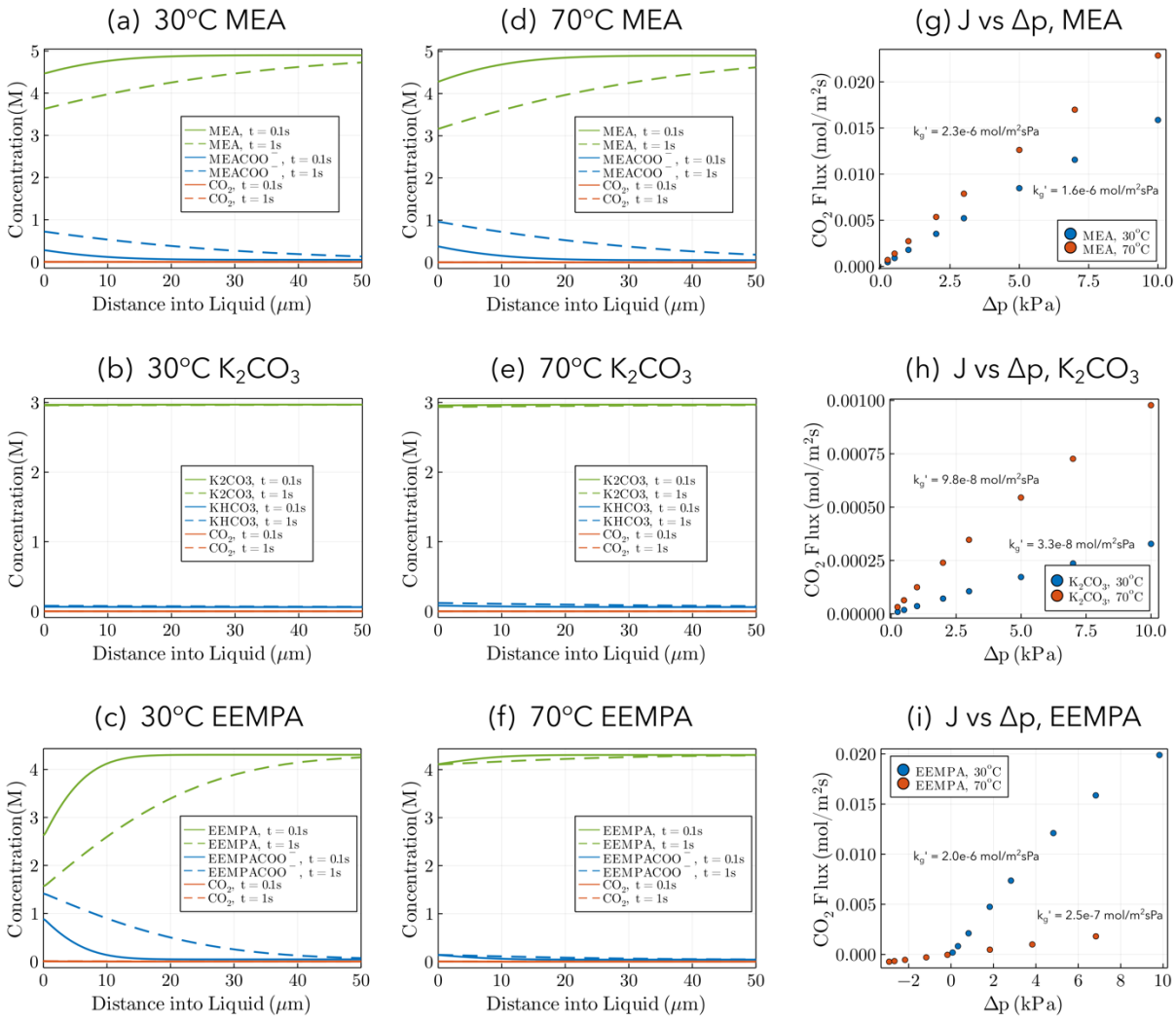


Figure S2: Generalization of system described in Figure 2 of the main text to other solvent systems. (a)-(f) Concentration profiles near the gas-liquid interface in 30wt% MEA, 30wt% K_2CO_3, and EEMPA at 30°C and 70°C, 0.1s and 1s after exposure to a gas with p_{CO2} = 10kPa. Bulk loading for all solvents is zero. DBU:Hexanol kinetics are used for EEMPA simulation, corresponding to lower bound in Figure 3 of the manuscript. (g)-(i) Plots of gas flux vs pressure driving force for each system, as predicted by surface renewal theory. Note that k_g' is given by the gradient of each line.

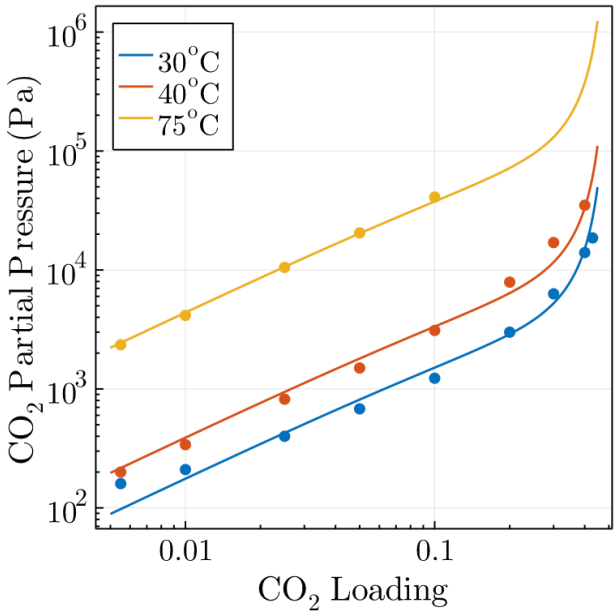


Figure S3: Vapor liquid equilibria for absorption of CO_2 into EEMPA. Data taken from Zheng et al. (2020).

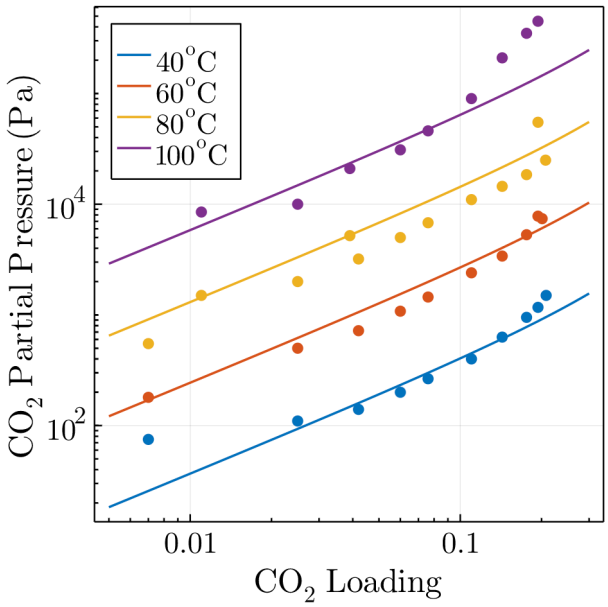


Figure S4: Vapor liquid equilibria for absorption of CO_2 into IPADM-2-BOL. Data taken from Mathias et al. (2015).

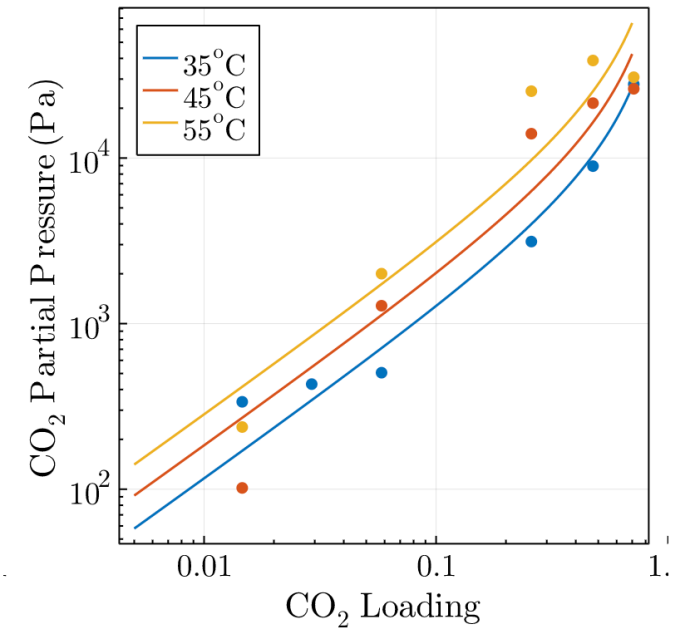


Figure S5: Vapor liquid equilibria for absorption of CO_2 into DBU-Hexanol. Data taken from Mathias et al. (2015).

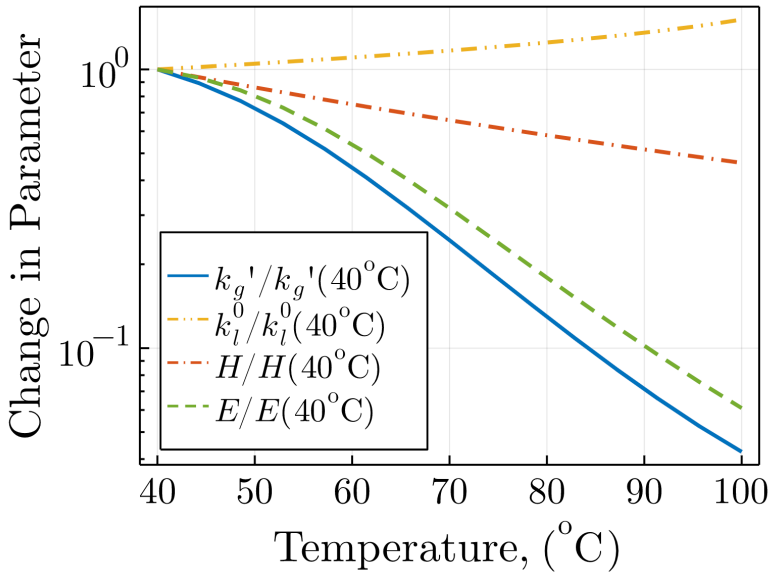


Figure S6: Relative change in k_g', k_l^0, H and E in IPADM-2-BOL at 1% CO_2 loading, as the temperature is varied from 40°C to 100°C, as predicted by the surface renewal model.

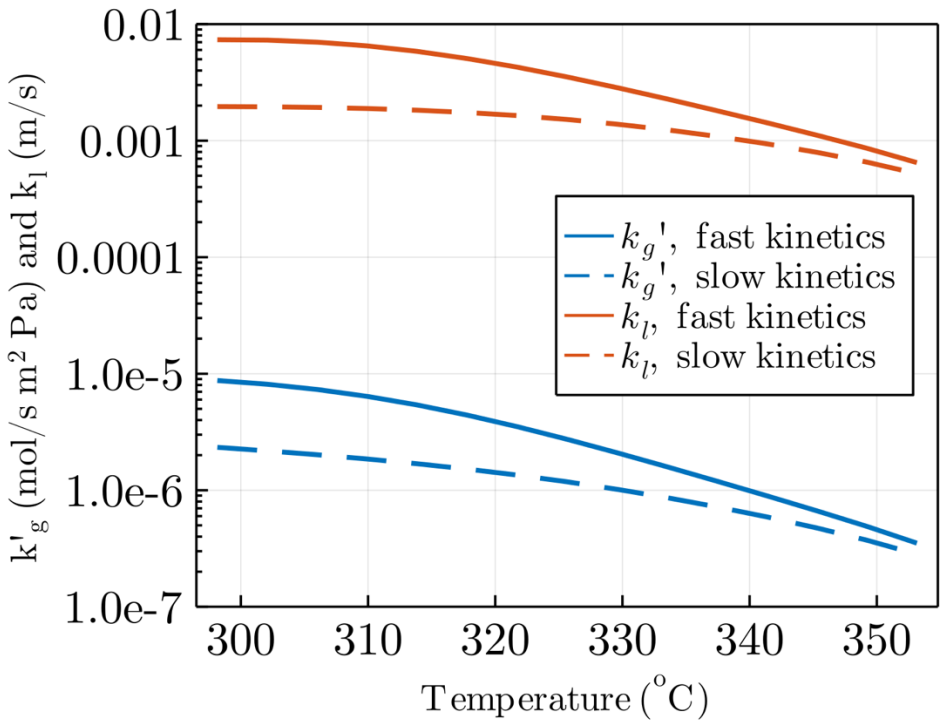


Figure S7: Plot of $k_g' = HEk_l^0$ and $k_l = Ek_l^0$ for IPADM at a range of temperatures. Bulk CO_2 loading: 1%. Solid line: instantaneous reaction kinetics. Dashed line: finite reaction kinetics equivalent to DBU:Hexanol.

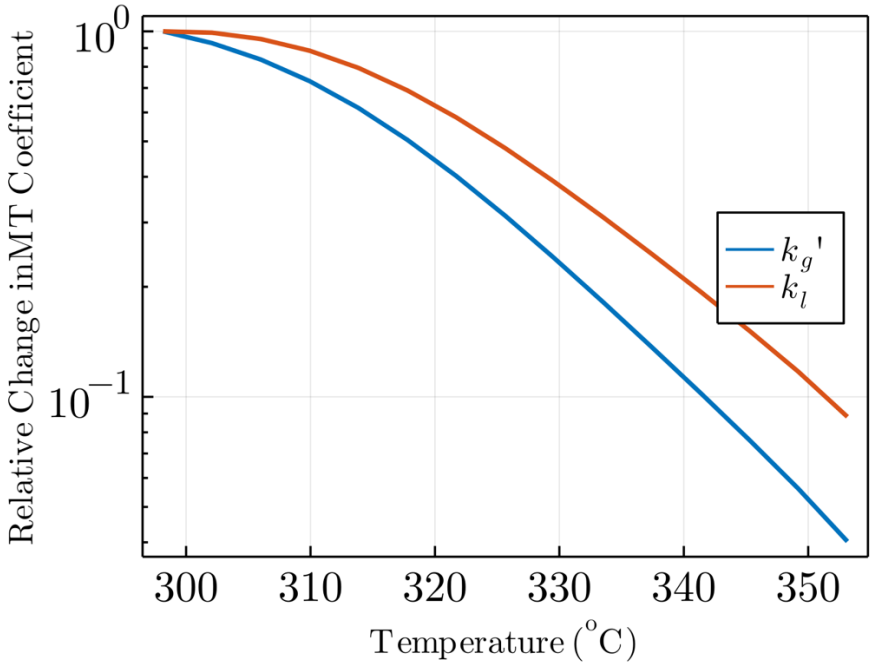


Figure S8 Relative change in $k_g' = HEk_l^0$ and $k_l = Ek_l^0$ for IPADM from 25°C. Bulk CO_2 loading: 1%. Instantaneous reaction kinetics.

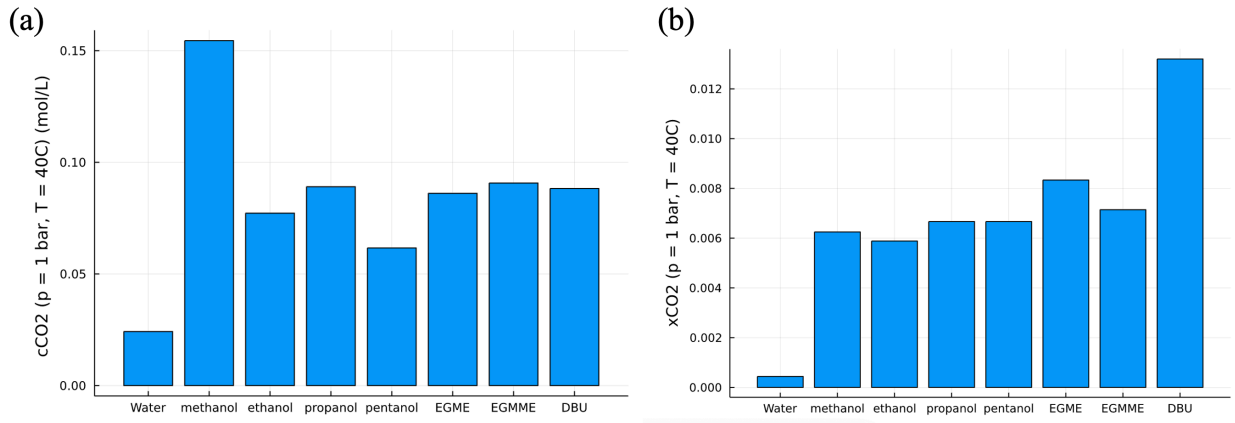


Figure S9: Equilibrium concentration of CO_2(aq) in a water and a range of non-aqueous solvents at 40°C, as measured on (a) a molar concentration basis, and (b) a mole fraction basis. Use of a mole-fraction basis typically exaggerates the ratio of the solubility of CO_2 in water to the solubility in non-aqueous solvents by about 3-10x, compared with a molar concentration basis, which is more appropriate for assessing mass transfer rates. Water data: Van Swaalj. DBU Data: reported by Mathias et al. (2015). All other data: Gui et al. (2011).

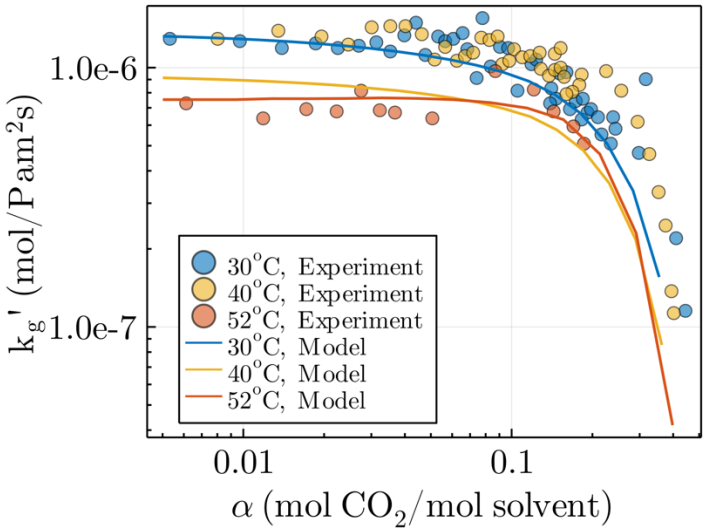


Figure S10: Comparison of EEMPA surface renewal model with experimental data of Zheng et al. (2020) at a range of temperatures and CO_2 loadings. EEMPA model uses finite reactions kinetics equivalent to value in DBU:Hexanol (i.e. lower bound in Figure 3 of manuscript).

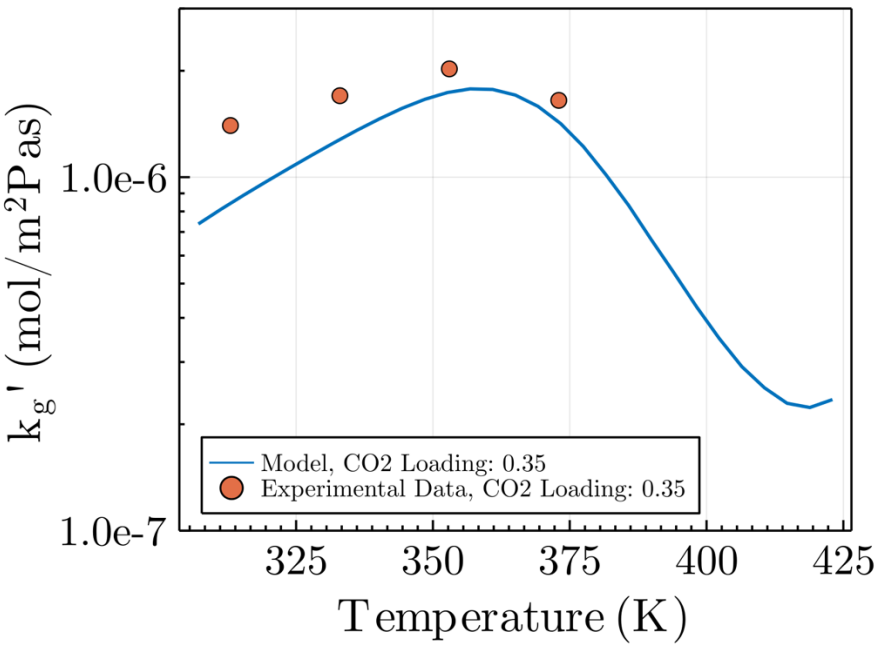


Figure S11: k_g' vs T for CO_2 absorption into 30wt% MEA, as predicted by surface renewal model. α = 0.35. Experimental data points taken from Dugas and Rochelle (2011). Values at 80°C and 100°C are interpolated from data at loadings of $\alpha = 0.271$ and $\alpha = 0.366$

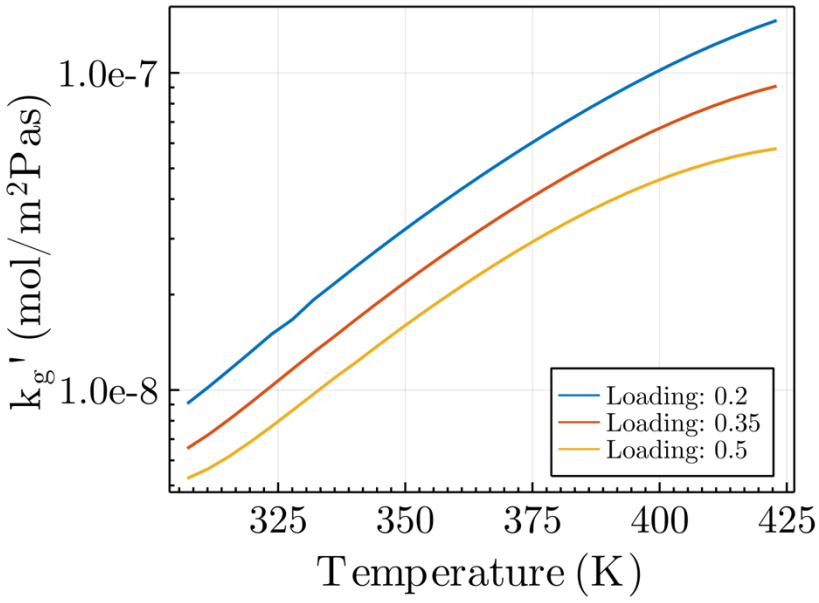


Figure S12: k_g' vs T for CO_2 absorption into 30wt% K_2CO_3 at a range of CO_2 loadings, as predicted by surface renewal model.

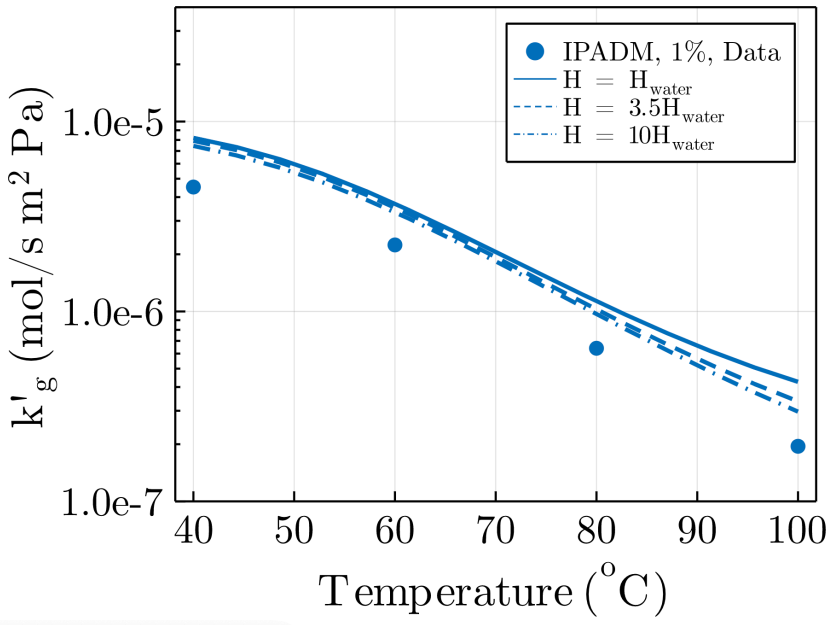


Figure S13: Predictions for k_g' for CO_2 absolution into IPADM-2-BOL for various choices of Henry's constant, in the instantaneous-reaction limit. Note that varying the Henry's constant by an order of magnitude has negligible effect on the prediction for k_g'. H_{water} is the Henry's constant of CO_2 in water.

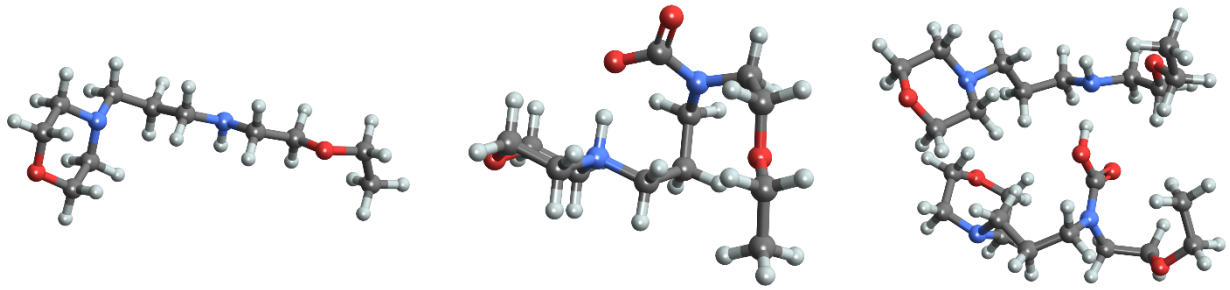


Figure S14: Molecular Structures for 2-EEMPA (left), Monomolecular 2-EEMPA-CO2 (middle), and Bimolecular 2-EEMPA-CO2 (right)

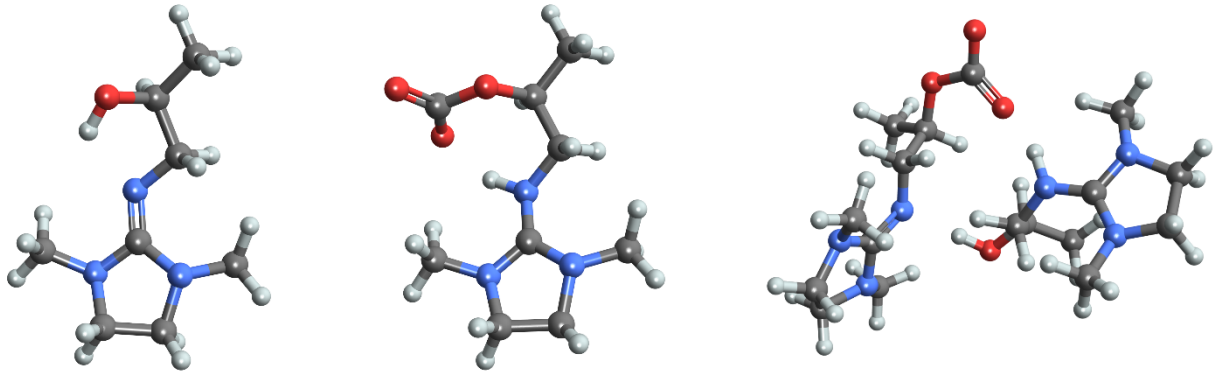


Figure S15: Molecular structure for IPADM-2-BOL (left), Monomolecular IPADM-2-BOL-CO2 (middle), and Bimolecular IPADM-2-BOL-CO2 (right)

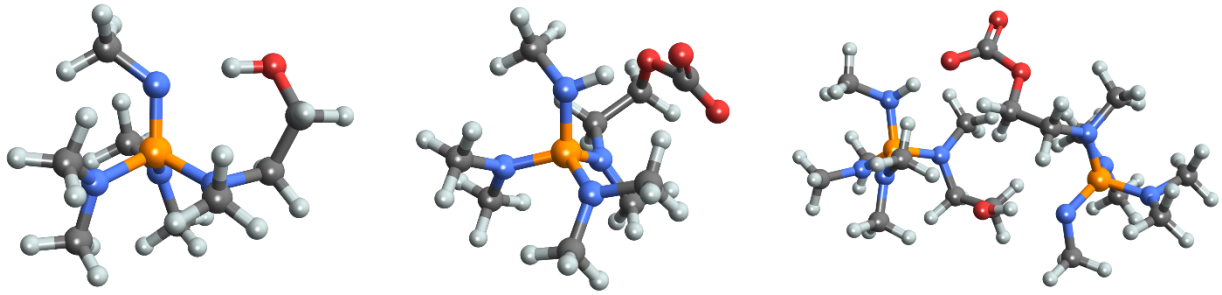


Figure S16: Molecular structures for Phos-BOL (left), Monomolecular Phos-BOL-CO2 (middle), and Bimolecular Phos-BOL-CO2 (right)

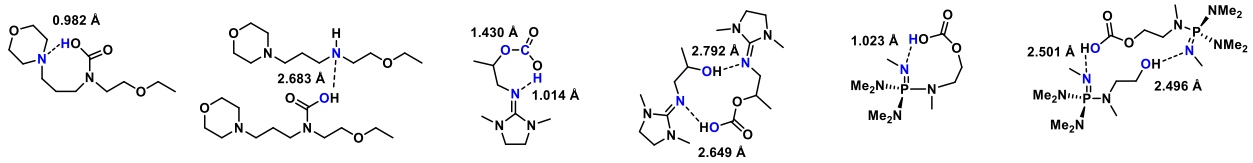


Figure S17: Scheme S1. Constrained interatomic distances applied in AIMD simulations for CO_2 bound species.

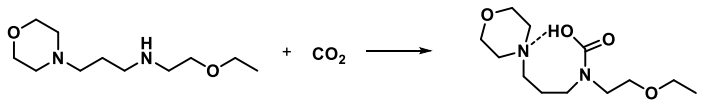


Figure S18: Scheme S2. Absorption of CO_2 by one 2-EEMPA molecule.

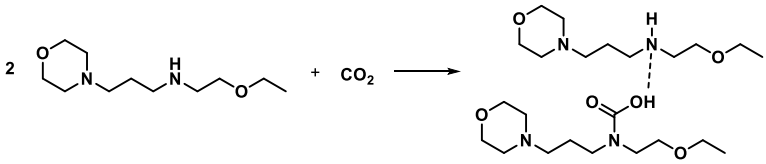
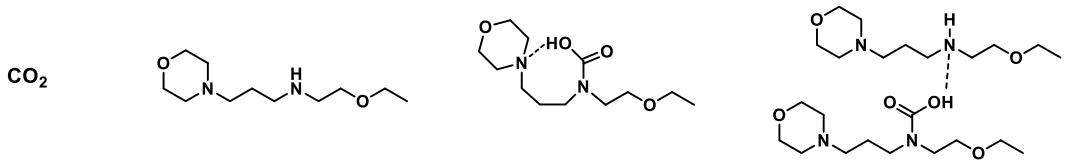


Figure S19: Scheme S3. Absorption of CO_2 by two 2-EEMPA molecules.

Section S2: Supplementary Tables



1 2 3 4

Species (see fig. above)	Solvent	Electronic Energy	Zero-Point Correction	Thermal Correction to Energy	Thermal Correction to Enthalpy	Thermal Correction to Gibbs Free Energy
1	H_2O	-188.584242	0.011735	0.014365	0.01531	-0.00963
1	MeOH	-188.584164	0.011737	0.014368	0.015312	-0.008973
1	2-butanol	-188.584031	0.011742	0.014372	0.015317	-0.008968
1	gas	-188.581585	0.011834	0.01446	0.015404	-0.008873
2	H_2O	-693.476794	0.354667	0.371667	0.372611	0.306862
2	MeOH	-693.476439	0.35468	0.371676	0.37262	0.30692
2	2-butanol	-693.475836	0.354702	0.371691	0.372635	0.307005
2	gas	-693.46655	0.354924	0.371904	0.372848	0.307302
3	H_2O	-882.077391	0.371839	0.390401	0.391345	0.324372
3	MeOH	-882.076315	0.371845	0.390404	0.391348	0.324381
3	2-butanol	-882.074469	0.371842	0.390402	0.391346	0.324364
3	gas	-882.043108	0.371337	0.390037	0.390981	0.323622
4	H_2O	-1575.57227	0.727747	0.764512	0.765456	0.654783
4	MeOH	-1575.571674	0.727792	0.764546	0.765491	0.654912
4	2-butanol	-1575.570662	0.727859	0.7646	0.765545	0.655089
4	gas	-1575.554781	0.728391	0.765137	0.766081	0.655992

Table S1. Thermochemical values for CO_2, 2-EEMPA, monomolecular 2-EEMPA-CO_2, and bimolecular 2-EEMPA-CO_2 (all values are in hartrees). For each structure, frequency calculations were performed with the polarizable continuum model using the integral equation formalism variant (IEFPCM) with the dielectric constant of H_2O (ε = 78.3553), methanol (ε = 32.613), and 2-butanol (ε = 15.944), as well as in gas phase.

Scheme	Solvent	ΔEE + ZPE	ΔEE + Thermal Energy	ΔEE + Thermal Enthalpies	ΔEE + Thermal Free Energies
1	H_2O	-28.665	-31.472	-33.948	28.313
1	MeOH	-27.001	-29.802	-32.283	28.153
1	2-butanol	-24.165	-26.946	-29.424	30.784
1	gas	25.221	22.844	20.366	79.343
2	H_2O	-72.889	-72.532	-77.489	42.659
2	MeOH	-73.349	-73.002	-77.962	40.467
2	2-butanol	-74.160	-73.811	-78.768	39.614
2	gas	-87.658	-87.235	-92.192	26.691

Table S2. Energy values (in kJ/mol) for the monomolecular (Scheme 1) and bimolecular (Scheme 2) CO_2 absorption processes by 2-EEMPA, calculated from the thermochemical values in Table S1.

Section S3: Development of Surface Renewal Models

Here, we describe the theory behind the surface renewal models used in this work, and also describe our physical parameter estimation methods. Julia code used to develop all figures in this work is also supplied in the Supporting Information.

Surface Renewal Theory

In Danckwerts' surface renewal theory (Danckwerts 1951; Danckwerts, 1970), the steady state absorption of gas into a flowing chemical solvent is modelled by first simulating the *unsteady* gas flux into a *stationary* chemical solvent. This may be justified as follows. As a liquid flows down an absorption column, random eddies, collisions with packing structures, and other similar flow events ensure that solvent is constantly circulated from the gas-liquid interface to the bulk and from the bulk to the interface. At any moment and at any given location, the fluid near the gas-liquid interface is regularly & randomly being 'renewed' or 'replaced' with fresh solvent from the bulk. Furthermore, the diffusion-reaction processes which control the flux of gas into the chemical solvent typically happen at very small length-scales, on the order of microns. At these length scales, the liquid solvent is, for all intents and purposes, stationary: advective flows normal to the surface (which could assist mass transport) may be ignored, and the local gas flux is controlled by an unsteady-state diffusion reaction process. This process begins the moment the fresh solvent is carried to the surface, and continues for some random quantity of time, θ, until a random eddy 'renews' the surface with fresh solvent and the process repeats again. Danckwerts' models this renewal process as a Poisson process (a natural choice for random events in continuous time) which implies θ is governed by an exponential probability distribution with probability density function:

$$f(\theta) = s \exp\left(-\frac{s}{\theta}\right)$$

where s is the mean surface lifetime – the one unknown parameter in the model. By analyzing diffusion-reaction phenomena in a physical solvent, it is possible to show that (Danckwerts 1970)

$$s = \frac{(k_l^0)^2}{D}$$

where k_l^0 is the liquid film mass transfer coefficient in the absence of chemical reactions (on the basis of a concentration driving force) and D is the diffusivity of the dissolving gas.

When using the surface renewal model, predicting the gas flux into a flowing fluid requires a model of the *unsteady-state* diffusion and reaction of gas into the *stationary* chemical solvent. Using this model, we may calculate the flux into the stationary solvent at some time, t, after the surface has been refreshed with solvent from the bulk, $J_s(t)$. Because of the time-symmetry of the Poisson process, at any given moment the probability that the time since the last surface renewal is in the interval $(t, d + dt)$ is given by $se^{-t/s}dt$. Hence, by the law of the unconscious statistician, the mean flux of gas over time for this Poisson process is given by:

$$J = \int_0^\infty J_s(\theta) s e^{-\frac{\theta}{s}} d\theta.$$

This is taken to be the gas flux into the flowing chemical solvent. $J_s(t)$ may be calculated by solving the unsteady-state diffusion-reaction problem for absorption into a stationary solvent which has uniform, bulk composition at $t = 0$, as described below.

Unsteady-state absorption of CO_2 into stationary CO_2BOLs.

We now describe the model developed for absorption of CO_2 into EEMPA, IPADM-2-BOL, and DBU-Hexanol. For absorption of CO_2 into IPADM-2-BOL, we assume the following 1-1 stoichiometry:

$$\mathrm{CO_2} + \mathrm{IPADM} \leftrightarrow \mathrm{IPADMCO_2}$$

In what follows, we will refer to $A \equiv \mathrm{IPADM}$; $\mathrm{B} \equiv \mathrm{IPADMCO_2}$, so the reaction is given by

$$\mathrm{CO_2} + \mathrm{A} \leftrightarrow \mathrm{B}$$

We assume the forward reaction is first order in $\mathrm{CO_2}$ and A. The surface renewal theory then requires we solve the following dynamic diffusion-reaction problem for the concentrations of $\mathrm{CO_2}, A$ and B in the vicinity of the gas-liquid interface, in order to calculate $J_s(t)$:

$$\frac{\partial c_{CO_2}}{\partial t} = D_{CO_2} \frac{\partial^2 c_{CO_2}}{\partial x^2} - k_f (c_{CO_2} c_A - c_B / K_{eq})$$

$$\frac{\partial c_A}{\partial t} = D_A \frac{\partial^2 c_A}{\partial x^2} - k_f (c_{CO_2} c_A - c_B / K_{eq})$$

$$\frac{\partial c_B}{\partial t} = D_B \frac{\partial^2 c_B}{\partial x^2} + k_f (c_{CO_2} c_A - c_B / K_{eq})$$

Where D_i are diffusivities, k_f is the second order rate constant, and K_{eq} is the equilibrium constant. At $\mathrm{t} = 0$, we assume the surface has just been replenished with solvent from the bulk,

$$c_{CO_2}(t = 0) = c_{CO_2}^{bulk}$$

$$c_A(t = 0) = c_A^{bulk}$$

$$c_B(t = 0) = c_B^{bulk} = K_{eq} c_{CO_2} c_A$$

At the gas-liquid interface, the flux of A and B are both zero, while $\mathrm{CO_2}$ is at equilibrium with the fixed partial pressure,

$$c_{CO_2}|_{x=0} = Hp_{CO_2}$$

$$\frac{\partial c_A}{\partial x}|_{x=0} = \frac{\partial c_B}{\partial x}|_{x=0} = 0$$

where H is the Henry's constant for CO_2 in the solvent. $J_s(t)$ is then given by

$$J_s(t) = -D_{CO_2}\frac{\partial c_{CO_2}}{\partial x}|_{t,x=0}$$

Similar equations may be derived for CO_2 absorption into DBU:Hexanol and EEMPA. For EEMPA, the equations were modified to account for the 1:2 stoichiometry described in Eq. (2) in the paper.

Solution of these equations requires multiple physical parameters, including diffusivities, D_i, the forward rate constant, k_f, the equilibrium constant, K_{eq}, and the Henry's constant, H. Furthermore, we need means of calculating these as a function of temperature. To apply the surface renewal model, we also need an estimate for the liquid-film mass transfer coefficient k_l^0, in order to calculate the surface renewal rate, s. We describe our approach to calculating each parameter below.

- *Diffusion Coefficients, D_i.* For EEMPA and DBU-Hexanol, for which no diffusivity data was available, the correlation of Wilke and Chang (1955) was used to estimate the diffusion coefficient, based on viscosity measurements by Zheng et al (2020) for EEMPA and Mathias et al. (2015) for DBU:Hexanol. For IPADM, diffusivity data of Yu et al. (2018) at 40°C was used; following the Stokes-Einstein equation, diffusivities at other temperatures were assumed to scale linearly with absolute temperature, so $D_T \approx D_{313K} \times T/313K$.
- *Forward rate constant. k_f.* For DBU Hexanol, k_f was set to the value of $0.6\ \mathrm{m^3/mol.\,s}$ experimentally measured by Ozturk et al. (2012). For EEMPA and IPADM-2-BOL, two cases were considered: a finite forward reaction rate, and an 'infinite' forward reaction rate. In the latter case, k_f was set to $10^4\ \mathrm{m^3/mol.\,s}$; further increases resulted in negligible change in flux. For the finite forward reaction case, k_f was given by the DBU Hexanol value above.
- *Equilibrium Constant, K_{eq}, and Henry's Constant H.* Vapor-liquid equilibria data was obtained from the papers of Zheng et al. (2020) (for EEMPA) and Mathias et al. (2015) (for IPADM-2-BOL and DBU-Hexanol.) The methodology of Gabrielsen et al. was used to regress this VLE data to functions of the form:

$$p_{CO_2}(T,\alpha) = \exp\left(A + \frac{B}{RT}\right)\frac{\alpha}{1-\alpha} \quad (\text{IPADM; DBUHex. Ideal soln. 1: 1 stoich})$$

$$p_{CO_2}(T,\alpha) = \exp\left(A + \frac{B}{RT} + C\alpha + D\sqrt{\alpha}\right)\frac{\alpha}{(1-2\alpha)^2} \quad (EEMPA.\ \text{Nonideal soln. 1: 2 stoich})$$

Here, A, B, C and D are fitting parameters, and α is the CO_2 loading in mol CO_2/mol amine. The lines of best fit are shown in Figures S3 – S5. The pre-factor in these fits is equal to $1/(K_{eq}H)$. For example, for IPADM-2-BOL

$$K_{eq}H = \frac{1}{\exp\left(A + \frac{B}{RT}\right)} = \exp\left(-A - \frac{B}{RT}\right)$$

In order to factorize K_{eq} and H, we require an expression for H. Based on Figure S9, we assume that the CO_2 solubility (on a molar basis) in a CO_2BOL at 40°C is about 3.5 times larger than for water at 40°C. Furthermore, Gui et al. (2012) found that the enthalpy of physical dissolution of CO_2 into a range of organic solvents was on the order of $-12.5\ kJ/mol$. Uainf these values, the Van't Hoff equation then gives

$$\frac{H(T)}{H(313)} = \exp\left(\frac{12500}{R}\left(\frac{1}{T} - \frac{1}{313}\right)\right)$$

This expression was used for all solvents, and K_{eq} was calculated as $K_{eq} = K_{eq}H/H$.

While this approach will only give an approximate estimate for the Henry's constant, we note that, in the instantaneous reaction limit, varying the Henry's constant by an order of magnitude has negligible effect on the gas flux (Figure S13). This occurs because we are in a reaction regime in which CO_2 is primarily carried into the solvent bound to the CO_2BOL. The equilibrium concentration of this CO_2-CO_2BOL complex at the gas-liquid interface depends only on the product $K_{eq}H$, and not on K_{eq} and H individually; the latter only gives the (much smaller) equilibrium concentration of CO_2, which has negligible effect on the overall CO_2 flux. In other words, the product $K_{eq}H$ (as determined with high confidence from the VLE) has a large impact on the flux, but once this is specified, the particular factorization into K_{eq} and H has negligible impact. CO_2BOLs with finite kinetics (e.g. DBU:Hexanol) are more sensitive to the choice of Henry's constant, as in this case a larger Henry's constant accelerates the (non-instantaneous) production of the CO_2-CO_2BOL complex at the gas-liquid interface.

- When comparing the surface renewal model to kinetic data measured in a wetted wall column (e.g. in Figure 3 of the manuscript), the correlation of Vivian and Peaceman (1956) was used to estimate k_l^0 under experimental conditions.

Development of Surface Renewal Models for Aqueous Solvents

Surface renewal models were also developed for two aqueous solvents: 30wt% MEA and 30wt% K_2CO_3. The stoichiometry of the MEA reaction is given by

$$CO_2 + 2MEA \rightarrow MEACOO^- + MEAH^+$$

While the stoichiometry for the K_2CO_3 systems is given by:

$$CO_2 + H_2O + CO_3^{2-} \rightarrow 2KHCO_3$$

The rate of reaction of CO_2 with MEA is given by

$$-r_{CO_2} = k_{MEA} c_{MEA} (c_{CO_2} - c^*_{CO_2})$$

Where $c^*_{CO_2}$ is the equilibrium CO_2 concentration for the local value of the solvent loading. For K_2CO_3

$$-r_{CO_2} = k_{OH} c_{OH} (c_{CO_2} - c^*_{CO_2})$$

Where c_{OH} is the local pH, which is in instantaneous equilibrium with the very fast carbonate/bicarbonate buffer reaction

$$K_{eqK2CO3buffer} = \frac{c_{OH} c_{HCO3}}{c_{CO32}}$$

Once again, a surface renewal model requires diffusivities, D_i, the forward rate constant, k_f, the equilibrium constant, K_{eq}, and the Henry's constant, H. Furthermore, we need means of calculating these as a function of temperature. We describe these below:

- *Diffusivities*: For MEA, diffusivities are estimated via the Wilke-Chang correlation. The viscosity of 30wt% MEA was interpolated from data of Arachchige (2013) and Arachchige (2013) between 40°C and 140°C. For K_2CO_3, ionic diffusivities at 25°C were taken from Weng et al. (2018) as follows:
    - $D_{CO_2} = 1.91 \times 10^{-9} m^2/s$
    - $D_{CO_3^{2-}} = 0.923 \times 10^{-9} m^2/s$
    - $D_{HCO_3^-} = 0.923 \times 10^{-9} m^2/s$

  These were assumed to scale linearly with absolute temperature, according to the Stokes-Einstein Equation.
- *Forward rate constant.* k_f. For MEA, the correlation of Versteeg et al. (1996) was used:

  $$k_{MEA}(T[K])[\mathrm{m^3/mol.\,s}] = 4.4 \times 10^8 \exp(-5400/T)$$

  For K_2CO_3, the correlation of Astarita (1983) was used:

  $$k_{OH}(T[K])[\mathrm{L/mol.\,s}] = 10^{13.65 - \frac{2895}{T} + 0.08I}$$

  Where I is the ionic strength in mol/L. Also required for K_2CO_3 kinetics is an estimate of the buffer equilibrium constant $K_{eqK2CO3buffer}$, which is used to calculate the local value of c_{OH} assuming instantaneous local equilibrium of the buffer reaction. At infinite dilution we used the correlation of Hikita et al. (1976):

$$K^{\infty}_{eqK2CO3buffer}(T[K])\left[\frac{mol}{m^3}\right] = 10^{-\frac{1568.9}{T}+2.5866+6.737\times10^{-3}T}$$

To correct for non-idealities with finite salt concentrations, we use the correlation of Cents et al. (2005).

$$\log_{10}\frac{K^{\infty}_{eqK2CO3buffer}}{K_{eqK2CO3buffer}} = \frac{1.01\sqrt{c_{K^+}}}{1+1.49\sqrt{c_{K^+}}} + 0.061c_{K^+}$$

c_{K^+} is the potassium ion concentration in mol/L.

- *VLE, $p^{eq}_{CO_2}(T,\alpha)$ and Henry's Constant H*. For MEA the Henry's constant expresson of Ma'Mum et al. (2009) was used, while for K_2CO_3, the model of Weisenberger and Schumpe (1996) was used, with the Henry's constant of CO2 in water taken from Versteeg and Van Swaalj (1988). For the partial pressure of CO_2 in concentrated MEA solutions, the expression of Gabrielsen et al. (2005) was used. For the partial pressure of CO_2 in 30wt% K_2CO_3 solutions, we used the following expression, regressed from the model of Kaur and Chen (2020), based on the methodology of Gabrielsen et al. (2005):

$$p_{CO_2}(T[K],\alpha,x_{K2CO30})[Pa] = x_{K2CO30} \times \exp\left(26.3,+\ -\frac{4311.5}{T}\ +\ 34.58\,x_{K2CO30}\alpha - 10.78\sqrt{x_{K2CO30}\alpha}\right)\frac{\alpha^2}{1-\alpha}$$

where x_{K2CO30} is the mole fraction of K_2CO_3 (ignoring dissociation) in the unloaded solvent.

Numerical Methods

The above PDEs were solved via the method of lines, with a finite volume spatial discretization. A geometrically-spaced non-uniform grid was used to ensure resolution of sharp changes in concentration profiles which arose close to the gas-liquid interface when $k_f = 10^4\ \mathrm{m^3/mol.\,s}$ (i.e. in the 'instantaneous reaction' limit.) The resulting set of ODEs was solved using DifferentialEquations.jl in Julia. The mass transfer coefficient was calculated by calculating the flux when a finite pressure driving force, Δp, was applied to a solvent at given loading and temperature, and then applying Eq. (1) in the manuscript,

$$k'_g = \frac{J}{\Delta p}$$

Section S4: Atomistic Simulations

Computational Details

Density Functional Theory (DFT) based ab initio molecular dynamics (AIMD) simulations were conducted with three-dimensional periodic boundary conditions (PBC) as implemented in the Vienna ab initio simulation package (VASP v. 5.4.4.18), a planewave pseudopotential code. (Kresse et al. 1996; Kresse et al. 1994; Kresse et al. 1993) The calculations employed the Perdew–Burke–Ernzerhof (PBE) (Perdew et al. 1996; Perdew et al. 1997) functional described within the generalized gradient approximation (GGA) (Perdew et al. 1992) and implemented the projector augmented wave (PAW) (Blochl et al. 1994; Kresse et al. 1999) approach for core–valence treatment. For all simulations, the temperature was set to 573 K with a time step of 1 fs, and a total simulated time span of 2-5 ps. A plane-wave energy cutoff of 400 eV was utilized for all unit cells. The self-consistent electronic convergence limit was set to 1 x 10^{-4} eV while the ionic convergence limit was set to 0.03 eV $Å^{-1}$. Dispersion corrections were implemented using Grimme's third generation corrections DFT-D3. (Grimme et al. 2012) For monomolecular and bimolecular CO_2 bound structures, selected interatomic distances were held constant as depicted in Figures S17. These values were generated by preliminary DFT structure optimizations for each species.

From the AIMD results, a series of lowest energy structures were identified for each species, and electronic structures were then further energy minimized using density functional theory (DFT) calculations in Gaussian 16 (Frisch et al. 2016) with the M06L functional and 6-31++G(d,p) basis set. For all calculations, the temperature was set to 298.15 K, using default convergence criterion. No structural constraints (e.g. fixed bond lengths, interatomic distances) were applied. Implicit solvent corrections to energies were applied using the Polarizable Continuum Model using the integral equation formalism variant (IEFPCM). While the data presented in the main text was calculated using the dielectric constant of water, calculations using additional solvents (as well as gas phase) were performed to evaluate the impact of dielectric constant on CO_2 absorption enthalpy (Tables S1-S2). The enthalpy of CO_2 absorption was calculated according to the following equation:

$$\Delta H_{abs} = \sum(\varepsilon_0 + H_{corr})_{products} - \sum(\varepsilon_0 + H_{corr})_{reactants}$$

Here, ε_0 corresponds to electronic energy, and H_{corr} corresponds to the thermal correction to enthalpy. The enthalpy of monomolecular CO_2 absorption by 2-EEMPA (Figures S18), for example, was calculated as follows:

$$\Delta H_{abs} = (\varepsilon_0 + H_{corr})_{2EEMPA-CO2} - ((\varepsilon_0 + H_{corr})_{2EEMPA} + (\varepsilon_0 + H_{corr})_{CO2})$$

Section S5: Atomistic Simulation Data

XYZ Coordinates

All energies listed in hartrees.

CO2

Zero-point correction: 0.011735
Thermal correction to energy: 0.014365
Thermal correction to enthalpy: 0.01531
Thermal correction to Gibbs free energy: -0.00963
Sum of electronic and zero-point energies: -188.572507
Sum of electronic and thermal energies: -188.569876
Sum of electronic and thermal enthalpies: -188.568932
Sum of electronic and thermal free energies: -188.593871

```
C 0.0000000000 -0.0000040000 -0.0000020000
O -1.1682760000 0.0000020000 0.0000010000
O 1.1682760000 0.0000020000 0.0000010000
```

2-EEMPA

Zero-point correction: 0.354667
Thermal correction to energy: 0.3716676
Thermal correction to enthalpy: 0.372611
Thermal correction to Gibbs free energy: 0.306862
Sum of electronic and zero-point energies: -693.122127
Sum of electronic and thermal energies: -693.105128
Sum of electronic and thermal enthalpies: -693.104184
Sum of electronic and thermal free energies: -693.169932

```
C 6.4796800000 12.7319900000 4.6633950000
C 7.7159100000 13.3914480000 5.2369430000
C 7.9601880000 12.0805630000 7.1970900000
C 9.0112450000 11.3484370000 8.0009980000
C 9.4330420000 10.1311550000 10.0447320000
C 8.7972090000 9.4930330000 11.2657520000
C 9.8062100000 8.9060570000 12.2388240000
C 11.7359480000 7.5391330000 12.6091660000
C 12.7229090000 6.5827060000 11.9773590000
C 11.1015380000 5.8579370000 10.4708480000
C 10.0816150000 6.8020790000 11.0695060000
H 5.9390800000 13.4395390000 4.0286660000
H 6.7474480000 11.8646140000 4.0530040000
H 5.7897430000 12.4012460000 5.4448250000
H 8.3542540000 13.7736050000 4.4347970000
H 7.4356260000 14.2465200000 5.8739760000
H 7.5795620000 12.9490180000 7.7605920000
H 7.1011800000 11.4145660000 7.0083930000
H 9.4700900000 10.5648590000 7.3690300000
H 9.8175760000 12.0431950000 8.2679080000
H 7.7135970000 10.1502470000 8.9825760000
H 10.1842330000 10.8693390000 10.3598740000
H 9.9848730000 9.3654940000 9.4673280000
H 8.0782790000 8.7254670000 10.9479090000
H 8.2079790000 10.2463440000 11.8013950000
H 10.4018530000 9.7163470000 12.6795980000
H 9.2674380000 8.4198280000 13.0779160000
```

```
H 12.2631420000 8.4187080000 12.9962010000
H 11.2440050000 7.0421680000 13.4709830000
H 13.4356190000 6.2082550000 12.7159270000
H 13.2817250000 7.0957980000 11.1771350000
H 10.6223810000 4.9496880000 10.0979420000
H 11.6166490000 6.3541980000 9.6310810000
H 9.3826260000 7.1154270000 10.2864390000
H 9.4943000000 6.2728860000 11.8483930000
N 8.4374390000 10.8214560000 9.2306240000
N 10.7502880000 7.9751770000 11.6250490000
O 8.5474070000 12.5061910000 5.9809600000
O 12.0615410000 5.4431080000 11.4365740000
```

2-EEMPA-CO2 Monomolecular

Zero-point correction: 0.371839
Thermal correction to energy: 0.390401
Thermal correction to enthalpy: 0.391345
Thermal correction to Gibbs free energy: 0.324372
Sum of electronic and zero-point energies: -881.705552
Sum of electronic and thermal energies: -881.686991
Sum of electronic and thermal enthalpies: -881.686046
Sum of electronic and thermal free energies: -881.753019

```
C 10.2630920000 6.2874670000 8.5697150000
C 11.4536490000 7.1981190000 8.7230670000
C 12.2702200000 9.3252510000 8.1277480000
C 11.8480110000 10.6577650000 7.5488360000
C 11.3012290000 12.0329170000 9.5126540000
C 9.5020480000 11.4607430000 7.8755320000
C 8.6192120000 10.2450660000 8.1714840000
C 8.6391690000 9.8183890000 9.6234540000
C 7.0250710000 11.5804010000 10.3598680000
C 6.8252130000 12.6862990000 11.3736040000
C 8.2176140000 11.6522740000 12.9224080000
C 8.4886810000 10.4938920000 11.9889120000
H 10.0755030000 6.0632820000 7.5160220000
H 9.3620350000 6.7485940000 8.9847330000
H 10.4325490000 5.3437350000 9.0938040000
H 11.6521700000 7.4167630000 9.7867230000
H 12.3660670000 6.7300330000 8.3170570000
H 12.5644640000 9.4576900000 9.1815580000
H 13.1450850000 8.9316810000 7.5828790000
H 11.4185260000 10.4975100000 6.5533480000
H 12.7417700000 11.2802440000 7.4329600000
H 9.5175390000 11.6217660000 6.7904390000
H 9.0636470000 12.3634880000 8.3142650000
H 8.9701290000 9.3821400000 7.5970640000
H 7.5969940000 10.4523050000 7.8338400000
H 9.6352910000 9.4487200000 9.8914500000
H 7.9112530000 9.0271410000 9.8282160000
H 9.1377740000 11.6824040000 10.4057370000
H 6.2642350000 10.7997670000 10.4611730000
H 6.9897920000 11.9790210000 9.3439320000
H 5.8287160000 13.1156470000 11.2614770000
H 7.5674380000 13.4846290000 11.2115160000
H 8.2509930000 11.3105500000 13.9578270000
H 8.9812770000 12.4340780000 12.7875340000
H 7.7741840000 9.6797730000 12.1458520000
H 9.5030630000 10.1082920000 12.1190310000
N 10.8675820000 11.3639850000 8.3569000000
```

```
N 8.3586870000 10.9449420000 10.5709390000
O 11.1901340000 8.4112130000 8.0351630000
O 12.5306290000 12.0513640000 9.7514860000
O 10.3879060000 12.5705410000 10.2443330000
O 6.9234100000 12.1963260000 12.7022320000
```

2-EEMPA-CO2 Bimolecular

Zero-point correction: 0.727747
Thermal correction to energy: 0.764512
Thermal correction to enthalpy: 0.765456
Thermal correction to Gibbs free energy: 0.654783
Sum of electronic and zero-point energies: -1574.844523
Sum of electronic and thermal energies: -1574.807758
Sum of electronic and thermal enthalpies: -1574.806814
Sum of electronic and thermal free energies: -1574.917487

```
C 11.3032870000 10.3110350000 7.6123420000
C 9.9871680000 10.5442870000 6.9013640000
C 9.2831610000 12.5570750000 7.9775010000
C 9.1197320000 12.8532080000 9.4544760000
C 11.3431710000 12.4787350000 10.3162070000
C 15.0555360000 13.1281620000 9.7711640000
C 14.8520010000 11.9526980000 8.8500530000
C 15.1656120000 9.6232190000 8.7503540000
C 15.9839150000 8.4958750000 9.3218820000
C 14.5306870000 13.9527890000 12.0175970000
C 13.8332820000 13.6059170000 13.3213170000
C 14.5981500000 12.6218590000 14.1952200000
C 12.8654630000 11.0521160000 14.7900320000
C 11.9922040000 10.5577340000 15.9217570000
C 13.6752770000 11.0393080000 17.4644540000
C 14.5787470000 11.5351230000 16.3559870000
C 9.5248530000 10.8897870000 10.9514700000
C 8.6594920000 11.2268580000 12.1584220000
C 9.4333630000 11.9017220000 13.2948600000
C 8.7309380000 14.2126760000 12.9820260000
C 10.0819910000 14.9086220000 12.9661600000
C 10.5410530000 14.1317830000 15.1312500000
C 9.1934890000 13.4341860000 15.1841000000
H 15.1986530000 12.0868770000 11.4957530000
H 11.7682820000 11.2568910000 7.9128400000
H 12.0096630000 9.7927130000 6.9563350000
H 11.1604270000 9.7060160000 8.5134160000
H 9.5325760000 9.5936080000 6.6065610000
H 10.1390330000 11.1322990000 5.9829000000
H 10.3021930000 12.8197230000 7.6676100000
H 8.5868040000 13.1791780000 7.3956470000
H 9.2699310000 13.9254140000 9.6231960000
H 8.1016410000 12.6061390000 9.7733700000
H 14.4623270000 13.9697040000 9.3995060000
H 16.1116330000 13.4402560000 9.7799520000
H 13.7763700000 11.7171800000 8.7912200000
H 15.1981330000 12.1868970000 7.8306500000
H 14.0879490000 9.4613640000 8.9238550000
H 15.3062270000 9.7035680000 7.6593570000
H 15.6919630000 7.5460790000 8.8672710000
H 17.0497560000 8.6498170000 9.1331070000
H 15.8357490000 8.4149140000 10.4022470000
H 15.5379590000 14.3609240000 12.2050120000
H 13.9628740000 14.7351380000 11.5007750000
```

```
H 13.6520590000 14.5227860000 13.8936040000
H 12.8433720000 13.1956560000 13.0787040000
H 15.4605430000 13.1284040000 14.6455960000
H 15.0128750000 11.7894740000 13.5897140000
H 13.4382520000 10.2026130000 14.3635230000
H 12.2355910000 11.4502930000 13.9858700000
H 11.3416920000 9.7440510000 15.5904750000
H 11.3598830000 11.3852760000 16.2910170000
H 13.1016540000 11.8843190000 17.8807870000
H 14.2534350000 10.5787590000 18.2688400000
H 15.2129890000 10.6997210000 15.9961060000
H 15.2452630000 12.3148110000 16.7409150000
H 10.3775660000 10.2747010000 11.2444100000
H 8.9495170000 10.3224880000 10.2114700000
H 8.1768990000 10.3106360000 12.5153410000
H 7.8384930000 11.8827100000 11.8419930000
H 13.0720790000 12.1022140000 11.0396090000
H 9.6079430000 11.1891520000 14.1101690000
H 10.4364010000 12.1891140000 12.9281450000
H 7.9697410000 14.9193480000 13.3369470000
H 8.4501740000 13.9126970000 11.9657350000
H 10.8572960000 14.2601080000 12.5202890000
H 10.0446160000 15.8307700000 12.3792400000
H 11.3261980000 13.4468120000 14.7651250000
H 10.8487410000 14.4879490000 16.1191850000
H 8.4570250000 14.1199880000 15.6239570000
H 9.2452460000 12.5464940000 15.8257520000
N 10.0376760000 12.0909920000 10.2912590000
N 13.7707080000 12.0925430000 15.2749150000
N 14.5759980000 12.7956010000 11.1151900000
N 8.6990090000 13.0368800000 13.8625180000
O 9.0181250000 11.1811170000 7.7310540000
O 12.1350730000 11.6828430000 11.0445530000
O 15.5584050000 10.8395660000 9.3732970000
O 12.7731000000 10.0420000000 16.9929860000
O 11.7556790000 13.4812050000 9.7198850000
O 10.4803600000 15.2809320000 14.2856170000
```

IPADM-2-BOL

Zero-point correction: 0.256485
Thermal correction to energy: 0.269967
Thermal correction to enthalpy: 0.270911
Thermal correction to Gibbs free energy: 0.216329
Sum of electronic and zero-point energies: -554.261994
Sum of electronic and thermal energies: -554.248512
Sum of electronic and thermal enthalpies: -554.247567
Sum of electronic and thermal free energies: -554.302150

```
C 7.2329960000 4.9176720000 8.6095620000
C 4.9963380000 5.8617310000 8.9191680000
C 4.2129910000 6.9431470000 8.2084000000
C 4.6020710000 8.1087840000 6.0460050000
C 6.2561140000 6.6842120000 7.1516790000
C 8.5662330000 6.7727150000 6.5443640000
C 9.3586470000 7.6147470000 5.5495950000
C 10.8381310000 7.6281020000 5.8436970000
H 7.1467250000 4.6172120000 9.6558410000
H 6.9569550000 4.0576930000 7.9818050000
H 8.2739980000 5.1709020000 8.4230410000
H 4.9853620000 5.9524440000 10.0082090000
```

```
H 4.6233570000 4.8604830000 8.6505460000
H 4.2639070000 7.9022640000 8.7505940000
H 3.1605730000 6.6899510000 8.0575210000
H 3.5248880000 8.1138190000 5.8663780000
H 4.8951260000 9.0872530000 6.4573210000
H 5.1200340000 7.9649480000 5.0977780000
H 8.8702600000 5.7200600000 6.4265620000
H 8.8532790000 7.0807470000 7.5656950000
H 9.1848650000 7.1986050000 4.5410330000
H 7.9121060000 8.8604250000 5.6388480000
H 11.0280300000 8.0353490000 6.8423160000
H 11.3785330000 8.2405510000 5.1174880000
H 11.2479860000 6.6146940000 5.8037210000
N 6.3507590000 6.0534870000 8.3932520000
N 4.9247100000 7.0228600000 6.9421620000
N 7.1616730000 6.9940630000 6.2860340000
O 8.8782000000 8.9600510000 5.5808130000
```

IPADM-2-BOL-CO2 Monomolecular

Zero-point correction: 0.27269
Thermal correction to energy: 0.288822
Thermal correction to enthalpy: 0.289766
Thermal correction to Gibbs free energy: 0.228208
Sum of electronic and zero-point energies: -742.841985
Sum of electronic and thermal energies: -742.825854
Sum of electronic and thermal enthalpies: -742.824910
Sum of electronic and thermal free energies: -742.886468

```
C 11.0219010000 13.5574440000 8.7006170000
C 9.4347950000 11.8116300000 7.9047280000
C 9.2280470000 10.3536260000 8.2620280000
C 10.1456480000 8.9421570000 10.1287980000
C 10.8620410000 11.2430900000 9.6024950000
C 12.9998150000 12.1021180000 10.5461630000
C 14.0013700000 11.5320880000 11.5418480000
C 15.2413470000 12.3963780000 11.5993320000
C 13.7078220000 9.0998060000 11.6762460000
H 10.5133820000 14.0372250000 9.5444610000
H 12.0952880000 13.7127600000 8.7835250000
H 10.6911370000 14.0332720000 7.7779150000
H 9.5405630000 11.9891040000 6.8336280000
H 8.6255930000 12.4459370000 8.2899420000
H 9.6822680000 9.6788780000 7.5238490000
H 8.1790350000 10.0806710000 8.3878810000
H 10.4694070000 9.0304690000 11.1662840000
H 9.1933880000 8.4119390000 10.1115710000
H 10.8904730000 8.3563930000 9.5748070000
H 12.7766920000 13.1380580000 10.8254790000
H 13.4462650000 12.1033570000 9.5440270000
H 13.5250610000 11.4744970000 12.5284340000
H 11.8362290000 10.5050470000 11.2223490000
H 14.9925560000 13.4139150000 11.9123230000
H 15.7264350000 12.4486150000 10.6197370000
H 15.9574790000 11.9847960000 12.3128990000
N 10.6866320000 12.1420920000 8.6041720000
N 9.9462350000 10.2495860000 9.5334080000
N 11.7877100000 11.2879950000 10.5508760000
O 14.4136740000 10.2126100000 11.1565430000
O 14.2586730000 8.0177110000 11.4254840000
O 12.6367920000 9.3374490000 12.2964110000
```

IPADM-2-BOL-CO2 Bimolecular
Zero-point correction: 0.531350
Thermal correction to energy: 0.562436
Thermal correction to enthalpy: 0.563380
Thermal correction to Gibbs free energy: 0.466716
Sum of electronic and zero-point energies: -1297.115850
Sum of electronic and thermal energies: -1297.084764
Sum of electronic and thermal enthalpies: -1297.083820
Sum of electronic and thermal free energies: -1297.180485

```
C 9.9217900000 9.1297050000 13.8826720000
C 8.3604670000 8.2858490000 12.2034350000
C 7.6595040000 8.9180510000 11.0220360000
C 7.8784750000 11.1394900000 9.9524620000
C 8.9572210000 10.5233890000 12.0660110000
C 9.7816970000 12.1864560000 13.5694380000
C 9.7466450000 13.7122290000 13.6044860000
C 11.6561770000 14.2002930000 15.0347730000
C 12.8602220000 11.7777390000 11.5747010000
C 12.2962940000 12.9613260000 10.7770210000
C 13.2636800000 13.4619150000 9.7273000000
C 15.1977390000 12.3265320000 12.1929800000
C 15.5353030000 14.5438280000 13.2409110000
C 17.2949350000 13.2407470000 12.0257370000
C 17.2967920000 11.8668230000 11.3749670000
C 15.4957210000 10.1331560000 11.0774120000
C 8.3466630000 14.2626350000 13.4640230000
H 10.8390840000 8.8199070000 13.3603360000
H 9.5881120000 8.2982790000 14.5070500000
H 10.1542460000 9.9659090000 14.5373490000
H 7.7053360000 7.6732550000 12.8276790000
H 9.2084440000 7.6636190000 11.8770340000
H 6.6091240000 9.1580300000 11.2552840000
H 7.6772870000 8.2976920000 10.1225960000
H 6.9431720000 11.5634370000 10.3488490000
H 7.6703710000 10.6771460000 8.9854290000
H 8.5897060000 11.9509420000 9.8034730000
H 10.8009410000 11.8779200000 13.8529720000
H 9.1006330000 11.8076920000 14.3501400000
H 10.3905060000 14.0928410000 12.7998780000
H 12.0592290000 11.3248350000 12.1670930000
H 13.2289710000 11.0127960000 10.8893440000
H 12.0845340000 13.7691820000 11.4992360000
H 13.5088540000 12.6640550000 9.0169490000
H 14.1968880000 13.8164040000 10.1769350000
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H 15.4432920000 15.2857910000 12.4370340000
H 16.2602270000 14.9076430000 13.9707960000
H 14.5690100000 14.4317280000 13.7364410000
H 18.1171150000 13.3890240000 12.7283250000
H 17.3215290000 14.0497060000 11.2831110000
H 17.8456700000 11.1272050000 11.9707940000
H 17.7060120000 11.8695170000 10.3630220000
H 14.7841740000 9.7670350000 11.8198420000
H 16.3920650000 9.5120670000 11.1275640000
H 15.0640760000 10.0341600000 10.0775140000
H 7.9043810000 13.9142810000 12.5260810000
H 8.3478050000 15.3556430000 13.4632730000
H 7.7111540000 13.9192960000 14.2878440000
```

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H 10.4525590000 12.3239920000 10.8329000000
N 8.8542590000 9.4497970000 12.9463480000
N 8.4341100000 10.1385380000 10.8385190000
N 16.0040740000 13.2740150000 12.7171660000
N 15.8738090000 11.5074970000 11.3636240000
N 13.9059070000 12.2019650000 12.5066540000
N 9.4068200000 11.7232770000 12.2508420000
O 10.2608180000 14.1650570000 14.8668980000
O 12.3615930000 13.9299600000 14.0282460000
O 11.1033520000 12.5564970000 10.1255940000
O 12.0058700000 14.5226130000 16.1844130000
```

Phos-BOL

Zero-point correction: 0.326944
Thermal correction to energy: 0.345966
Thermal correction to enthalpy: 0.346911
Thermal correction to Gibbs free energy: 0.281030
Sum of electronic and zero-point energies: -953.881998
Sum of electronic and thermal energies: -953.862975
Sum of electronic and thermal enthalpies: -953.862031
Sum of electronic and thermal free energies: -953.927912

```
C 5.0760260000 5.8698230000 5.2026930000
C 7.8677690000 4.7038680000 8.5732720000
C 5.4535160000 4.9229220000 8.3580690000
C 8.5667290000 5.8298010000 4.9497140000
C 9.7363380000 6.8646590000 6.8198610000
C 6.3199750000 8.0782260000 9.1143330000
C 7.5619070000 9.3133170000 7.3916810000
C 6.4129800000 10.1368710000 6.8244740000
H 5.3036960000 5.9496610000 4.1289100000
H 3.9837230000 5.9392060000 5.2958890000
H 5.3565110000 4.8510380000 5.5133710000
H 7.9880000000 5.1454130000 9.5751160000
H 8.8035130000 4.8243220000 8.0264340000
H 7.6890370000 3.6304200000 8.6971580000
H 4.6714900000 5.4794970000 7.8390210000
H 5.2804250000 3.8504960000 8.2071130000
H 5.3699630000 5.1304350000 9.4352390000
H 9.2974310000 6.2936690000 4.2776580000
H 8.8911200000 4.7959660000 5.1451410000
H 7.6049940000 5.8010510000 4.4336190000
H 10.3088920000 5.9379000000 6.9723750000
H 9.5793710000 7.3402870000 7.7889790000
H 10.3449880000 7.5324210000 6.1963080000
H 6.3398440000 7.1335010000 9.6620660000
H 6.6952450000 8.8591200000 9.7828280000
H 5.2728980000 8.3120760000 8.8701350000
H 8.0401210000 9.8819760000 8.2016730000
H 8.3150290000 9.1573890000 6.6121360000
H 6.7694710000 11.1610230000 6.6653270000
H 5.6018270000 10.1988390000 7.5703830000
H 5.7366110000 8.7017630000 5.6689730000
N 5.7127160000 6.9206520000 5.9741750000
N 6.7622110000 5.2922600000 7.8365880000
N 8.4604420000 6.6091030000 6.1709710000
N 7.1936740000 8.0038310000 7.9487120000
O 5.9300530000 9.6717710000 5.5811100000
P 6.9558990000 6.6912050000 6.9175840000
```

Phos-BOL-CO2 Monomolecular
Zero-point correction: 0.342828
Thermal correction to energy: 0.364510
Thermal correction to enthalpy: 0.365454
Thermal correction to Gibbs free energy: 0.293891
Sum of electronic and zero-point energies: -1142.467867
Sum of electronic and thermal energies: -1142.446185
Sum of electronic and thermal enthalpies: -1142.445240
Sum of electronic and thermal free energies: -1142.516804

```
C 8.3713490000 11.2713920000 8.6028700000
C 11.7390150000 11.9804310000 11.7596130000
C 10.5397010000 10.4880910000 13.2916240000
C 8.5454030000 8.0709780000 11.3866170000
C 7.3933410000 10.2236700000 11.6453530000
C 12.1514090000 8.7402470000 10.6241790000
C 10.7157120000 8.7442720000 8.6087590000
C 11.6381630000 9.3424620000 7.5600860000
C 12.2855850000 11.5707690000 8.2570710000
H 8.8386470000 11.0058320000 7.6486970000
H 7.7750590000 12.1770590000 8.4661090000
H 7.6986190000 10.4658730000 8.9037740000
H 11.6301610000 12.8194190000 12.4542090000
H 11.7569890000 12.3725850000 10.7393960000
H 12.7025730000 11.4899030000 11.9545150000
H 10.3982420000 11.2985060000 14.0137700000
H 9.6922910000 9.8063150000 13.3718370000
H 11.4537600000 9.9416810000 13.5623950000
H 8.5172750000 7.8672950000 12.4646180000
H 7.6602020000 7.6211890000 10.9258480000
H 9.4326770000 7.5981810000 10.9652040000
H 6.4789690000 9.8227770000 11.1958020000
H 7.4652390000 11.2848670000 11.4038770000
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H 12.0675110000 7.6513390000 10.7256640000
H 13.0530840000 8.9864870000 10.0533400000
H 12.2526270000 9.1701790000 11.6205740000
H 10.8270330000 7.6516080000 8.6386400000
H 9.6729470000 8.9484740000 8.3426850000
H 11.3970820000 8.9184070000 6.5798530000
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N 10.6276850000 11.0523100000 11.9506600000
N 8.5516660000 9.5038010000 11.1212610000
N 10.9775680000 9.2819740000 9.9489600000
O 11.4238310000 10.7438130000 7.4903140000
O 13.3807570000 11.1110380000 8.6192750000
O 11.7756730000 12.7038520000 8.4533290000
P 9.9050130000 10.3214860000 10.6549400000
```

Phos-BOL-CO2 Bimolecular
Zero-point correction: 0.671009
Thermal correction to energy: 0.713636
Thermal correction to enthalpy: 0.714580
Thermal correction to Gibbs free energy: 0.595040
Sum of electronic and zero-point energies: -2096.365938

Sum of electronic and thermal energies: -2096.323312
Sum of electronic and thermal enthalpies: -2096.322368
Sum of electronic and thermal free energies: -2096.441908

C 15.6610750000 10.5098970000 13.3714760000
C 15.9409230000 10.7236530000 9.7770190000
C 14.0195990000 12.1604670000 9.4098190000
C 17.8742180000 13.2001430000 10.5675920000
C 17.7396870000 13.1761510000 12.9777450000
C 13.6371000000 14.3732230000 12.7363400000
C 12.1997980000 14.0619830000 12.3853450000
C 10.5281470000 14.7140300000 10.7754210000
C 6.8035600000 12.4897690000 12.4942040000
C 9.6821420000 9.8895180000 14.9932340000
C 9.7943610000 12.2823270000 14.5601090000
C 7.6351630000 8.7420540000 11.3023070000
C 6.9049660000 9.1807020000 13.5894860000
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C 12.4617050000 9.9418070000 12.1435980000
C 10.3643110000 11.2498560000 10.2645180000
C 14.9809980000 14.9949060000 10.7492140000
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H 17.3568840000 12.9374710000 9.6445910000
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H 9.4058420000 12.5257240000 15.5544690000
H 10.8897800000 12.2372060000 14.5977590000
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H 8.4369190000 8.9177590000 10.5839360000
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O 10.3334380000 15.1280210000 9.6188330000
P 15.4419940000 12.5388770000 11.7474460000
P 8.8609690000 10.7928550000 12.5381380000

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