

Supporting Information for: Simulating the reactions of CO₂ in aqueous monoethanolamine solution by Reaction Ensemble Monte Carlo using the Continuous Fractional Component method

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1 Molecular Partition Function

Consider the RxMC algorithm for a single reaction system involving n species. Equilibrium is achieved when

$$\sum_{i=1}^n \nu_i \mu_i = 0 \quad (\text{S1})$$

where ν_i and μ_i are the stoichiometric coefficient and the chemical potential of species i , respectively.¹ The molecular partition function q_i , of an isolated molecule of type i in the ideal gas phase is defined by²

$$q_i = q_{i,\text{qm}} q_{i,\text{cl}} = \frac{q_{i,\text{qm}}}{\hbar^{f_i}} \int \exp[-\beta \mathcal{H}_{i,\text{cl}}(p_i, r_i)] dp_i dr_i \quad (\text{S2})$$

where \hbar is Planck's constant, $q_{i,\text{cl}}$ is the classical molecular partition function, $q_{i,\text{qm}}$ is the quantum molecular partition function of isolated molecules of type i , $\beta = 1/(k_B T)$, p_i and r_i are the momenta and generalized coordinates associated with all the classical degrees of freedom of species i , and $\mathcal{H}_{i,\text{cl}}$ is the classical Hamiltonian of the system. The molar standard chemical potential of an isolated molecule in the gas phase μ_i^0 is related to the total molecular partition function q_i by²

$$\frac{\mu_i^0}{k_B T} = -\ln \left(\frac{q_i}{\beta p^0 \Lambda_i^3} \right) \quad (\text{S3})$$

where p^0 is the standard state pressure (1 bar) and Λ_i is the thermal de Broglie wavelength of molecules of type i . The Hamiltonian of a molecule \mathcal{H}_i can be written as a sum of Hamiltonians for the various degrees of freedom of the molecule³

$$\mathcal{H}_i \approx \mathcal{H}_{i,\text{trans}} + \mathcal{H}_{i,\text{rot}} + \mathcal{H}_{i,\text{vib}} + \mathcal{H}_{i,\text{elec}} \quad (\text{S4})$$

where $\mathcal{H}_{i,\text{trans}}$, $\mathcal{H}_{i,\text{rot}}$, $\mathcal{H}_{i,\text{vib}}$, $\mathcal{H}_{i,\text{elec}}$ are the Hamiltonian of the translational, rotational, vibrational and electronic degrees of freedom respectively of a molecule of type i . Consequently, the molecular partition function q_i can be expressed in terms of the various degrees of freedom of the molecule as³

$$q_i = q_{i,\text{trans}} q_{i,\text{rot}} q_{i,\text{vib}} q_{i,\text{elec}} \quad (\text{S5})$$

$$= q_{i,\text{trans}} q_{i,\text{int}} \quad (\text{S6})$$

where $q_{i,\text{trans}}$, $q_{i,\text{rot}}$, $q_{i,\text{vib}}$, $q_{i,\text{elec}}$ are the translational, rotational, vibrational and electronic contributions to the molecular partition function of a molecule of type i . The internal contributions to the molecular partition function $q_{i,\text{int}}$ are the rotational, vibrational and electronic degrees of freedom:

$$q_{i,\text{int}} = q_{i,\text{rot}}q_{i,\text{vib}}q_{i,\text{elec}} \quad (\text{S7})$$

The translational partition function depends on temperature as well as the volume. The translational partition function equals,³

$$q_{i,\text{trans}} = \left(\frac{2\pi m_i k_B T}{h^2} \right)^{3/2} V \quad (\text{S8})$$

$$= \frac{V}{\Lambda_i^3} \quad (\text{S9})$$

$$= \frac{q_i}{q_{i,\text{int}}} \quad (\text{S10})$$

where m_i is the mass of the molecule of type i and V is the volume of the system. In our case, the volume V is the volume of the simulation box. This molecular partition function q_i can be split into two parts, one part which depends on only the temperature $\hat{q}_i(T)$ and the other which depends only on the volume. Incorporating this in Eq. (S5), we obtain,

$$q_i = \hat{q}_i(T)V \quad (\text{S11})$$

Quantum mechanical simulations using GAUSSIAN 09⁴ are performed to obtain the molecular partition functions. The output of GAUSSIAN 09⁴ provides the values for the individual contributions to the partition functions (translational, rotational, vibrational and electronic). The volume term in the translational partition function is calculated in GAUSSIAN 09 using the ideal gas law for a single isolated molecule: $V = k_B T/P$.⁵ Since the volume changes in our Monte Carlo simulations one needs to consider that q_i changes when V changes. To this end, we have explicitly separated the volume term and used $\hat{q}_i(T)$ as input to our simulations. The values of the computed partition functions are listed in Table S1.

2 Osmotic Ensemble with Continuous Fractional Component Monte Carlo

The reaction ensemble is best described by taking the osmotic ensemble as the starting point since most chemical reactions take place in a system at constant pressure. Let N denote the number of molecules, P the imposed hydrostatic pressure, V the volume and μ the chemical potential. The expression for the partition function for the osmotic ensemble is,^{6,7}

$$\Xi(\mu, p, T) = \beta P \sum_{N=0}^{\infty} \frac{\exp(\beta\mu N)}{\Lambda^{3N} N!} \int dV V^N \exp[-\beta PV] \int ds^N \exp[-\beta U(s^N)] \quad (\text{S12})$$

where s^N are the configurations of the N molecules and $U(s^N)$ is the potential energy of the system. Approximating Q semi-classically, the expression becomes,⁸

$$\Xi(\mu, p, T) = \beta P \sum_{N=0}^{\infty} \int \exp \left[\beta\mu N - \ln(N!) + N \ln \frac{V q_{i,\text{int}}}{\Lambda^3} - \beta PV - \beta U(s^N, \omega^N) \right] ds^N d\omega^N dV \quad (\text{S13})$$

where ω^N are the orientations and internal configuration of the N molecules. $q_{i,\text{int}}$ is the internal contribution (electronic, rotational, vibrational) to the partition function of the isolated molecule (see Eq. S7). Substituting Eqs. (S5),(S7),(S9),(S11) in Eq. (S13) we obtain,

$$\Xi(\mu, p, T) = \beta P \sum_{N=0}^{\infty} \int \exp \left[\beta\mu N - \ln(N!) + N \ln(\hat{q}_i(T)V) - \beta PV - \beta U(s^N, \omega^N) \right] ds^N d\omega^N dV \quad (\text{S14})$$

where $q_i = q_{i,\text{int}}V/\Lambda^3 = \hat{q}_i(T)V$. Consider now a multicomponent system. Let N_i denote the number of molecules of type i and μ_i the chemical potential of the species i . In a mixture of n species, the expression for the partition function is

$$\begin{aligned} \Xi(\mu_1, \dots, \mu_n, p, T) = \beta P \sum_{N_1=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \int \cdots \int \exp \left[\beta \sum_{i=1}^n N_i \mu_i - \sum_{i=1}^n \ln N_i! + \sum_{i=1}^n N_i \ln(\hat{q}_i(T)V) \right. \\ \left. - \beta PV - \beta U(s^N, \omega^N) \right] ds^{N_1} d\omega^{N_1} \cdots ds^{N_n} d\omega^{N_n} dV \end{aligned} \quad (\text{S15})$$

where s^{N_i} are the configurations of the N_i molecules of type i and ω^{N_i} are the orientations and internal configurations of the N_i molecules of type i . $\hat{q}_i(T)$ is the temperature dependent term in the molecular

partition function for the molecule of type i (Eq. (S11)). The Reaction Ensemble Monte Carlo method inserts and deletes the reactant and product molecules in the system according to the stoichiometry of the reaction.² In dense systems, the efficiency of the insertions and deletions of molecules decreases greatly, since the acceptance probabilities for the insertions/deletions are very low.^{9–11} The reason for this is that inserting molecules in these dense systems can lead to overlaps between atoms. To circumvent this problem, Shi *et al.*^{10,12} have developed the Continuous Fractional Component Monte Carlo (CFCMC) method. In this method, the molecules are gradually inserted or deleted in many trial moves and not in a single move. A fractional molecule is introduced into the system for species that is inserted/deleted. The parameter to describe the interactions of the fractional molecule with the surrounding molecules is defined as λ , with $\lambda \in [0, 1]$. By changing the value of λ , the molecule is gradually inserted/deleted in the system as interactions with the surrounding molecules are gradually turned on/off. For the combination of the Reaction Ensemble Monte Carlo and the Continuous Fractional Component methods, we introduce fractional molecules for each reacting species (both reactants and products) in the mixture according to their stoichiometry.^{10,12,13} For the reaction move, λ is defined as the extent of interactions of the fractional reactant molecules with the surrounding molecules. The extent of the interactions of the fractional product molecules with the surrounding molecules is $1 - \lambda$. If $\lambda = 0$, the forward reaction takes place and the interactions of the product molecules with the surrounding molecules are at full strength while for $\lambda = 1$, the backward reaction takes place and the interactions of the reactant molecules with the surrounding molecules are at full strength. The potential energy of this system now also depends on λ and is therefore denoted by $U(s^N, \omega^N, \lambda)$. Let us now consider a system of n species. For such an expanded osmotic ensemble, the partition function for a system becomes¹³

$$\begin{aligned} \Xi(\mu_1, \dots, \mu_n, p, T) = & \beta P \int_0^1 d\lambda \sum_{N_i=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \int \exp \left[\beta \sum_{i=1}^n N_i \mu_i - \sum_{i=1}^n \ln N_i! + \sum_{i=1}^n N_i \ln(\hat{q}_i(T)V) \right. \\ & \left. - \beta PV - \beta U(s^N, \lambda) \right] ds^{N_1} d\omega^{N_1} \cdots ds^{N_n} d\omega^{N_n} dV \end{aligned} \quad (\text{S16})$$

For efficiency reasons, changes in λ should be made in such a way that there is a flat distribution of λ .¹⁰ This enables all the λ states to be visited with equal probability and forces the molecules in and out of the system.^{10,12,13} Suitable bias factors $\eta(\lambda)$ are introduced to improve the probabilities of transitions in λ . The Wang-Landau algorithm^{14,15} can be used to compute these bias factors on the fly. The partition functions

including the biasing factors are now expressed as

$$\begin{aligned} \Xi_{\text{biased}}(\mu_1, \dots, \mu_n, p, T) = & \beta P \int_0^1 d\lambda \sum_{N_1=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \int \exp \left[\beta \sum_{i=1}^n N_i \mu_i - \sum_{i=1}^n \ln N_i! + \sum_{i=1}^n N_i \ln(\hat{q}_i(T)V) \right. \\ & \left. - \beta PV - \beta U(s^N, \omega^N, \lambda) \right] \exp[\eta(\lambda)/k_B T] ds^{N_1} d\omega^{N_1} \cdots ds^{N_n} d\omega^{N_n} dV \end{aligned} \quad (\text{S17})$$

The probability that the system is in a certain state is

$$p_{\text{biased}} \sim \exp \left[\beta \sum_{i=1}^n N_i \mu_i - \sum_{i=1}^n \ln N_i! + \sum_{i=1}^n N_i \ln(\hat{q}_i(T)V) - \beta PV - \beta U(s^N, \omega^N, \lambda) \right] \exp[\eta(\lambda)/k_B T] \quad (\text{S18})$$

3 Equilibrium constants for ideal gas reactions

For an ideal gas reacting mixture consisting of four species A, B, C and D, the expression for the chemical equilibrium constant for the reaction,



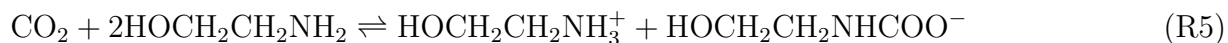
is given by,

$$\begin{aligned} K_{\text{idealgas}} &= \frac{\left[\frac{q_C}{V}\right]^c \left[\frac{q_D}{V}\right]^d}{\left[\frac{q_A}{V}\right]^a \left[\frac{q_B}{V}\right]^b} \\ &= \frac{[q_C]^c [q_D]^d}{[q_A]^a [q_B]^b} V^{(c+d-a-b)} \end{aligned} \quad (\text{S20})$$

where q_i is the ideal gas partition function of species i ¹⁶ (Eq. (S5)). The equilibrium constants for the different CO₂-MEA reactions at 293 K and 353 K when the species are considered as ideal gas molecules are listed in Table S2. It is clear from the values of K_{idealgas} that the reaction will not occur (as expected as one needs ion solvation).

4 Probability distribution in λ space

For flat distributions in the λ probability, the biasing factors represent the free energy cost of inserting and deleting the molecules taking part in the reaction.^{10,11} Figure S1 shows the biasing factors for the reaction of CO_2 and aqueous MEA solutions for the overall Reaction R5



at 293 K when we intermolecular interactions are included. From Fig S1, we notice that increasing λ leads to low biasing values. This corresponds to the state where increasing the interactions of the fractional molecule with the surrounding molecules are very favorable and increasing λ leads to low free energies. The acceptance rates for the reaction where only the λ changes between 0 to 1 (first case, see main text) is kept fixed around 50%. The acceptance rates for the successful forward/reverse reactions (second and third cases) are of the order 0.2 % to 0.5 %, which is somewhat low but still sufficiently large to obtain accurate statistics during the MC simulations.

5 Force Field parameters

This section includes all the force field parameters of the different molecules in the system. The force field for the linear CO₂ molecule was taken from the TraPPE force field.¹⁷ For water, the four-site rigid model TIP4P¹⁸ was used. The 4-site TIP4P water model uses a dummy atom (labeled M) along the bisector of H-O-H angle. Force field parameters for the HCO₃⁻ and CO₃²⁻ have been taken from the OPLS force field.^{19,20} The force field parameters for H₃O⁺ molecule have been taken from Vacha *et al.*²¹ All molecular models for CO₂, water, MEA, MEAH⁺, MEACOO⁻, H₃O⁺, HCO₃⁻ and CO₃²⁻ have been treated as rigid in the simulations. The partial charges for HCO₃⁻, CO₃²⁻, MEACOO⁻ and MEAH⁺ have been computed from quantum mechanical simulations in GAUSSIAN.^{4,22} σ and ϵ are the Lennard-Jones (LJ) parameters, q the atomic partial charges, L the bond distance between two atoms and θ the angle of bonded atoms. Due to the scaling of the LJ potential and charges in the RxMC/CFC method, the hydrogen atoms in HCO₃⁻, water and H₃O⁺ are assigned values of $\sigma = 1.0\text{\AA}$ and $\epsilon/k_B = 1.0\text{ K}$ to avoid overlaps on the end hydrogen atoms.^{10,12,13} Electrostatic interactions were handled by the Ewald summation algorithm²³ with a relative precision of 10^{-5} .²⁴ The cut off radius was set at 12\AA for the Lennard-Jones interactions. The Lorentz-Berthelot mixing rules were adopted for Lennard-Jones interactions.²⁵ The scaled Lennard-Jones interaction potential is given by^{10,12}

$$U(r_{ij}, \lambda_{ij}) = \lambda_{ij} 4\epsilon_{ij} \left[\frac{1}{\left(\tau(1 - \lambda_{ij})^2 + \left(\frac{r_{ij}}{\sigma_{ij}} \right)^6 \right)^2} - \frac{1}{\left(\tau(1 - \lambda_{ij})^2 + \left(\frac{r_{ij}}{\sigma_{ij}} \right)^6 \right)} \right] \quad (\text{S21})$$

where $\lambda_{ij} = \lambda_i \times \lambda_j$ and $\tau = 1/2$.^{10,12,13} To obtain the electrostatic scaled potentials, the partial charges on the fractional molecule were scaled as $q_f = \lambda_i^5 q_i$.¹³

Table S1: Partition Functions ($\hat{q}_i(T)$) of the isolated molecules at different temperatures 293 K, 333 K, 353 K computed using quantum mechanical simulations using GAUSSIAN 09.^{4,5} Details of these calculations can be found in the main text and Section 1 of Supplementary Information.

Molecule	\hat{q}_i (293 K) (\AA^{-3})	\hat{q}_i (333 K) (\AA^{-3})	\hat{q}_i (353 K) (\AA^{-3})
CO ₂	$7.8752 \cdot 10^4$	$1.1294 \cdot 10^5$	$1.3368 \cdot 10^5$
MEA	$6.9980 \cdot 10^7$	$1.4048 \cdot 10^8$	$1.9685 \cdot 10^8$
MEAH ⁺	$8.8994 \cdot 10^7$	$1.8468 \cdot 10^8$	$2.6286 \cdot 10^8$
MEACOO ⁻	$5.1046 \cdot 10^9$	$1.3078 \cdot 10^{10}$	$2.0653 \cdot 10^{10}$
H ₂ O	$3.0134 \cdot 10^3$	$4.4259 \cdot 10^3$	$5.2742 \cdot 10^3$
H ₃ O ⁺	$4.8631 \cdot 10^3$	$7.2028 \cdot 10^3$	$8.6279 \cdot 10^3$
HCO ₃ ⁻	$1.6616 \cdot 10^7$	$2.7090 \cdot 10^7$	$3.4201 \cdot 10^7$
CO ₃ ²⁻	$6.8336 \cdot 10^6$	$1.0663 \cdot 10^7$	$1.3155 \cdot 10^7$

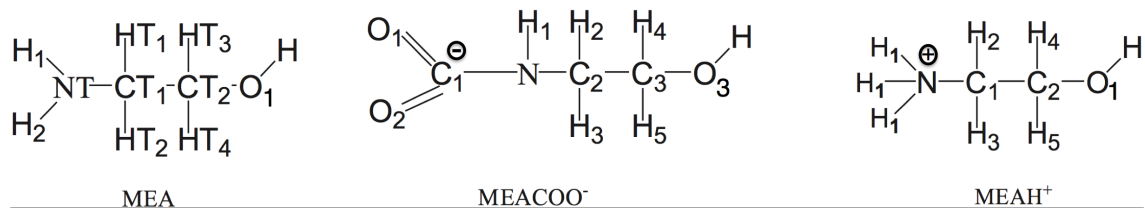
Table S2: Equilibrium constants for the different ideal gas reactions at 293 K and 353 K as obtained from the computed partition functions (Table S1).

Reactions	K_{idealgas} (293 K)	K_{idealgas} (353 K)
R1	$2.8302 \cdot 10^{-06}$	$1.6498 \cdot 10^{-06}$
R2	$6.6368 \cdot 10^{-01}$	$6.2920 \cdot 10^{-01}$
R3	$7.8802 \cdot 10^{-01}$	$8.1627 \cdot 10^{-01}$
R4	$1.3229 \cdot 10^{-02}$	$1.6179 \cdot 10^{-02}$
R5	$2.9504 \cdot 10^{-08}$	$2.1787 \cdot 10^{-08}$

Table S3: Force field parameters for H₂O,¹⁸ CO₂,¹⁷ HCO₃⁻,^{19,20} CO₃²⁻^{19,20} and H₃O⁺.²¹ H₂O, CO₂, HCO₃⁻, CO₃²⁻ and H₃O⁺ are modeled as rigid molecules.

H₂O (TIP4P)¹⁸							
$\theta_{\text{H-O-H}} [^\circ]$	104.52	$\sigma_{\text{O-O}} [\text{\AA}]$	3.154	$\varepsilon_{\text{O-O}}/k_{\text{B}} [\text{K}]$	78.020	$q_{\text{O}} [e]$	0
$L_{\text{O-H}} [\text{\AA}]$	0.9572	$\sigma_{\text{H-H}} [\text{\AA}]$	0	$\varepsilon_{\text{H-H}}/k_{\text{B}} [\text{K}]$	0	$q_{\text{H}} [e]$	+0.52
$L_{\text{O-M}} [\text{\AA}]$	0.15	$\sigma_{\text{M-M}} [\text{\AA}]$	0	$\varepsilon_{\text{M-M}}/k_{\text{B}} [\text{K}]$	0	$q_{\text{M}} [e]$	-1.04
CO₂ (TraPPE)¹⁷							
$\theta_{\text{O-C-O}} [^\circ]$	180	$\sigma_{\text{C-C}} [\text{\AA}]$	2.75	$\varepsilon_{\text{C-C}}/k_{\text{B}} [\text{K}]$	28.129	$q_{\text{C}} [e]$	+0.70
$L_{\text{O-C}} [\text{\AA}]$	1.16	$\sigma_{\text{O-O}} [\text{\AA}]$	3.05	$\varepsilon_{\text{O-O}}/k_{\text{B}} [\text{K}]$	80.507	$q_{\text{O}} [e]$	-0.35
HCO₃⁻ (OPLS)^{19,20}							
$\theta_{\text{O1-C-O2}} [^\circ]$	113.98	$\sigma_{\text{H-H}} [\text{\AA}]$	1.0	$\varepsilon_{\text{H-H}}/k_{\text{B}} [\text{K}]$	1.0	$q_{\text{H}} [e]$	+0.254
$\theta_{\text{O1-C-O3}} [^\circ]$	132.7	$\sigma_{\text{O2-O2}} [\text{\AA}]$	3.0	$\varepsilon_{\text{O2-O2}}/k_{\text{B}} [\text{K}]$	85.5479	$q_{\text{O2}} [e]$	-0.632
$\theta_{\text{O2-C-O3}} [^\circ]$	113.32	$\sigma_{\text{C-C}} [\text{\AA}]$	3.75	$\varepsilon_{\text{C-C}}/k_{\text{B}} [\text{K}]$	52.8384	$q_{\text{C}} [e]$	+0.978
$\theta_{\text{H-O2-C}} [^\circ]$	101	$\sigma_{\text{O1-O1}} [\text{\AA}]$	2.96	$\varepsilon_{\text{O-O}}/k_{\text{B}} [\text{K}]$	105.6768	$q_{\text{O1}} [e]$	-0.773
$L_{\text{H-O2}} [\text{\AA}]$	0.96	$\sigma_{\text{O3-O3}} [\text{\AA}]$	3.0	$\varepsilon_{\text{O3-O3}}/k_{\text{B}} [\text{K}]$	85.5479	$q_{\text{O3}} [e]$	-0.827
$L_{\text{O2-C}} [\text{\AA}]$	1.45	$L_{\text{O3-C}} [\text{\AA}]$	1.25	$L_{\text{O1-C}} [\text{\AA}]$	1.24		
CO₃²⁻ (OPLS)^{19,20}							
$\theta_{\text{O-C-O}} [^\circ]$	120	$\sigma_{\text{C-C}} [\text{\AA}]$	3.75	$\varepsilon_{\text{C-C}}/k_{\text{B}} [\text{K}]$	52.8384	$q_{\text{C}} [e]$	+0.928
$\theta_{\text{O2-C-O}} [^\circ]$	120	$\sigma_{\text{O2-O2}} [\text{\AA}]$	2.96	$\varepsilon_{\text{O2-O2}}/k_{\text{B}} [\text{K}]$	105.6768	$q_{\text{O2}} [e]$	-0.976
$L_{\text{O-C}} [\text{\AA}]$	1.31	$\sigma_{\text{O-O}} [\text{\AA}]$	3.0	$\varepsilon_{\text{O-O}}/k_{\text{B}} [\text{K}]$	85.5479	$q_{\text{O}} [e]$	-0.976
$L_{\text{O2-C}} [\text{\AA}]$	1.31						
H₃O²⁻ (Vacha)²¹							
$\theta_{\text{H-O-H}} [^\circ]$	111.28	$\sigma_{\text{H-H}} [\text{\AA}]$	1.0	$\varepsilon_{\text{H-H}}/k_{\text{B}} [\text{K}]$	1.0	$q_{\text{H}} [e]$	+0.4722
$L_{\text{O-H}} [\text{\AA}]$	0.98	$\sigma_{\text{O-O}} [\text{\AA}]$	3.05	$\varepsilon_{\text{O-O}}/k_{\text{B}} [\text{K}]$	74.2085	$q_{\text{O}} [e]$	-0.4166
$L_{\text{H-H}} [\text{\AA}]$	1.63						

Table S4: Force field parameters for monoethanolamine (MEA), the carbamate ion ($\text{HOCH}_2\text{CH}_2\text{NHCOO}^-$), and the amine ion ($\text{HOCH}_2\text{CH}_2\text{NH}_3^+$), which are all modeled as rigid objects. These two ions are abbreviated as MEACOO^- and MEA^+ and their partial charges sum up to -1 and $+1$ respectively. Parameter values were taken from Chen *et al.*²²



#	Atom type	Molecule	ϵ/k_B [K]	σ [Å]	Partial charge [e]
1	NT	MEA	85.6	3.300	-0.900
2	H1	MEA	1.0	1.0	0.360
3	H2	MEA	1.0	1.0	0.360
4	CT1	MEA	33.2	3.500	0.060
5	HT1	MEA	7.5	2.500	0.060
6	HT2	MEA	7.5	2.500	0.060
7	CT2	MEA	33.2	3.500	0.145
8	HT3	MEA	15.1	2.500	0.060
9	HT4	MEA	15.1	2.500	0.060
10	O1	MEA	85.6	3.120	-0.683
11	H	MEA	1.0	1.0	0.418
12	C1	MEACOO ⁻	52.9	3.75	+0.914
13	O1	MEACOO ⁻	106	2.96	-0.798
14	O2	MEACOO ⁻	106	2.96	-0.863
15	N	MEACOO ⁻	85.6	3.25	-0.510
16	H1	MEACOO ⁻	1.0	1.0	+0.158
17	C2	MEACOO ⁻	33.2	3.5	+0.100
18	H2	MEACOO ⁻	15.1	2.5	+0.005
19	H3	MEACOO ⁻	15.1	2.5	+0.039
20	C1	MEACOO ⁻	33.2	3.5	+0.218
21	H4	MEACOO ⁻	15.1	2.5	-0.009
22	H5	MEACOO ⁻	15.1	2.5	+0.005
23	O3	MEACOO ⁻	85.6	3.12	-0.679

#	Atom type	Molecule	ε/k_B [K]	σ [Å]	Partial charge [e]
24	H	MEACOO ⁻	1.0	1.0	+0.420
25	N	MEAH ⁺	85.6	3.25	-0.367
26	H1	MEAH ⁺	1.0	1.0	+0.335
27	H1	MEAH ⁺	1.0	1.0	+0.335
28	H1	MEAH ⁺	1.0	1.0	+0.335
29	C1	MEAH ⁺	33.2	3.5	+0.063
30	H2	MEAH ⁺	15.1	2.5	+0.080
31	H3	MEAH ⁺	15.1	2.5	+0.124
32	C2	MEAH ⁺	33.2	3.5	+0.149
33	H4	MEAH ⁺	15.1	2.5	+0.058
34	H5	MEAH ⁺	15.1	2.5	+0.086
35	O1	MEAH ⁺	85.6	3.12	-0.663
36	H	MEAH ⁺	1.0	1.0	+0.465

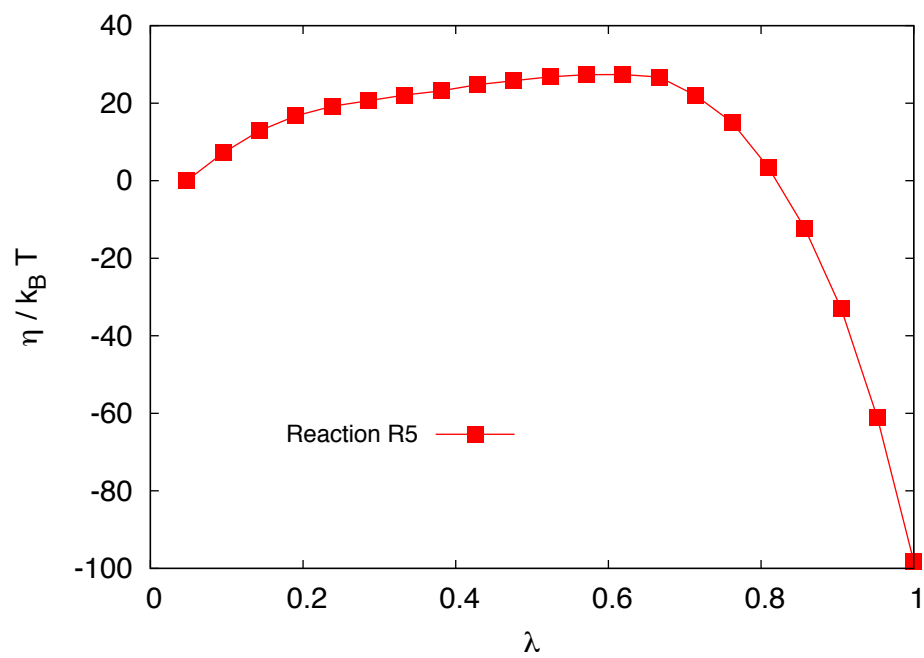


Figure S1: Biasing factors η as a function of λ for the reaction of CO_2 with aqueous MEA solutions via reaction R5 at 293 K and 1 bar. The line is a guide to the eye.

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