Supplementary Materials: Solvation Dynamics of CO_2(g) by Monoethanolamine at the Gas–Liquid Interface: A Molecular Mechanics Approach

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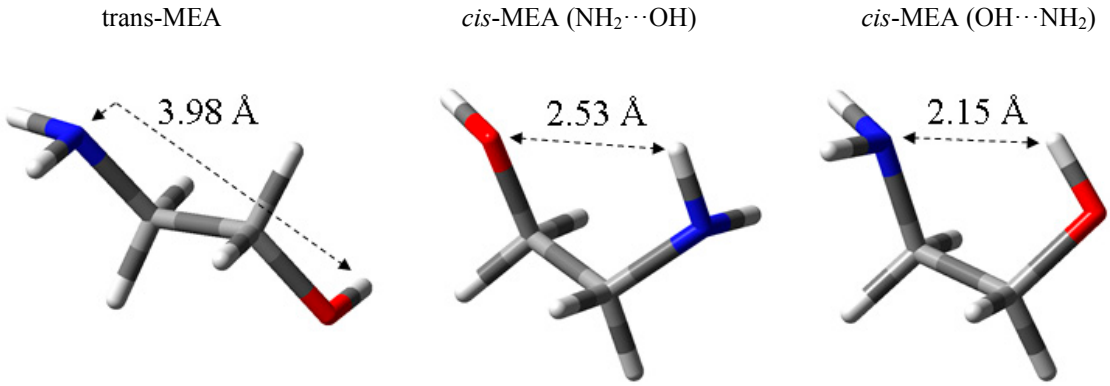

Figure S1. MP2/aug-cc-pVTZ optimized monomeric MEA geometries using PCM model in EtOH. The distance between N of NH_2 group to H of OH group is labeled.

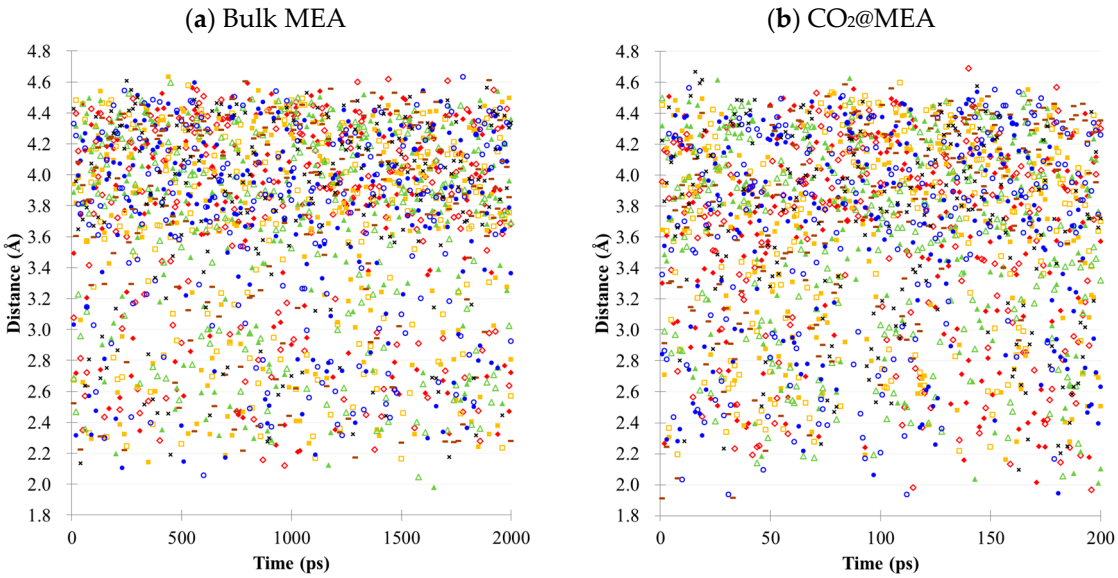

Figure S2. History of intramolecular N_{NH2}-H_{OH} distance in Å of (**a**) 2 ns $(MEA)_{128}$ bulk simulation at 400 K and (**b**) $(CO_2)_{44}$ in $(MEA)_{804}$ simulations at 400 K. The sampled potential energy surface of simulation (**a**) is shown in Figure S3. Ten MEA molecules are randomly selected and N-H distance is recorded per 10 ps for (**a**). The 10 MEA molecules positioning closest to $(CO_2)_{44}$ at t = 0 ps are chosen and N-H distance is recorded per 1 ps for (**b**).

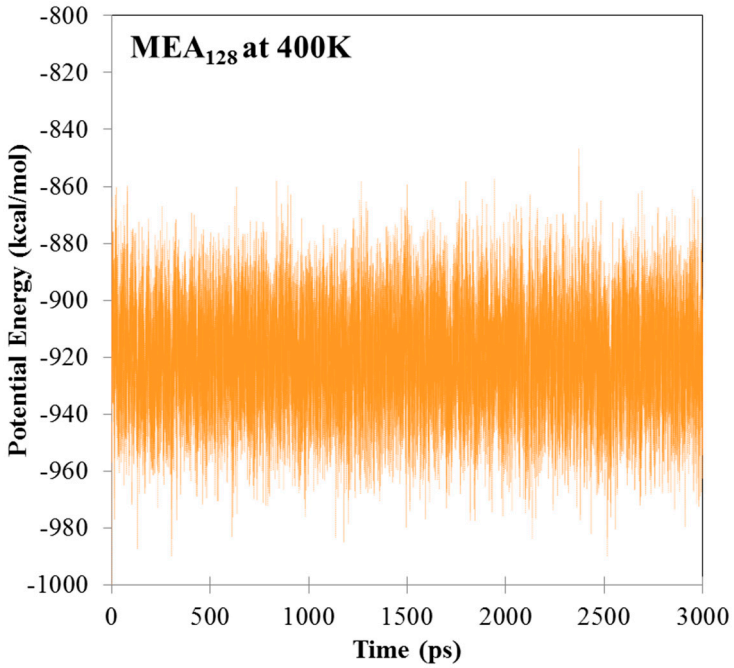

Figure S3. The 3 ns history of the sampled potential energy for bulk MEA at 400 K and the last 2 ns trajectory is used for intramolecular HB analysis.

Table S1. The energetics of various stable geometries calculated at MP2/aug-cc-pVTZ using PCM model and MM level in vacuum.

kcal/mol (AU)	E_{PCM}(MP2)	G_{PCM}(MP2)	ΔU(MM)
trans-MEA	0.00 (−210.02476)	0.00 (−209.95389)	0.00
cis-MEA (NH_2···OH)	−1.01 (−210.02636)	−0.91 (−209.95534)	−0.02
cis-MEA (OH···NH_2)	−2.55 (−210.02881)	−1.83 (−209.95682)	0.18

Table S2. Cartesian coordinates at BLYP-D2/aug-cc-pVTZ level for the OHO and NHN.

OHO				NHN			
N	3.023	−0.080	−1.310	N	−1.655	1.716	0.176
H	2.112	−0.453	−1.585	H	−1.684	2.590	−0.348
H	3.719	−0.524	−1.910	H	−1.883	1.944	1.146
C	3.263	−0.433	0.107	C	−2.645	0.753	−0.369
H	4.225	−0.001	0.419	C	−2.431	−0.613	0.288
H	3.304	−1.523	0.291	H	−2.473	0.661	−1.449
C	2.156	0.153	0.985	H	−3.695	1.059	−0.219
H	2.397	−0.028	2.045	H	−1.435	−0.997	0.027
H	2.090	1.237	0.811	H	−2.489	−0.504	1.387
O	0.893	−0.480	0.674	O	−3.478	−1.493	−0.187
H	0.249	0.221	0.436	H	−3.227	−2.402	0.038
O	−0.970	1.548	−0.015	H	0.165	0.525	−0.201
H	−1.265	1.978	0.806	N	1.010	−0.028	−0.375
N	−3.638	−1.087	−0.274	H	1.420	0.303	−1.250
H	−3.265	−1.653	−1.038	C	1.982	0.188	0.713
H	−4.065	−1.735	0.388	C	3.270	−0.580	0.445
C	−2.542	−0.335	0.379	H	1.548	−0.190	1.651
H	−1.664	−0.946	0.646	H	2.244	1.252	0.872
H	−2.940	0.103	1.306	H	3.941	−0.508	1.318
C	−2.095	0.797	−0.558	H	3.032	−1.637	0.249
H	−1.729	0.385	−1.506	O	3.903	0.016	−0.722
H	−2.939	1.468	−0.772	H	4.603	−0.584	−1.024

parameter set for CO_2 + MEA parameterized by MKT (2016)#

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atom      1   C   "CSP3 ALKANE"              6   12.000   4
atom      5   H   "EXCEPT ON N,O,S"          1   1.008    1
atom      3   C   "C of CO2"                 6   12.000   2
atom      7   O   "O of CO2"                 8   15.999   1
atom      6   O   "C-O-H, C-O-C, O-O"        8   15.995   2
atom     21   H   "-OH ALCOHOL"              1   1.008    1
atom      8   N   "NSP3"                     7   14.003   3
atom     23   H   "NH AMINE/IMINE"           1   1.008    1
bond      1   5       4.86    1.0969
bond      6  21       7.57    0.9718
bond      8  23       6.42    1.0222
bond      1   8       5.30    1.4811
bond      1   6       5.70    1.4478
bond      1   1       4.49    1.5297
bond      3   7      14.50    1.1739
angle     7   3   7    0.70    180.00
angle     5   1   5    0.51    109.44
angle    21   6  21    0.66    104.56
angle    23   8  23    0.45    106.78
angle     5   1   8    0.82    109.30
angle     1   8  23    0.60    110.20
angle     1   6  21    0.75    108.00
angle     1   1   5    0.59    109.80
angle     1   1   6    0.83    107.50
angle     1   1   8    0.78    109.47
angle     5   1   6    0.82    110.00
torsion   5   1   1   8    0.000 0.0 1  0.000 180.0 2  0.374 0.0 3
torsion   6   1   1   8    0.000 0.0 1  −1.050 180.0 2  1.850 0.0 3
torsion   5   1   1   5    0.000 0.0 1  0.000 180.0 2  0.238 0.0 3
torsion   5   1   1   6    0.000 0.0 1  0.000 180.0 2  0.300 0.0 3
torsion   1   1   6  21    0.400 0.0 1  0.000 180.0 2  0.100 0.0 3
torsion   5   1   6  21    0.000 0.0 1  0.000 180.0 2  0.200 0.0 3
torsion   1   1   8  23    0.073 0.0 1  −0.422 180.0 2  0.327 0.0 3
torsion   5   1   8  23    0.121 0.0 1  −0.648 180.0 2  0.199 0.0 3
vdw       6         1.820   0.059
vdw       8         1.930   0.043
vdw       1         2.040   0.800
vdw       3         1.412   0.030
vdw       7         1.513   0.100
dipole 1  8  1.65 0.5
dipole 1  6  1.94 0.5
dipole 3  7  1.80 0.5
dipole 6  21  −1.94 0.5
dipole 8  23  −1.65 0.5
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