Supporting Information available for

Uptake of Water by an Acid-Base Nanoparticle: Theoretical and Experimental Studies of the Methanesulfonic Acid-Methylamine System

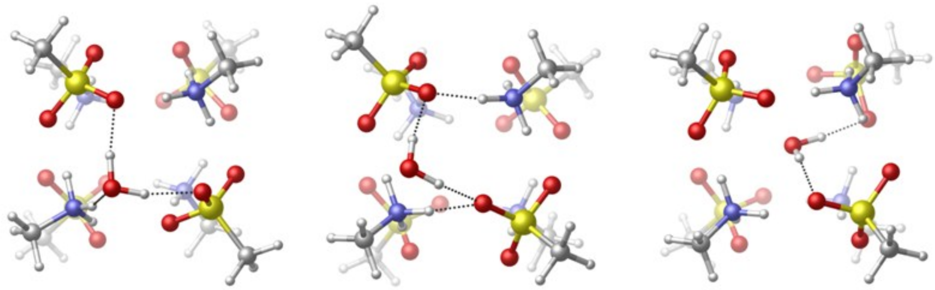
Jing Xu[a], Véronique Perraud,[a] Barbara J. Finlayson-Pitts,[a] and R. Benny Gerber*,[a,b]*

[a]Department of Chemistry
University of California, Irvine
Irvine, CA 92697, USA

[b]Institute of Chemistry, Fritz Haber Research Center
Hebrew University of Jerusalem
Jerusalem 91904, Israel

For submission to:

Physical Chemistry Chemical Physics



	iso-1	iso-2	iso-3
BLYP-D/6-31+G(d)	0.00	3.05	3.45
BLYP-D/aug-cc-pVDZ	0.00	2.51	3.82
BLYP-D/6-311++G(3df,3dp)	0.00	2.29	3.55
B3LYP-D3/aug-cc-pVDZ	0.00	2.15	3.47

Figure S1. Structures and relative energies corrected with zero-point energies (in kcal/mol) of three low-lying isomers of $(MSA\text{-}MA)_4\text{-}H_2O$ at BLYP-D/6-31+G(d), BLYP-D/aug-cc-pVDZ, BLYP-D/6-311++G(3df, 3dp) and B3LYP-D3/aug-cc-pVDZ levels.

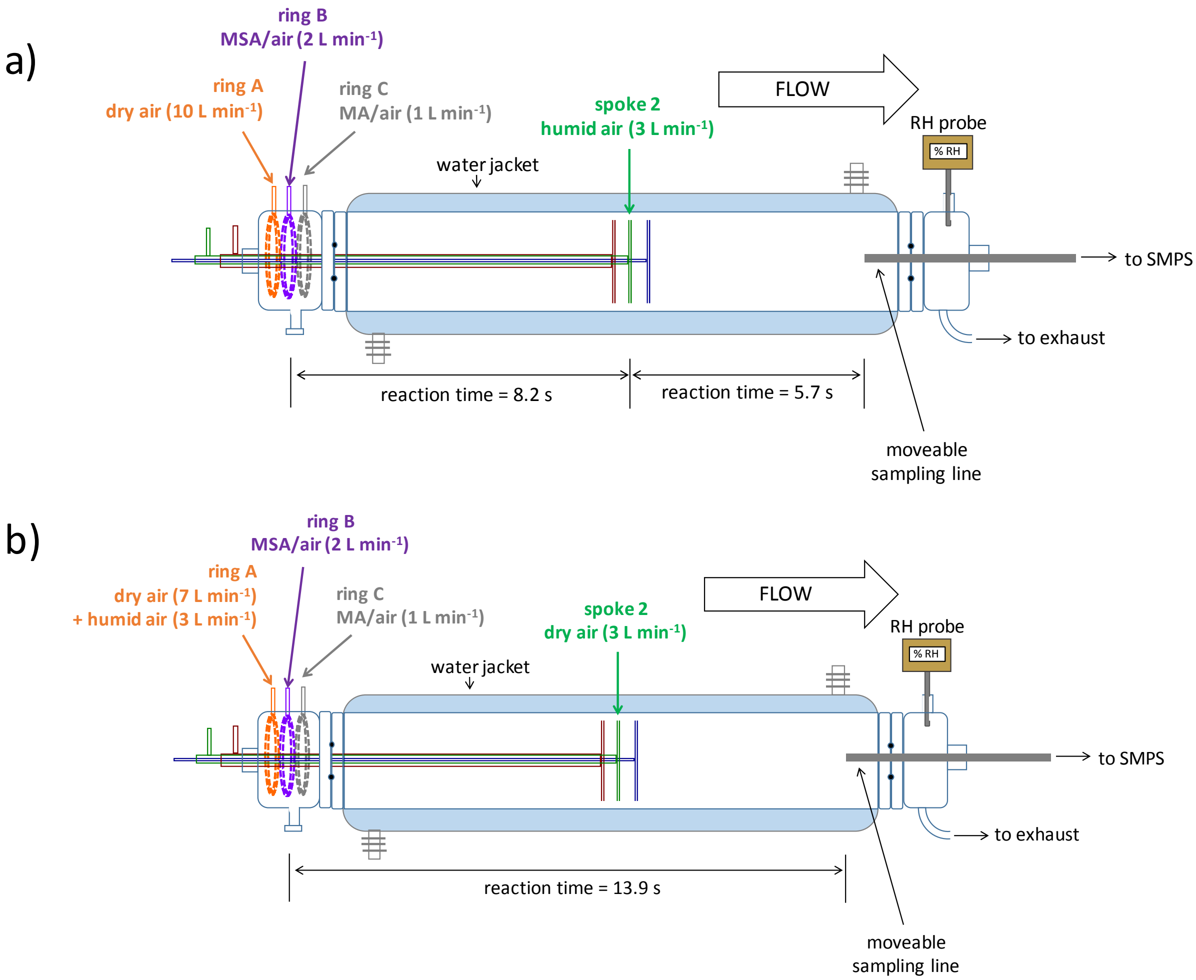


Figure S2. Schematic of the flow reactor (adapted from ref. 43) corresponding to the two conditions studied: (a) with water added at spoke 2, downstream of the formation of MSA-MA particles; (b) with water added at ring A and MSA reacting with MA and H_2O *at the same time*.

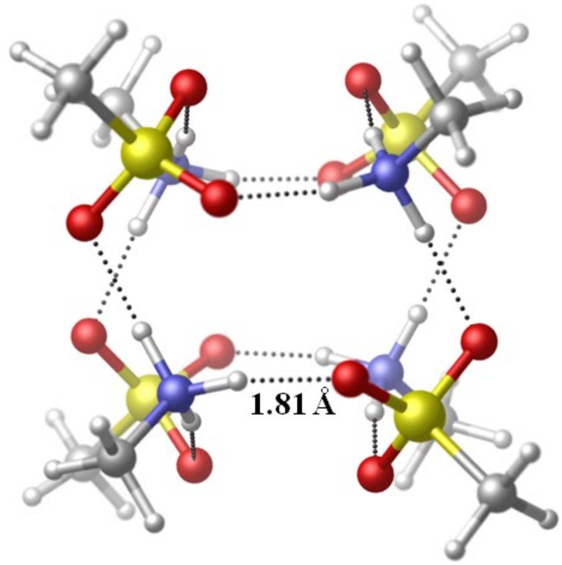


Figure S3. Structures of $(MSA\text{-}MA)_4$ and bond length of hydrogen bond at the level of BLYP-D/6-31+G(d).

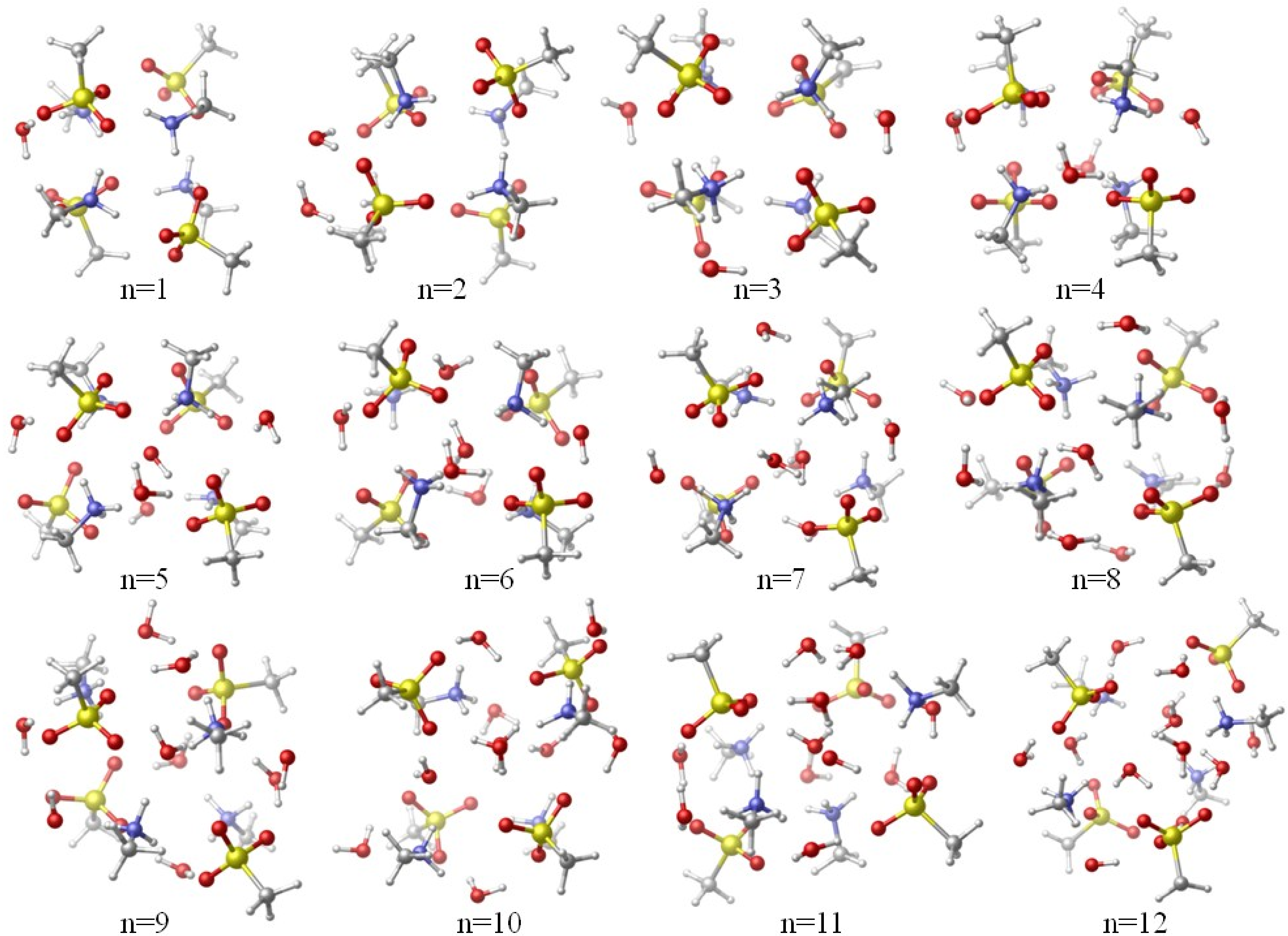


Figure S4. Structures of $(MSA\text{-}MA)_4\text{-}(H_2O)_n$, n=1 to 12 at 10 ps from the dynamic simulations (T=300 K) at the level of BLYP-D/6-31+G(d).

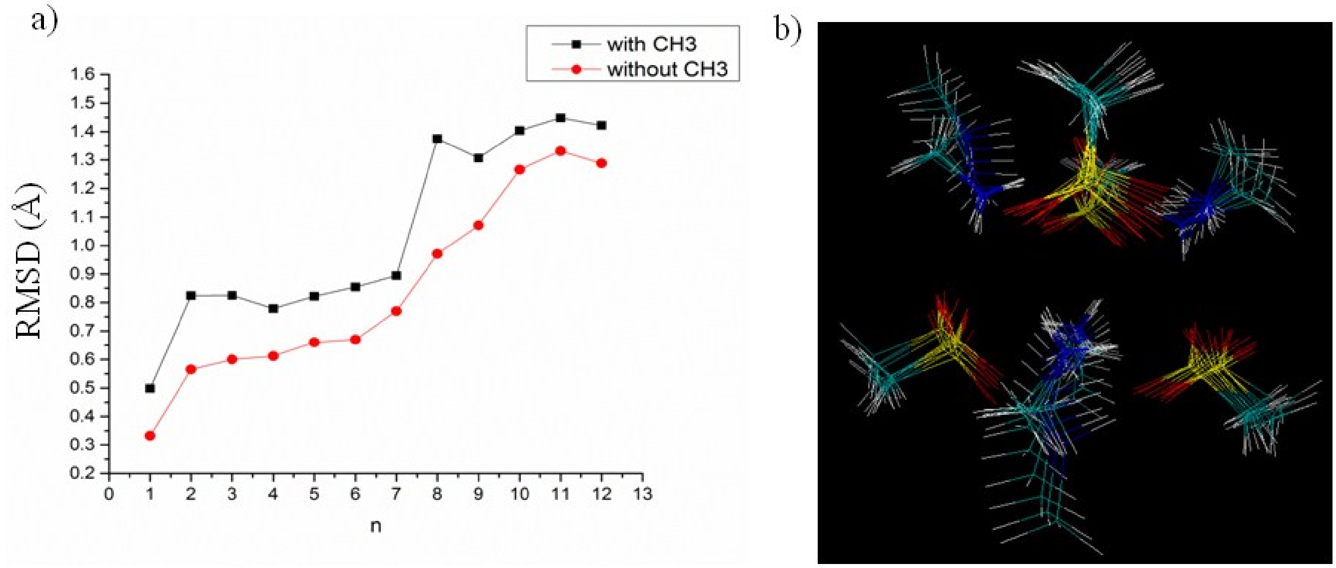
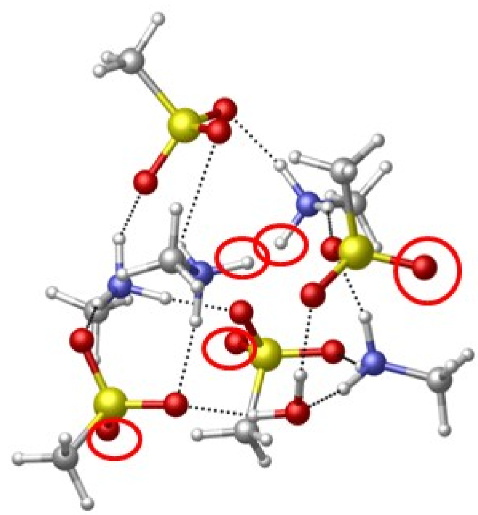


Figure S5. a) Root-mean-square deviation (RMSD) values of the geometry of $(MSA\text{-}MA)_4$ in $(MSA\text{-}MA)_4\text{-}(H_2O)_n$, n=1 to 12 with anhydrous $(MSA\text{-}MA)_4$ as the reference. Values in red are calculated when all the CH_3 groups are omitted. b) The skeleton of $(MSA\text{-}MA)_4$ in each system.



4MSA-4MA-H_2O

Figure S6. The structure of one isomer composed of 4 MSA, 4 MA and 1 H_2O.

Table S1 Partial charges of $(MSA\text{-}MA)_4\text{-}(H_2O)_n$ n= 0 to 12. S and N represent the MSA^{-} fragment and $H^{+}MA$ fragment, respectively. See Scheme 1 of text for S and N atom numbering. The values for H_2O are the charges on each water molecules, and the location of each water molecules is given in parenthesis.

n	S1	N10	S17	N26	S33	N42	S49	N58	H_2O
n=0	-0.82	0.82	-0.82	0.82	-0.82	0.82	-0.82	0.82	
n=1	-0.82	0.82	-0.84	0.83	-0.84	0.82	-0.82	0.82	0.01(F3)
n=2	-0.83	0.83	-0.83	0.83	-0.83	0.82	-0.84	0.83	0.01(F3), 0.01(F3)
n=3	-0.83	0.83	-0.84	0.82	-0.84	0.82	-0.82	0.82	0.02(F3), 0.01(F4), 0.01(F6)
n=4	-0.83	0.83	-0.85	0.84	-0.85	0.82	-0.83	0.83	0.01(F2), 0.01(F3), 0.01(F4), 0.01(F5)
n=5	-0.82	0.84	-0.83	0.84	-0.83	0.82	-0.82	0.82	0.01(F2), 0.01(F3), 0.01(F4), 0.01(F5), -0.06 (In)
n=6	-0.83	0.85	-0.83	0.81	-0.84	0.82	-0.83	0.82	0.03(F1), 0.00(F2), 0.02(F3), 0.02(F4), 0.01(F5), -0.05 (In)
n=7	-0.84	0.85	-0.86	0.83	-0.83	0.81	-0.83	0.83	0.02(F1), 0.01(F2), 0.01(F3), 0.01(F4), 0.01(F5), 0.02(F6), -0.04 (In)
n=8	-0.84	0.80	-0.85	0.83	-0.82	0.80	-0.83	0.79	0.02(F1), 0.01(F3), 0.02(F3), 0.02(F4), 0.02(F4), 0.02(F6),

									0.02(F6), -0.01 (In)
n=9	-0.83	0.81	-0.83	0.79	-0.83	0.76	-0.84	0.83	0.02(F1), 0.03(F1), 0.02(F3), 0.01(F3), 0.01(F4), 0.02(F4), 0.02(F5), 0.03(F6), -0.02 (In)
n=10	-0.82	0.76	-0.83	0.77	-0.83	0.80	-0.83	0.81	0.01(F1), 0.02(F1), 0.02(F2), 0.02(F3), 0.02(F3), 0.02(F4), 0.02(F4), 0.01(F5), 0.02(F6), 0.01 (In)
n=11	-0.83	0.79	-0.83	0.77	-0.82	0.80	-0.82	0.78	0.01(F1), 0.02(F1), 0.03(F2), 0.01(F3), 0.02(F3), 0.01(F4), 0.02(F4), 0.02(F5), 0.02(F6), 0.02(In), -0.02 (In)
n=12	-0.83	0.76	-0.84	0.77	-0.83	0.80	-0.81	0.80	0.02(F1), 0.03(F1), 0.02(F2), 0.01(F3), 0.03(F3), 0.00(F4), 0.02(F4), 0.04(F5), 0.01(F6), 0.02(F6), 0.00(In), -0.02 (In)