1 Supporting Information available for

Nanoparticles Grown from Methanesulfonic Acid and Methylamine: Microscopic Structures and Formation Mechanism

5

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

7
8 [a]Department of Chemistry
9 University of California, Irvine
10 Irvine, CA 92697
11

12 [b]Institute of Chemistry, Fritz Haber Research Center
13 Hebrew University of Jerusalem
14 Jerusalem 91904, Israel
15

16 For submission to:

17 *Physical Chemistry Chemical Physics*

18

19

20

21 *Corresponding author, R. Benny Gerber Email: benny@fh.huji.ac.il; phone: (949) 824-6758

22

23

24

25

26

28 Table S1. Parameters of the unit cell of the MSA-NH$_3$ crystal obtained in this work and
29 corresponding experimental values.

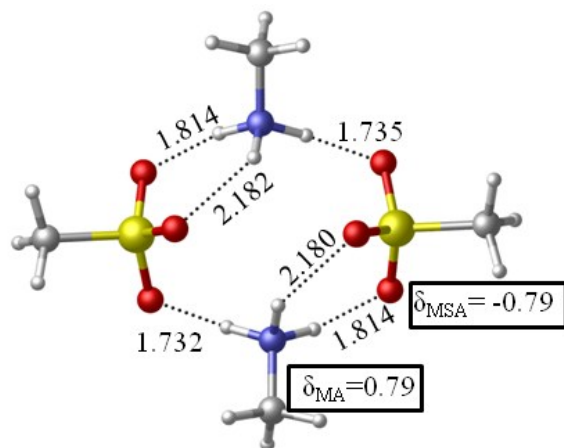| Parameter	This work	Exp.[105]
a (Å)	7.729	7.499
b (Å)	7.312	7.288
c (Å)	9.371	9.234
α	90.0	90.0
β	93.8	93.3
γ	90.0	90.0
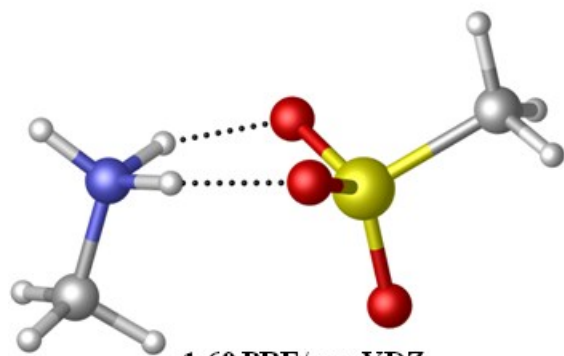
1.69 PBE/cc-pVDZ
1.68 B3LYP-D3/aug-cc-pVDZ
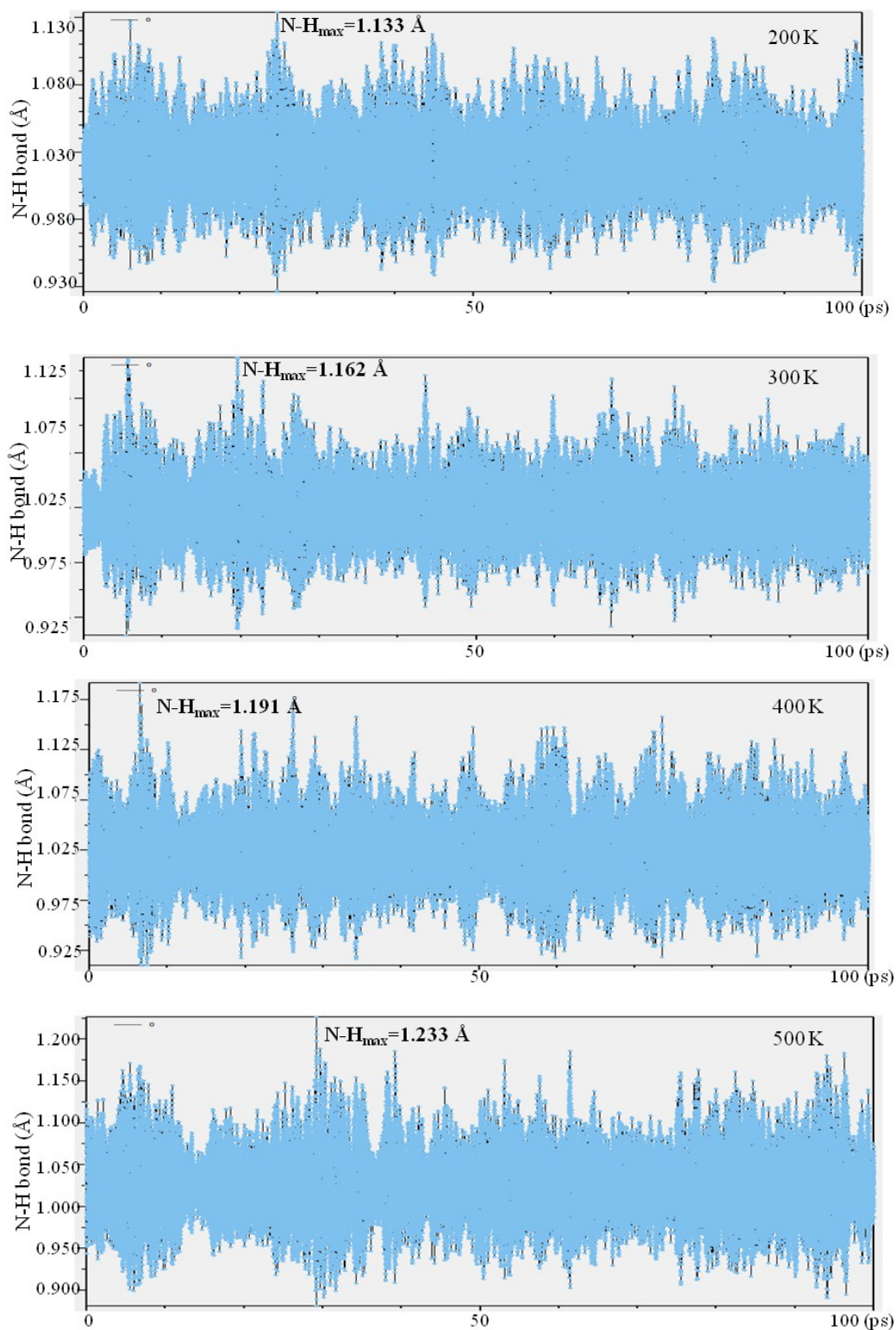**1.65 MP2/aug-cc-pVDZ**
1.72 PM3

31

32 Figure S1. The structure of MSA-MA and the average bond lengths of H-bonds (Å) at four
33 methods. The values at B3LYP-D3/aug-cc-pVDZ and MP2/aug-cc-pVDZ are from ref 54.
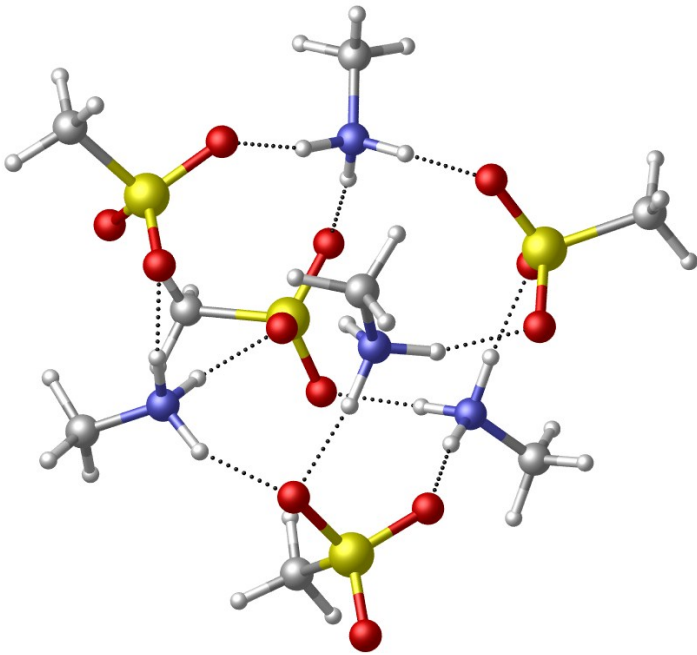
35

36

Figure S2. Key geometrical parameters (Å) and partial charges δ (in atomic units) of (MSA-MA)$_2$ at PBE/cc-pVDZ level.

200 K — N-H$_{max}$=1.133 Å

300 K — N-H$_{max}$=1.162 Å

400 K — N-H$_{max}$=1.191 Å
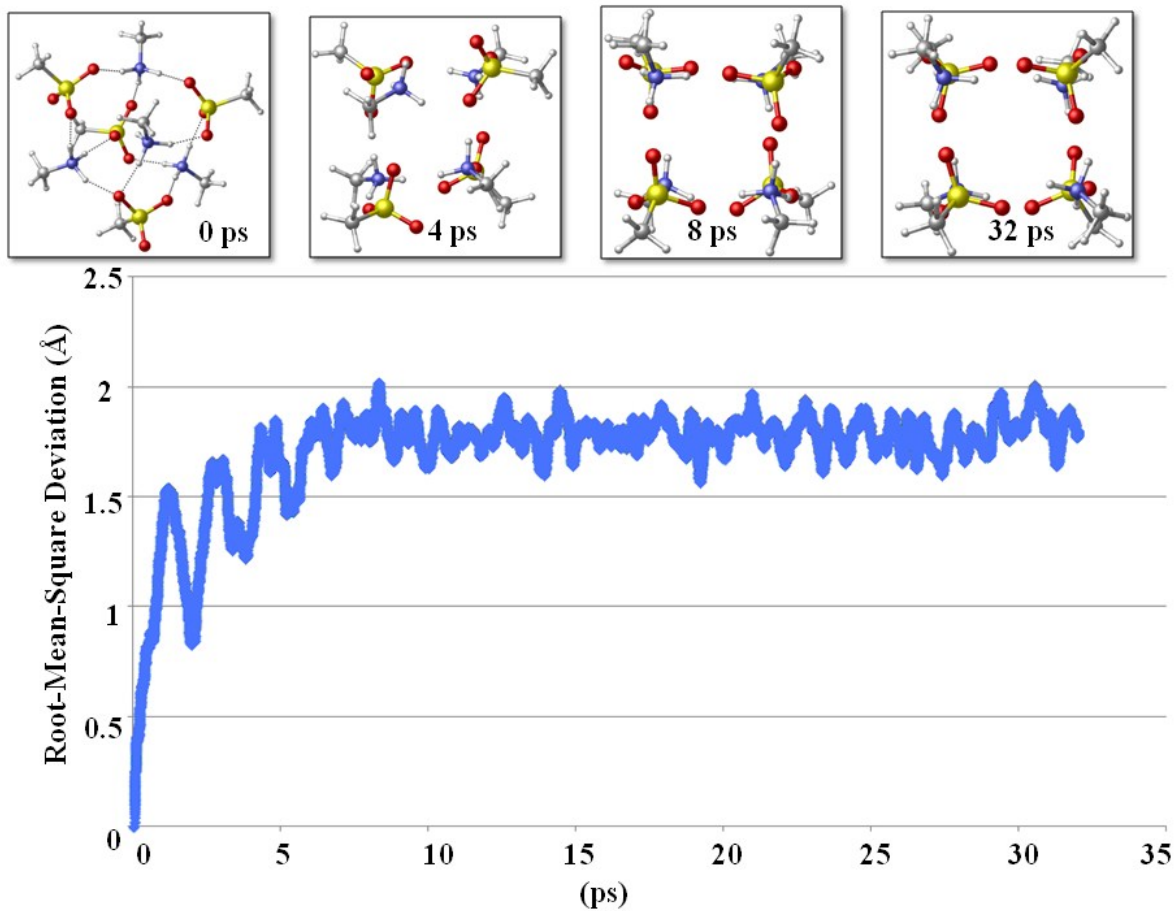
500 K — N-H$_{max}$=1.233 Å

40

41 Figure S3 Bond lengths (Å) of one N-H bond in (MSA-MA)$_4$ from dynamics simulation at four
42 temperatures (200 K, 300 K, 400 K and 500 K) during 100 ps.

43

44   Figure S4. The structure of the second 4MSA-4MA isomer at PBE/cc-pVDZ level.

46

47 Figure S5 The structural evolutions of the second isomer of 4MSA-4MA described by Root-
48 Mean-Square Deviation during 32 ps at 300 K.