



Supplement of

Cluster-to-particle transition in atmospheric nanoclusters

Haide Wu et al.

Correspondence to: Jonas Elm (jelm@chem.au.dk)

The copyright of individual parts of the supplement might differ from the article licence.

Table S1. Binding free energies ΔG_{bind} and size-averaged binding free energy $\Delta G_{\text{bind}}/m$ of $(\text{SA})_n(\text{Base})_n$ clusters (Lowest energy configurations, monomer count $m = 2n, n = 1 \sim 15$).

Monomer Count m	SA-DMA		SA-AM		SA-MA		SA-TMA	
	ΔG_{bind}	$\Delta G_{\text{bind}}/m$	ΔG_{bind}	$\Delta G_{\text{bind}}/m$	ΔG_{bind}	$\Delta G_{\text{bind}}/m$	ΔG_{bind}	$\Delta G_{\text{bind}}/m$
2	-12.209	-6.104	-8.166	-4.083	-9.773	-4.886	-11.216	-5.608
4	-42.431	-10.608	-30.828	-7.707	-37.800	-9.450	-34.788	-8.697
6	-69.758	-11.626	-54.908	-9.151	-66.329	-11.055	-51.874	-8.646
8	-97.628	-12.203	-82.281	-10.285	-96.796	-12.100	-78.304	-9.788
10	-125.943	-12.594	-109.191	-10.919	-126.638	-12.664	-94.996	-9.500
12	-154.808	-12.901	-137.574	-11.465	-161.491	-13.458	-117.489	-9.791
14	-180.523	-12.895	-167.116	-11.937	-191.728	-13.695	-135.217	-9.658
16	-207.598	-12.975	-196.250	-12.266	-224.950	-14.059	-156.430	-9.777
18	-237.180	-13.177	-228.335	-12.685	-254.913	-14.162	-182.792	-10.155
20	-264.325	-13.216	-256.266	-12.813	-288.369	-14.418	-204.435	-10.222
22	-288.533	-13.115	-281.994	-12.818	-322.734	-14.670	-224.055	-10.184
24	-320.280	-13.345	-313.074	-13.045	-352.506	-14.688	-246.493	-10.271
26	-348.137	-13.390	-337.161	-12.968	-383.187	-14.738	-265.303	-10.204
28	-372.227	-13.294	-368.948	-13.177	-415.376	-14.835	-284.866	-10.174
30	-402.285	-13.409	-394.024	-13.134	-447.527	-14.918	-303.211	-10.107

Table S2. Binding free energies ΔG_{bind} of $(\text{SA})_n(\text{Base})_n$ clusters (thermal averaged by configurations, monomer count $m = 2n, n = 1 \sim 15$).

Monomer Count m	SA-DMA	SA-AM	SA-MA	SA-TMA
2	-12.209	-8.166	-9.773	-11.216
4	-42.650	-30.992	-37.976	-34.788
6	-70.372	-55.312	-66.565	-52.311
8	-97.787	-82.874	-97.101	-78.362
10	-126.510	-109.538	-127.144	-95.330
12	-155.499	-137.958	-161.886	-118.001
14	-181.120	-167.771	-192.437	-135.259
16	-207.614	-196.791	-224.986	-156.635
18	-237.561	-228.720	-255.359	-183.054
20	-264.561	-256.340	-288.672	-204.491
22	-288.788	-282.219	-323.091	-224.484
24	-320.294	-313.223	-352.618	-247.057
26	-348.541	-337.389	-383.600	-265.490
28	-372.436	-368.999	-415.691	-284.993
30	-402.738	-394.181	-447.846	-303.439

Table S3. Binding free energies ΔG_{bind} of $(\text{SA})_n(\text{Base})_n$ clusters (four lowest energy configurations, monomer count $m = 2n$, $n = 1 \sim 8$).

Monomer Count m	SA-DMA	SA-AM	SA-MA	SA-TMA
2	-12.209	-8.166	-9.773	-11.216
2				
2				
2				
4	-37.696	-29.700	-37.172	-29.776
4	-40.737	-29.784	-37.800	-34.788
4	-41.874	-30.828		
4	-42.431			
6	-68.917	-52.860	-63.549	-50.590
6	-68.923	-53.663	-65.015	-50.724
6	-69.694	-54.780	-65.725	-51.203
6	-69.758	-54.908	-66.329	-51.874
8	-95.469	-81.083	-95.402	-74.874
8	-95.880	-81.988	-95.976	-75.440
8	-96.247	-82.212	-96.067	-76.882
8	-97.628	-82.281	-96.796	-78.304
10	-124.873	-107.517	-125.622	-93.553
10	-124.991	-108.299	-125.831	-93.890
10	-125.056	-108.787	-126.000	-94.139
10	-125.943	-109.191	-126.638	-94.996
12	-153.877	-136.098	-160.474	-116.340
12	-153.946	-136.416	-160.784	-116.523
12	-154.300	-137.197	-160.829	-117.338
12	-154.808	-137.574	-161.491	-117.489
14	-179.810	-166.355	-191.220	-131.630
14	-180.074	-166.533	-191.298	-132.640
14	-180.161	-166.928	-191.500	-133.453
14	-180.523	-167.116	-191.728	-135.217
16	-204.181	-195.274	-222.043	-154.504
16	-204.334	-195.456	-222.145	-155.144
16	-204.691	-196.007	-222.995	-155.254
16	-207.598	-196.250	-224.950	-156.430

Table S4. Binding free energies ΔG_{bind} of $(\text{SA})_n(\text{Base})_n$ clusters (four lowest energy configurations, monomer count $m = 2n$, $n = 9 \sim 15$).

Monomer Count m	SA-DMA	SA-AM	SA-MA	SA-TMA
18	-235.665	-227.000	-253.660	-180.888
18	-236.082	-227.468	-253.951	-181.213
18	-236.625	-227.741	-254.101	-182.228
18	-237.180	-228.335	-254.913	-182.792
20	-262.824	-253.764	-286.936	-201.569
20	-262.926	-254.473	-287.440	-202.415
20	-263.228	-254.544	-287.674	-202.695
20	-264.325	-256.266	-288.369	-204.435
22	-287.161	-279.301	-320.817	-221.999
22	-287.280	-279.467	-320.886	-223.379
22	-287.482	-281.469	-322.549	-223.821
22	-288.533	-281.994	-322.734	-224.055
24	-316.966	-311.012	-350.430	-245.640
24	-317.138	-311.794	-350.442	-245.666
24	-317.435	-311.803	-350.864	-246.146
24	-320.280	-313.074	-352.506	-246.493
26	-346.227	-335.598	-381.153	-260.385
26	-346.460	-335.851	-381.289	-262.671
26	-348.056	-336.184	-383.136	-264.695
26	-348.137	-337.161	-383.187	-265.303
28	-370.165	-362.961	-412.315	-281.602
28	-370.928	-365.580	-414.138	-283.107
28	-371.393	-367.498	-415.040	-283.863
28	-372.227	-368.948	-415.376	-284.866
30	-400.950	-391.275	-445.279	-301.338
30	-401.865	-391.705	-446.564	-301.598
30	-401.876	-393.251	-447.074	-302.495
30	-402.285	-394.024	-447.527	-303.211