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A Surprisingly High Enhancing Potential of Nitric Acid in Sulfuric Acid–Methylamine Nucleation

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Table S1. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-MA system and SA-MA system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecules cm^{-3}).

Table S2. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-DMA system and SA-DMA system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecules cm^{-3}).

Table S3. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-A system and SA-A system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecule cm^{-3}).

Table S4. Coordinates of all optimized $(NA)_x(SA)_y(MA)_z$ ($1 \le x$, $1 \le y$, $x + y \le 3$, $1 \le z \le 3$), $(NA)_x(SA)_y(DMA)_z$ ($1 \le x$, $1 \le y$, $1 \le z \le x + y \le 3$) and $(NA)_x(SA)_y(A)_z$ ($1 \le x$, $1 \le y$, $1 \le z \le x + y \le 3$) clusters.

Table S5. Single point energies (kcal mol^{-1}) at the DLPNO-CCSD(T)/aug-cc-pVTZ level and the corresponding Gibbs free energy correction G_{corr} (kcal mol^{-1}) and Gibbs free energy G (kcal mol^{-1}) at 298.15K for all the most stable configurations of the NA-SA-MA, NA-SA-DMA and NA-SA-A systems.

Figure S1. Lowest Gibbs free energy conformations of the $(NA)_{1-3}(MA)_{1-3}$ clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, 298.15 K and 1 atm. The dashed red lines indicate hydrogen bonds.

Figure S2. Formation free energy (ΔG) of (A) $(NA)_x(SA)_y(MA)_z$ ($1 \le x$, $1 \le y$, $x + y \le 3$, $1 \le z \le 3$), (B) $(NA)_x(SA)_y(A)_z$ ($x \ge 1$, $y \ge 1$, $1 \le z \le x + y \le 3$) and (C) $(NA)_x(SA)_y(DMA)_z$ ($x \ge 1$, $y \ge 1$, $1 \le z \le x + y \le 3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, 298.15 K and 1 atm.

Figure S3. Cluster growth pathways for the NA-SA-MA system at (A) 238.15 K, [NA] = 10^{10} molecules cm^{-3}, [SA] = 10^6 molecules cm^{-3} and [MA] = 10^8 molecules cm^{-3}, (B) 278.15 K, [NA] = 10^{12} molecules cm^{-3}, [SA] = 10^6 molecules cm^{-3} and [MA] = 10^8 molecules cm^{-3}.

Table S1. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-MA system and SA-MA system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecules cm^{-3}).

T	[NA]	[SA]	[MA]	$J_{NA\text{-}SA\text{-}MA}$	$J_{SA\text{-}MA}$	r
238.15	1.00E+10	1.00E+06	1.00E+08	3.41E-01	8.93E-05	3818.8
238.15	1.00E+10	1.00E+06	1.00E+09	3.88E+01	2.70E-03	14369.1
238.15	1.00E+10	1.00E+07	1.00E+08	1.76E+02	6.37E-01	276.1
238.15	1.00E+10	1.00E+07	1.00E+09	5.13E+03	1.72E+01	297.6
258.15	1.00E+10	1.00E+06	1.00E+08	2.15E-03	2.75E-07	7796.5
258.15	1.00E+10	1.00E+06	1.00E+09	1.44E-01	2.91E-05	4942.9
258.15	1.00E+10	1.00E+07	1.00E+08	1.43E+00	2.15E-03	662.4
258.15	1.00E+10	1.00E+07	1.00E+09	7.90E+01	2.20E-01	359.7
278.15	1.00E+10	1.00E+06	1.00E+08	1.26E-05	8.03E-10	15698.5
278.15	1.00E+10	1.00E+06	1.00E+09	9.40E-04	1.27E-07	7391.2
278.15	1.00E+10	1.00E+07	1.00E+08	9.41E-03	6.70E-06	1404.1
278.15	1.00E+10	1.00E+07	1.00E+09	6.81E-01	9.99E-04	682.1
298.15	1.00E+10	1.00E+06	1.00E+08	1.83E-09	8.46E-14	21570.9
298.15	1.00E+10	1.00E+06	1.00E+09	9.03E-07	6.29E-11	14370.1
298.15	1.00E+10	1.00E+07	1.00E+08	1.70E-06	8.33E-10	2036.2
298.15	1.00E+10	1.00E+07	1.00E+09	7.73E-04	5.78E-07	1337.5
278.15	1.00E+08	1.00E+06	1.00E+08	1.59E-07	8.03E-10	197.6
278.15	1.00E+08	1.00E+06	1.00E+09	2.01E-05	1.27E-07	157.9
278.15	1.00E+08	1.00E+07	1.00E+08	1.25E-04	6.70E-06	18.7
278.15	1.00E+08	1.00E+07	1.00E+09	1.58E-02	9.99E-04	15.8
278.15	1.00E+09	1.00E+06	1.00E+08	1.39E-06	8.03E-10	1731.5
278.15	1.00E+09	1.00E+06	1.00E+09	1.57E-04	1.27E-07	1231.7
278.15	1.00E+09	1.00E+07	1.00E+08	1.05E-03	6.70E-06	156.5
278.15	1.00E+09	1.00E+07	1.00E+09	1.17E-01	9.99E-04	117.0
278.15	1.00E+11	1.00E+06	1.00E+08	8.87E-05	8.03E-10	110366.9
278.15	1.00E+11	1.00E+06	1.00E+09	5.84E-03	1.27E-07	45913.6
278.15	1.00E+11	1.00E+07	1.00E+08	6.46E-02	6.70E-06	9630.9
278.15	1.00E+11	1.00E+07	1.00E+09	3.83E+00	9.99E-04	3838.0
278.15	1.00E+12	1.00E+06	1.00E+08	6.76E-04	8.03E-10	841918.9
278.15	1.00E+12	1.00E+06	1.00E+09	1.26E-01	1.27E-07	993776.4
278.15	1.00E+12	1.00E+07	1.00E+08	4.55E-01	6.70E-06	67895.6
278.15	1.00E+12	1.00E+07	1.00E+09	3.63E+01	9.99E-04	36335.5

Table S2. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-DMA system and SA-DMA system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecules cm^{-3}).

T	[NA]	[SA]	[DMA]	$J_{NA\text{-}SA\text{-}DMA}$	$J_{SA\text{-}DMA}$	r
238.15	1.00E+10	1.00E+06	1.00E+08	6.24E+01	3.06E+01	2.0
238.15	1.00E+10	1.00E+06	1.00E+09	3.35E+04	1.23E+04	2.7
238.15	1.00E+10	1.00E+07	1.00E+08	2.61E+04	2.46E+04	1.1
238.15	1.00E+10	1.00E+07	1.00E+09	7.63E+05	6.49E+05	1.2
258.15	1.00E+10	1.00E+06	1.00E+08	1.70E+01	1.60E+01	1.1
258.15	1.00E+10	1.00E+06	1.00E+09	9.64E+03	8.58E+03	1.1
258.15	1.00E+10	1.00E+07	1.00E+08	1.98E+04	1.97E+04	1.0
258.15	1.00E+10	1.00E+07	1.00E+09	6.25E+05	6.16E+05	1.0
278.15	1.00E+10	1.00E+06	1.00E+08	2.32E-01	2.29E-01	1.0
278.15	1.00E+10	1.00E+06	1.00E+09	6.83E+01	6.43E+01	1.1
278.15	1.00E+10	1.00E+07	1.00E+08	1.17E+03	1.17E+03	1.0
278.15	1.00E+10	1.00E+07	1.00E+09	9.61E+04	9.56E+04	1.0
298.15	1.00E+10	1.00E+06	1.00E+08	2.20E-03	2.19E-03	1.0
298.15	1.00E+10	1.00E+06	1.00E+09	1.84E-01	1.82E-01	1.0
298.15	1.00E+10	1.00E+07	1.00E+08	1.57E+01	1.57E+01	1.0
298.15	1.00E+10	1.00E+07	1.00E+09	1.02E+03	1.02E+03	1.0
278.15	1.00E+08	1.00E+06	1.00E+08	2.29E-01	2.29E-01	1.0
278.15	1.00E+08	1.00E+06	1.00E+09	6.43E+01	6.43E+01	1.0
278.15	1.00E+08	1.00E+07	1.00E+08	1.17E+03	1.17E+03	1.0
278.15	1.00E+08	1.00E+07	1.00E+09	9.56E+04	9.56E+04	1.0
278.15	1.00E+09	1.00E+06	1.00E+08	2.29E-01	2.29E-01	1.0
278.15	1.00E+09	1.00E+06	1.00E+09	6.47E+01	6.43E+01	1.0
278.15	1.00E+09	1.00E+07	1.00E+08	1.17E+03	1.17E+03	1.0
278.15	1.00E+09	1.00E+07	1.00E+09	9.57E+04	9.56E+04	1.0
278.15	1.00E+11	1.00E+06	1.00E+08	2.54E-01	2.29E-01	1.1
278.15	1.00E+11	1.00E+06	1.00E+09	1.11E+02	6.43E+01	1.7
278.15	1.00E+11	1.00E+07	1.00E+08	1.18E+03	1.17E+03	1.0
278.15	1.00E+11	1.00E+07	1.00E+09	1.00E+05	9.56E+04	1.0
278.15	1.00E+12	1.00E+06	1.00E+08	7.08E-01	2.29E-01	3.1
278.15	1.00E+12	1.00E+06	1.00E+09	1.56E+03	6.43E+01	24.2
278.15	1.00E+12	1.00E+07	1.00E+08	1.30E+03	1.17E+03	1.1
278.15	1.00E+12	1.00E+07	1.00E+09	1.46E+05	9.56E+04	1.5

Table S3. Cluster formation rates (J, cm^{-3} s^{-1}) of NA-SA-A system and SA-A system, and the enhancement factor r at different temperatures (K) and precursor concentrations (molecule cm^{-3}).

T	[NA]	[SA]	[A]	$J_{NA\text{-}SA\text{-}A}$	$J_{SA\text{-}A}$	r
238.15	1.00E+10	1.00E+06	1.00E+10	6.35E-03	5.51E-05	115.3
238.15	1.00E+10	1.00E+07	1.00E+10	8.85E+00	4.36E-01	20.3
258.15	1.00E+10	1.00E+06	1.00E+10	9.79E-09	4.82E-09	2.0
258.15	1.00E+10	1.00E+07	1.00E+10	6.10E-05	4.13E-05	1.5
278.15	1.00E+10	1.00E+06	1.00E+10	1.53E-14	1.42E-14	1.1
278.15	1.00E+10	1.00E+07	1.00E+10	1.43E-10	1.42E-10	1.0
298.15	1.00E+10	1.00E+06	1.00E+10	8.76E-20	8.58E-20	1.0
298.15	1.00E+10	1.00E+07	1.00E+10	8.58E-16	8.58E-16	1.0
278.15	1.00E+08	1.00E+06	1.00E+10	1.42E-14	1.42E-14	1.0
278.15	1.00E+08	1.00E+07	1.00E+10	1.42E-10	1.42E-10	1.0
278.15	1.00E+09	1.00E+06	1.00E+10	1.42E-14	1.42E-14	1.0
278.15	1.00E+09	1.00E+07	1.00E+10	1.42E-10	1.42E-10	1.0
278.15	1.00E+11	1.00E+06	1.00E+10	1.09E-13	1.42E-14	7.7
278.15	1.00E+11	1.00E+07	1.00E+10	1.56E-10	1.42E-10	1.1
278.15	1.00E+12	1.00E+06	1.00E+10	9.47E-12	1.42E-14	665.8
278.15	1.00E+12	1.00E+07	1.00E+10	1.13E-09	1.42E-10	7.9

Table S4. Coordinates of all optimized $(NA)_x(SA)_y(MA)_z$ ($1 \le x$, $1 \le y$, $x + y \le 3$, $1 \le z \le 3$), $(NA)_x(SA)_y(DMA)_z$ ($1 \le x$, $1 \le y$, $1 \le z \le x + y \le 3$) and $(NA)_x(SA)_y(A)_z$ ($1 \le x$, $1 \le y$, $1 \le z \le x + y \le 3$) clusters.

$(NA)_1(SA)_1(MA)_1$

S	-1.763993	-0.540643	-0.095694
O	-1.313723	-0.549069	1.483712
O	-2.313648	0.815115	-0.333043
H	-1.021023	1.789988	-0.665148
H	-1.989379	-1.030175	1.979839
O	-0.443346	-0.651846	-0.776703
O	-2.68498	-1.643031	-0.265959
O	2.262357	0.553079	-0.329879
O	1.80602	-1.582745	-0.053336
H	0.889422	-1.215771	-0.311821
O	3.804684	-0.847613	0.264068
N	2.675333	-0.571573	-0.037919
N	-0.037345	2.176958	-0.631046
C	0.231219	2.725458	0.721369
H	0.577717	1.365048	-0.799787
H	-0.417295	3.583327	0.895225
H	1.279944	3.008782	0.797977
H	0.004713	1.942588	1.444791
H	0.107649	2.864945	-1.36631

$(NA)_1(SA)_1(MA)_2$

S	-2.070602	0.00165	-0.061157
O	-3.502245	0.001971	0.705947
O	-2.052668	1.236009	-0.877959
H	-0.541036	2.06901	-0.691216
H	-4.203162	0.005274	0.03993
O	-1.091968	-0.001457	1.027829
O	-2.055126	-1.229922	-0.882169
O	1.759748	-0.001126	-0.884451
O	3.325614	-1.088074	0.150571
H	0.746068	-3.058054	-1.126769
O	3.326918	1.086244	0.148171
N	2.845344	-0.001014	-0.171682
N	0.443924	-2.329564	-0.484318
C	0.597968	-2.743503	0.932289
H	1.021824	-1.466373	-0.675212
H	0.033214	-3.65942	1.10694
H	0.19957	-1.938149	1.548238
H	1.656853	-2.891848	1.139581
H	-0.5449	-2.065391	-0.692312

N	0.448737	2.329884	-0.483578
C	0.605692	2.737219	0.934686
H	1.024238	1.46598	-0.678393
H	0.04432	3.654354	1.113798
H	1.665397	2.880681	1.141318
H	0.205021	1.930582	1.547501
H	0.752043	3.060352	-1.123217

$(NA)_1(SA)_1(MA)_3$

N	-1.736883	1.925536	-0.012661
O	-0.981804	1.732943	-1.040375
O	-1.322028	2.656133	0.896729
O	-2.830094	1.353411	0.032356
H	-1.320236	-0.004745	-1.40304
S	1.892678	-1.082733	-0.125394
O	1.037196	-0.476175	0.910374
O	1.18066	-1.971136	-1.061223
O	2.869605	-2.051404	0.742993
O	2.767744	-0.100082	-0.795741
H	0.556048	2.103577	-0.449669
H	3.424233	-2.54835	0.12642
N	-1.468211	-1.027577	-1.31065
C	-2.544379	-1.499663	-2.197125
H	-0.558823	-1.490582	-1.465564
H	-3.456823	-0.954597	-1.954186
H	-2.700903	-2.567608	-2.04139
H	-2.279008	-1.319032	-3.239249
H	-1.705564	-1.186278	-0.27567
N	1.450366	2.182544	0.099127
C	1.817489	3.589451	0.344299
H	1.25386	1.661908	0.958991
H	2.010982	4.076396	-0.611189
H	2.710457	3.634531	0.967896
H	0.979189	4.076988	0.840976
H	2.169526	1.615014	-0.380699
N	-1.829319	-1.239234	1.417758
C	-2.234172	-2.437124	2.154433
H	-0.855836	-1.003964	1.612606
H	-3.275654	-2.675525	1.922561
H	-2.138938	-2.334196	3.242558
H	-1.614938	-3.280005	1.836529
H	-2.395945	-0.434184	1.672872

$(NA)_2(SA)_1(MA)_1$

S	-0.477653	1.555334	0.550439
O	0.28103	2.977302	0.595651
O	-0.29539	1.013954	1.89947
H	0.086689	-0.692816	1.728593
H	-0.11725	3.559722	-0.066419
O	-1.862348	1.865112	0.150997
O	0.212537	0.728941	-0.478117
O	-2.251008	-1.252228	0.155041
O	-3.157313	0.120214	-1.291028
H	-2.674209	0.751475	-0.666714
O	-3.255887	-2.009488	-1.615477
N	-2.869833	-1.125026	-0.900459
O	2.688126	-1.196165	-0.23822
O	2.652079	0.742214	-1.283094
H	1.711369	0.706266	-0.908858
O	4.43025	-0.471884	-1.3031
N	3.29752	-0.372267	-0.922739
N	0.312197	-1.605602	1.278112
C	0.787224	-2.626202	2.23744
H	-0.543423	-1.882518	0.783512
H	1.693747	-2.258994	2.716499
H	1.003692	-3.551149	1.704367
H	0.015299	-2.799069	2.986448
H	1.027398	-1.384566	0.569529

$(NA)_2(SA)_1(MA)_2$

S	2.229663	-0.251122	-0.131187
O	1.651521	0.316219	1.127584
O	3.818858	-0.363217	0.138253
H	3.974077	-1.053166	0.797737
H	0.378016	-0.2965	1.74161
O	1.763681	-1.6317	-0.359123
O	2.137428	0.667594	-1.258641
O	-0.465332	-0.771174	2.066081
O	-1.038775	1.3397	2.284498
H	0.602774	2.324139	0.750877
O	-2.499765	-0.246318	2.564053
N	-1.400127	0.177479	2.318425
O	-1.361054	0.3276	-0.55953
O	-2.056788	-0.75297	-2.30325
H	-1.419862	-1.896287	-1.182791
O	-1.737797	1.392832	-2.410674

N	-1.727388	0.337436	-1.784471
N	0.219693	2.456999	-0.187508
C	-0.370929	3.791087	-0.411092
H	0.973805	2.211595	-0.842358
H	-1.137169	3.962241	0.34451
H	-0.828109	3.797646	-1.399687
H	0.401246	4.557191	-0.341364
H	-0.49993	1.691759	-0.309631
N	-0.900829	-2.416235	-0.433896
C	-1.076145	-3.879934	-0.50905
H	0.098462	-2.136133	-0.505672
H	-2.135286	-4.121066	-0.422042
H	-0.520369	-4.354875	0.299214
H	-0.697767	-4.231208	-1.468448
H	-1.217304	-2.022572	0.456044

$(NA)_2(SA)_1(MA)_3$

N	-1.493394	1.940803	0.810025
O	-1.92085	2.257073	-0.317599
O	-2.143095	1.174885	1.556065
O	-0.378887	2.380156	1.195958
H	1.904597	1.85617	-0.823833
N	2.98139	-0.20625	-0.523754
O	3.017722	-0.051995	-1.746195
O	2.996392	0.816874	0.239573
O	2.886379	-1.336932	0.000657
H	1.643168	-2.265543	-0.866146
S	-0.356489	-1.827566	-0.306348
O	0.751482	-2.564452	-1.175785
O	-0.081393	-2.103354	1.116469
O	-0.25675	-0.366354	-0.5889
O	-1.629459	-2.384685	-0.799136
H	-2.760562	-1.1547	-0.645993
H	1.928357	0.332401	1.605498
N	0.97756	1.990898	-1.266919
C	1.074004	2.530494	-2.636344
H	0.406835	2.562931	-0.630296
H	1.680484	1.848185	-3.230542
H	0.072332	2.615749	-3.056617
H	1.545441	3.512474	-2.604994
H	0.540476	1.049657	-1.245435
N	1.101122	0.145452	2.206529
C	1.471176	-0.022562	3.62507

H	0.645713	-0.716552	1.83152
H	1.93382	0.893008	3.993481
H	0.574296	-0.241724	4.203868
H	2.174789	-0.850318	3.708662
H	0.450937	0.934555	2.057325
N	-3.314653	-0.274074	-0.496626
C	-4.771858	-0.479912	-0.608246
H	-2.963039	0.423349	-1.155793
H	-5.082936	-1.200982	0.146772
H	-5.285213	0.467817	-0.446764
H	-5.007137	-0.869098	-1.59852
H	-3.034976	0.128027	0.422852

$(NA)_1(SA)_2(MA)_1$

S	-0.185159	2.04559	0.368374
O	0.692363	2.481302	-0.854893
O	0.840205	1.802023	1.532536
H	1.366812	0.959964	1.371708
H	1.383279	1.787398	-1.067995
O	-1.04907	3.130594	0.719114
O	-0.794627	0.734733	0.051579
S	2.524918	-0.639081	-0.429511
O	1.864758	-1.761386	-1.092097
O	4.057688	-1.107273	-0.31376
H	4.61134	-0.333228	-0.138096
H	0.262251	-2.135907	-0.256502
O	2.549903	0.640251	-1.1605
O	2.033265	-0.450323	0.973784
O	-3.004948	-1.436669	0.078781
O	-3.309662	0.569473	-0.774276
H	-2.363529	0.618716	-0.451463
O	-4.922752	-0.859056	-0.751486
N	-3.779627	-0.648548	-0.464795
N	-0.29199	-2.060711	0.614883
C	-0.533489	-3.380546	1.239244
H	0.297205	-1.447334	1.192343
H	-1.152297	-3.978669	0.571978
H	-1.050264	-3.238192	2.187329
H	0.42437	-3.872724	1.403275
H	-1.170041	-1.565418	0.409279

$(NA)_1(SA)_2(MA)_2$

S	-2.539468	-1.321708	-0.519993

O	-3.472398	-0.463943	0.243879
O	-3.457435	-2.319856	-1.398905
H	-4.000785	-1.792893	-2.000407
H	-3.023614	1.171061	0.189379
O	-1.75442	-0.522904	-1.488567
O	-1.751583	-2.252589	0.290928
S	0.639545	1.563798	-0.133262
O	0.059915	1.032567	1.129592
O	0.744394	0.30308	-1.124172
H	-0.169198	-0.016713	-1.350558
H	-0.123877	-1.997369	0.834213
O	-0.265247	2.550972	-0.752657
O	2.033932	2.006549	-0.011447
O	3.33106	-0.87288	0.462632
O	4.084915	0.697234	-0.870918
H	3.262495	1.140988	-0.478422
O	5.044573	-1.230582	-0.820401
N	4.158221	-0.543992	-0.385576
N	-2.776095	2.188968	0.207932
C	-2.692964	2.677953	1.605406
H	-1.843094	2.311464	-0.262245
H	-3.636629	2.484711	2.114918
H	-2.473724	3.745452	1.600331
H	-1.87733	2.140899	2.08795
H	-3.477081	2.692928	-0.330801
N	0.744986	-1.618086	1.258401
C	1.102702	-2.29788	2.520248
H	1.512258	-1.659287	0.581896
H	0.280069	-2.186226	3.225807
H	2.006782	-1.842641	2.922948
H	1.277381	-3.355427	2.325405
H	0.555246	-0.600239	1.392735

$(NA)_1(SA)_2(MA)_3$

N	2.212679	1.963693	0.169625
O	1.176287	2.682487	0.173533
O	2.634281	1.518877	-0.929611
O	2.783087	1.6859	1.231851
H	-0.010677	0.400148	1.549128
S	-3.133819	-0.152023	0.125672
O	-4.559422	-0.11549	0.334406
O	-2.487982	1.208332	0.032328
O	-2.914874	-0.815825	-1.324277

O	-2.34371	-0.978129	1.08334
H	-1.252703	-2.183162	0.757466
H	-1.974095	-1.094395	-1.41783
S	0.540515	-1.782892	-0.291446
O	-0.22138	-1.220322	-1.443347
O	-0.456098	-2.727634	0.49244
O	0.962715	-0.697378	0.638335
O	1.673893	-2.625143	-0.6849
H	3.168886	-1.646733	-0.327155
H	-0.140163	0.551777	-1.764672
N	-0.462777	1.536018	-1.791577
C	-0.649139	2.014359	-3.175838
H	-1.347592	1.533158	-1.239834
H	0.309084	1.989269	-3.69378
H	-1.031748	3.034396	-3.155184
H	-1.363633	1.365808	-3.682195
H	0.224784	2.099069	-1.256781
N	3.683717	-0.838003	0.071455
C	5.142728	-1.029676	0.179269
H	3.431774	0.012287	-0.480562
H	5.351371	-1.900337	0.800436
H	5.582116	-0.137989	0.625578
H	5.556639	-1.183853	-0.816684
H	3.238088	-0.654008	0.974085
N	-0.501736	1.229359	1.940729
C	-0.91247	1.009802	3.342346
H	0.13475	2.022462	1.802468
H	-1.595721	0.16104	3.36117
H	-1.416788	1.900244	3.716918
H	-0.030529	0.799955	3.947128
H	-1.325248	1.359727	1.313597

$(NA)_1(SA)_1(DMA)_1$

S	-1.845105	-0.620669	-0.070256
O	-0.53684	-1.01474	-0.608455
O	-2.919718	-1.565383	-0.076857
O	-2.324134	0.66731	-0.850569
O	-1.627497	-0.106675	1.403533
H	-1.633752	1.375636	-0.785876
H	-0.826638	0.502304	1.423456
N	0.742887	1.852948	0.077844
O	0.606172	1.220813	1.169794
H	1.135511	-0.932547	-0.158256

O	1.874859	1.899558	-0.440306
O	-0.237519	2.383867	-0.468115
N	2.167908	-0.830952	-0.086102
H	2.320787	0.19877	-0.132188
C	2.792461	-1.482449	-1.258592
H	2.56706	-2.549205	-1.237797
H	2.378693	-1.036167	-2.162396
H	3.871389	-1.326344	-1.225128
C	2.619785	-1.342866	1.226501
H	2.106101	-0.776884	2.002705
H	2.373167	-2.402542	1.302547
H	3.697754	-1.202415	1.315175

$(NA)_1(SA)_1(DMA)_2$

S	-0.014576	1.832225	-0.179359
O	-1.469363	1.92957	-0.436506
O	0.707566	3.066938	0.035314
O	0.649241	1.212323	-1.527191
O	0.225238	0.779576	0.867191
H	0.128084	0.432222	-1.818004
H	1.579227	-0.064555	0.745712
N	-0.000543	-1.887478	-0.957871
O	-0.756402	-1.202608	-1.685787
H	-2.13777	0.475611	0.106204
O	-0.405793	-2.274957	0.16506
O	1.16252	-2.15188	-1.329808
N	2.461923	-0.623912	0.566119
H	2.179294	-1.319665	-0.151215
C	2.863552	-1.321061	1.802856
H	3.042372	-0.58268	2.58593
H	2.055047	-1.990195	2.097425
H	3.772906	-1.896286	1.620681
C	3.474607	0.29906	0.006987
H	3.054816	0.756413	-0.889126
H	3.688566	1.075335	0.742881
H	4.383353	-0.255262	-0.233388
N	-2.491752	-0.401241	0.5611
H	-1.721456	-1.094432	0.461163
C	-3.673785	-0.892966	-0.172751
H	-4.451809	-0.128451	-0.154358
H	-3.370768	-1.097206	-1.199313
H	-4.038715	-1.808346	0.296226
C	-2.717706	-0.114763	1.991638

H	-1.784942	0.270349	2.403745
H	-3.501639	0.638049	2.086986
H	-3.014812	-1.031396	2.504189

$(NA)_2(SA)_1(DMA)_1$

N	-2.739257	0.671563	-0.096972
O	-2.200523	0.682871	1.063998
H	0.118529	1.199834	0.00315
O	-2.735266	1.725142	-0.750214
O	-3.223614	-0.377434	-0.541263
N	3.034552	-0.004803	0.043739
O	3.159489	-1.285887	-0.354024
H	2.363422	-1.773581	-0.013047
O	2.16894	0.250939	0.866678
O	3.807122	0.770307	-0.461227
N	-0.02705	2.219685	-0.059488
H	-1.035763	2.308457	-0.29069
C	0.805306	2.72754	-1.174509
H	1.85662	2.561181	-0.934873
H	0.539323	2.180802	-2.078983
H	0.613188	3.792292	-1.310474
C	0.245936	2.850715	1.252306
H	-0.44093	2.423066	1.981472
H	1.278729	2.64177	1.530139
H	0.081122	3.925416	1.166943
S	-0.304789	-1.734221	0.003759
O	-0.112776	-0.497973	-0.750442
O	0.830282	-2.623829	0.143839
O	-1.455895	-2.565508	-0.685476
O	-0.855203	-1.405508	1.419749
H	-2.239689	-1.97305	-0.76627
H	-1.503546	-0.59826	1.361823

$(NA)_2(SA)_1(DMA)_2$

S	-0.363647	-2.382178	-0.530081
O	-1.234401	-2.602402	0.769825
O	-0.589324	-3.523704	-1.371858
O	0.990249	-1.996655	-0.158475
O	-1.057962	-1.095525	-1.154029
H	2.306459	-0.128833	1.10043
H	-0.357785	-0.390416	-1.380395
N	0.428735	1.898953	-1.614078
O	0.760953	0.657268	-1.558959

H	-2.037594	0.602427	0.860689
O	-0.783388	2.181964	-1.709764
O	1.303898	2.749039	-1.573354
N	0.069416	0.267225	1.984575
O	-1.087579	-0.275012	2.037627
H	-1.108294	-1.839749	1.397105
O	1.042457	-0.333026	2.457307
O	0.181736	1.376392	1.438295
N	-2.544907	1.215471	0.186065
H	-1.862912	1.426861	-0.570968
C	-2.865464	2.487214	0.870701
H	-3.568558	2.290395	1.681357
H	-1.937973	2.896594	1.269506
H	-3.302653	3.181159	0.151842
C	-3.71351	0.50356	-0.374893
H	-3.358286	-0.404032	-0.861039
H	-4.402196	0.253578	0.433546
H	-4.210771	1.14927	-1.100036
N	2.8035	0.261411	0.281238
H	2.063367	0.39913	-0.441635
C	3.799639	-0.707258	-0.227844
H	4.559553	-0.874668	0.537011
H	3.283378	-1.637275	-0.460545
H	4.260762	-0.294784	-1.126094
C	3.364434	1.581882	0.649726
H	2.552844	2.194397	1.039156
H	4.135049	1.441807	1.409449
H	3.783037	2.048466	-0.24174

$(NA)_2(SA)_1(DMA)_3$

S	-0.599047	-0.574069	-1.639981
O	-1.134155	-1.932835	-1.508865
O	0.151198	-0.129627	-0.433
O	-1.641976	0.420905	-2.005347
O	0.452298	-0.547135	-2.833817
H	-2.795058	0.009476	0.863716
H	1.365987	-0.400536	-2.463789
N	2.963802	-0.549809	-0.609559
O	2.73351	0.202513	-1.618795
H	1.062544	1.753839	0.638993
O	3.281631	-0.012523	0.467402
O	2.829873	-1.772644	-0.714081
N	-0.899554	0.952165	1.928674

O	-1.538747	-0.125596	2.146499
H	0.8795	-1.219035	0.805126
O	0.309328	1.011129	2.22971
O	-1.478696	1.911219	1.402947
N	-3.426195	0.097547	0.03935
H	-2.791445	0.336903	-0.76451
C	-4.381086	1.199287	0.275614
H	-5.048256	0.928241	1.095637
H	-3.812804	2.089488	0.541138
H	-4.9595	1.369494	-0.633626
C	-4.057139	-1.211108	-0.244199
H	-3.269003	-1.918529	-0.505174
H	-4.609532	-1.54273	0.636757
H	-4.736213	-1.101569	-1.091006
N	0.717397	-1.862998	1.600941
H	-0.129938	-1.45468	2.028843
C	1.846315	-1.826911	2.555887
H	2.756982	-2.089012	2.018744
H	1.929759	-0.814232	2.945546
H	1.646317	-2.535504	3.361997
C	0.437711	-3.204981	1.03989
H	-0.340979	-3.104906	0.282551
H	1.349811	-3.569154	0.566918
H	0.128957	-3.873762	1.845325
N	1.530958	2.278366	-0.11844
H	1.971402	1.551681	-0.72323
C	2.591105	3.119911	0.472887
H	2.140293	3.821034	1.17668
H	3.295538	2.462861	0.98101
H	3.100334	3.662968	-0.32479
C	0.51543	3.025763	-0.893912
H	-0.222077	2.318943	-1.274283
H	0.027405	3.743545	-0.23414
H	1.011727	3.538354	-1.71973

$(NA)_1(SA)_2(DMA)_1$

S	-2.705907	0.274439	-0.393567
O	-1.551619	1.054142	0.058085
O	-3.902399	0.951323	-0.793183
O	-3.086747	-0.747969	0.743995
O	-2.231346	-0.637615	-1.593478
H	-2.284299	-1.261743	1.028087
H	-1.326576	-1.008476	-1.410218

S	0.42923	-1.677461	0.572199
O	1.162249	-0.553797	1.16246
O	-0.809321	-2.077254	1.232409
O	1.362899	-2.974258	0.687349
O	0.232804	-1.458866	-0.911424
H	2.233589	-2.76077	0.315589
H	1.211567	-0.381056	-1.467969
N	2.942588	0.225778	-0.946116
O	1.76626	0.470284	-1.562235
H	0.239603	1.412809	0.41082
O	3.466969	1.206989	-0.453158
O	3.362762	-0.907982	-0.942752
N	0.838925	2.203311	0.69219
H	1.803748	1.918804	0.487771
C	0.660858	2.399199	2.150993
H	-0.386319	2.637594	2.33699
H	0.923127	1.466726	2.648908
H	1.304122	3.21393	2.485086
C	0.483518	3.377517	-0.138612
H	0.673842	3.128879	-1.181952
H	-0.575922	3.588571	0.002617
H	1.093396	4.229188	0.164808

$(NA)_1(SA)_2(DMA)_2$

S	0.856683	2.508037	-0.434047
O	-0.582241	2.655416	-0.286247
O	1.706787	3.650585	-0.606882
O	1.171587	1.51912	-1.628769
O	1.378625	1.659626	0.819126
H	0.615769	0.690849	-1.508446
H	1.772853	-1.731324	0.46339
S	-0.576787	-1.88801	-1.139702
O	-0.151109	-0.489323	-0.787802
O	0.097586	-2.418938	-2.306486
O	-2.039625	-1.999195	-1.06113
O	0.029895	-2.762832	0.100189
H	-2.565286	-0.471395	-0.183777
H	-0.498346	-2.553659	0.903694
N	-0.43759	-0.490653	2.183182
O	-0.684758	0.749663	2.064936
H	0.592971	1.381498	1.404308
O	0.719496	-0.864273	2.416166
O	-1.363332	-1.309191	2.027807

N	2.521727	-1.042933	0.29012
H	2.048621	-0.129111	0.367789
C	3.058984	-1.22281	-1.082977
H	3.598851	-2.169212	-1.123488
H	2.230411	-1.250084	-1.789248
H	3.727525	-0.39213	-1.308995
C	3.551241	-1.12824	1.353992
H	3.066047	-0.964524	2.314171
H	4.011958	-2.115854	1.321345
H	4.302401	-0.358785	1.173396
N	-2.754131	0.529891	0.014096
H	-1.874184	0.901103	0.403538
C	-3.815469	0.654664	1.03647
H	-4.732847	0.207814	0.651249
H	-3.482436	0.130088	1.930657
H	-3.9741	1.711229	1.254458
C	-3.052027	1.200308	-1.27109
H	-2.209861	1.040774	-1.941896
H	-3.956781	0.761591	-1.693316
H	-3.18161	2.267772	-1.096258

$(NA)_1(SA)_2(DMA)_3$

S	-0.474514	-1.736933	-1.059669
O	-1.599582	-1.756957	-2.011874
O	0.476362	-2.929292	-1.510533
O	-0.902962	-1.975568	0.330408
O	0.341969	-0.490727	-1.172363
H	-2.699941	0.074015	0.256927
H	-0.613102	0.851197	-1.260008
S	-1.002982	2.137171	0.403226
O	-1.583004	0.988999	1.178269
O	-1.756637	3.368994	0.506059
O	-1.149255	1.684275	-1.143989
O	0.456062	2.234553	0.654988
H	-0.259658	-0.278389	1.786359
H	1.649105	1.527632	-0.47102
N	2.91306	-1.309099	0.126156
O	2.385838	-2.410843	0.37993
H	1.289004	-2.899283	-0.947654
O	3.425125	-1.082337	-0.985941
O	2.903995	-0.398796	1.000464
N	2.443696	1.542311	-1.140107
H	2.831718	0.578389	-1.173442

C	3.464944	2.453517	-0.582248
H	3.016884	3.436861	-0.435512
H	3.794091	2.041458	0.371038
H	4.307071	2.515952	-1.273082
C	1.93934	1.929929	-2.474945
H	1.250162	1.157917	-2.814426
H	1.419937	2.885413	-2.393821
H	2.78028	2.010577	-3.165492
N	0.528879	-0.500293	2.419703
H	1.388275	-0.521719	1.829333
C	0.344066	-1.833999	3.032262
H	-0.557709	-1.819926	3.647125
H	0.245617	-2.563808	2.232233
H	1.21552	-2.058647	3.648785
C	0.67258	0.59502	3.404211
H	0.826919	1.525666	2.859682
H	-0.240543	0.661527	3.996955
H	1.526482	0.378545	4.048115
N	-3.404526	-0.395626	-0.360115
H	-2.849467	-0.865109	-1.106941
C	-4.281025	0.643972	-0.941446
H	-4.798058	1.164144	-0.133907
H	-3.654664	1.34965	-1.486782
H	-5.003001	0.175264	-1.611874
C	-4.103607	-1.437181	0.421876
H	-3.353614	-2.147092	0.770708
H	-4.611383	-0.968765	1.266486
H	-4.828841	-1.942279	-0.217766

$(NA)_1(SA)_1(A)_1$

N	-2.910015	0.359662	-0.025069
O	-2.548211	-0.622442	-0.867441
H	-1.584173	-0.831481	-0.697948
O	-2.063273	0.788678	0.757184
O	-4.043922	0.734669	-0.118797
S	1.067781	-0.569887	0.096954
O	2.293337	-1.253166	0.428598
O	-0.032815	-1.310853	-0.511914
O	1.352098	0.657711	-0.814341
O	0.531216	0.065536	1.453145
H	-0.396078	0.358429	1.316223
H	2.344891	1.005908	-0.665765
N	3.796676	1.34593	-0.416246

H	4.193186	0.488262	-0.037563
H	3.932085	2.084439	0.26754
H	4.311531	1.592428	-1.256015

$(NA)_1(SA)_1(A)_2$

N	2.632962	-0.040759	-0.122286
O	2.851036	-1.209963	-0.512575
H	1.476577	-2.069208	0.086188
O	1.911867	0.116474	0.920869
O	3.069068	0.941641	-0.720456
S	-1.801481	0.009084	-0.120856
O	-1.480549	-1.120884	-1.01903
O	-1.234768	-0.126023	1.224072
O	-3.403609	-0.053188	0.124863
O	-1.546858	1.329121	-0.744548
H	-0.220163	2.084173	-0.074205
H	-3.846711	0.045136	-0.729164
N	0.657774	2.403324	0.411532
H	0.42059	3.007004	1.193536
H	1.27448	2.885217	-0.239429
H	1.174082	1.533145	0.746886
N	0.517282	-2.309252	0.439081
H	-0.200465	-2.096466	-0.28756
H	0.305606	-1.652439	1.19991
H	0.454095	-3.272529	0.753696

$(NA)_2(SA)_1(A)_1$

S	-2.002215	-0.216458	-0.18978
O	-1.713148	0.957981	-1.032882
O	-1.024735	-1.3163	-0.387992
O	-3.42582	-0.765516	-0.694375
O	-2.232638	0.057922	1.235778
H	-0.9198	-0.486091	2.096269
H	-3.441958	-0.746733	-1.661809
N	1.139256	2.183935	0.156216
O	0.840176	1.15794	0.767176
O	2.088565	2.888015	0.3635
O	0.330667	2.556025	-0.840641
H	-0.432369	1.895513	-0.869925
N	2.247426	-1.541719	-0.494634
O	1.833508	-1.945552	0.593358
O	3.39177	-1.518322	-0.851294
O	1.347394	-1.090861	-1.376934

H	0.429522	-1.175035	-0.959642
N	0.025285	-0.809113	2.436098
H	-0.048787	-1.384262	3.270718
H	0.604681	0.014569	2.604529
H	0.474479	-1.337023	1.66702

$(NA)_2(SA)_1(A)_2$

S	-1.866122	-0.358571	0.08024
O	-2.076213	-0.066219	1.513665
O	-0.457842	-0.156832	-0.319907
O	-2.740323	0.700706	-0.758846
O	-2.394949	-1.665437	-0.353662
H	-1.039689	-2.546096	-0.856184
H	-2.273271	1.553504	-0.76256
N	0.518177	2.414999	-0.460584
O	0.67566	2.441827	0.7521
O	-0.429306	2.856193	-1.065636
O	1.488821	1.881575	-1.209287
H	2.033072	1.293515	-0.600528
N	2.241278	-1.024061	-0.013835
O	2.575168	0.109907	0.413588
O	2.365171	-1.326924	-1.19847
O	1.748574	-1.854129	0.813847
H	0.976382	-0.725887	2.030982
N	-0.062354	-2.852675	-1.09954
H	-0.028639	-3.804876	-1.45221
H	0.557848	-2.734257	-0.272169
H	0.31839	-2.200524	-1.788786
N	0.488424	0.093348	2.444827
H	0.687233	0.180817	3.436879
H	-0.540907	0.01926	2.254662
H	0.830772	0.915055	1.930845

$(NA)_2(SA)_1(A)_3$

S	0.058576	1.828903	-0.062453
O	-0.931369	2.689444	-0.739802
O	0.08402	1.980476	1.404932
O	1.460566	2.299452	-0.643748
O	-0.115742	0.396824	-0.431303
H	2.156916	1.699579	-0.275031
H	0.998022	-1.098053	1.731458
N	-1.987863	-1.702784	0.181418
O	-2.359269	-1.065249	1.193014

H	-2.941176	0.206573	-0.821197
O	-2.470046	-1.423302	-0.948935
O	-1.125065	-2.592932	0.284656
N	2.637292	-0.767306	-0.012117
O	2.943015	-0.870349	-1.216491
H	1.468371	-1.805026	-1.80133
O	2.089079	-1.740541	0.570178
O	2.836047	0.295664	0.61358
N	0.43547	-1.783991	-1.901865
H	0.149946	-0.816949	-1.645411
H	-0.020716	-2.39111	-1.198149
H	0.131885	-2.025566	-2.839743
N	-3.174685	1.182373	-0.501586
H	-4.022234	1.525593	-0.944652
H	-2.359127	1.831154	-0.680033
H	-3.310626	1.101901	0.506292
N	0.286287	-0.624888	2.339242
H	0.306522	0.395953	2.124597
H	0.49494	-0.793148	3.318691
H	-0.655346	-0.973085	2.099471

$(NA)_1(SA)_2(A)_1$

S	0.542869	1.571866	0.243973
O	-0.714878	2.081948	0.774321
O	0.373703	0.855082	-1.066108
O	1.367773	0.773237	1.171582
O	1.389276	2.88888	-0.08462
H	2.277257	2.631058	-0.375598
H	1.039199	-0.795923	1.702578
S	-2.633193	-0.62008	-0.178759
O	-1.506963	-1.218015	0.540845
O	-3.824763	-1.377921	-0.404133
O	-2.093432	-0.119447	-1.577052
O	-3.037241	0.706209	0.574165
H	-2.235492	1.265295	0.738131
H	-1.193171	0.286065	-1.476288
N	2.929703	-1.127278	-0.561902
O	3.470039	-0.143537	-1.0041
O	3.39133	-1.952669	0.203574
O	1.65308	-1.383361	-0.939329
H	1.237769	-0.494776	-1.177112
N	0.829566	-1.819091	1.794709
H	-0.068671	-1.950968	1.301852

H	0.748326	-2.091066	2.77101
H	1.581689	-2.336928	1.329171

$(NA)_1(SA)_2(A)_2$

S	-2.195562	-0.21369	-0.075895
O	-1.822227	-0.470577	-1.47557
O	-1.726423	-1.21787	0.899595
O	-3.79588	-0.391013	0.007392
O	-1.920848	1.179334	0.35384
H	-4.208692	0.191912	-0.645058
H	-0.720758	1.954715	-0.267968
S	1.608771	-1.422356	0.060042
O	0.898457	-0.118343	0.031501
O	2.529073	-1.574761	-1.073392
O	0.471636	-2.529233	-0.254662
O	2.135762	-1.705358	1.40661
H	-0.362113	-2.261866	0.185809
H	1.031401	-0.679617	2.424598
N	1.033028	2.641922	0.101258
O	0.037012	2.402187	-0.778723
O	0.769282	2.544431	1.290018
O	2.083535	2.957786	-0.389281
H	0.867462	0.903496	-2.196533
N	0.708602	-0.015306	-2.621843
H	0.674119	0.046677	-3.635676
H	-0.199956	-0.342831	-2.230097
H	1.470987	-0.649049	-2.295865
N	0.217324	-0.059008	2.634691
H	0.068572	0.056052	3.633095
H	-0.612534	-0.47383	2.169485
H	0.392458	0.845176	2.17448

$(NA)_1(SA)_2(A)_3$

S	-0.808004	1.86623	-0.056068
O	-0.773764	0.418188	-0.409444
O	-2.002202	2.525012	-0.622555
O	0.417767	2.558872	-0.778216
O	-0.658217	2.042958	1.401362
H	1.253416	2.119513	-0.462305
H	-0.306761	0.517338	2.136755
S	2.803764	-0.23268	-0.056086
O	2.794471	-0.601712	-1.485784
O	2.516164	1.194399	0.182222

O	4.317527	-0.458218	0.473504
O	2.027719	-1.166865	0.775996
H	4.882505	0.213628	0.067589
H	0.013001	-2.306861	-1.102145
N	-2.14061	-2.05324	0.160243
O	-2.635138	-1.999972	-0.978645
O	-1.101798	-2.701392	0.38483
O	-2.677674	-1.412864	1.116935
H	-3.772272	-0.030633	-1.278174
N	-3.843488	0.54837	-0.440411
H	-3.49899	-0.081159	0.323148
H	-4.805417	0.83332	-0.280292
H	-3.203093	1.385869	-0.532732
N	0.275316	-1.623052	-1.830479
H	-0.075934	-1.926095	-2.733407
H	1.302342	-1.448265	-1.839127
H	-0.171896	-0.729741	-1.53662
N	-0.154189	-0.499242	2.32236
H	0.047125	-0.670649	3.302828
H	0.651229	-0.805383	1.733798
H	-1.005447	-1.004773	2.031509

Table S5. Single point energies (kcal mol^{-1}) at the DLPNO-CCSD(T)/aug-cc-pVTZ level and the corresponding Gibbs free energy correction G_{corr} (kcal mol^{-1}) and Gibbs free energy G (kcal mol^{-1}) at 298.15K for all the most stable configurations of the NA-SA-MA, NA-SA-DMA and NA-SA-A systems.

clusters	single point	G_{corr}	G
$(NA)_1(SA)_1(MA)_1$	-1075.773484	0.091878	-1075.681606
$(NA)_1(SA)_1(MA)_2$	-1171.525076	0.157342	-1171.367734
$(NA)_1(SA)_1(MA)_3$	-1267.254704	0.21914	-1267.035564
$(NA)_1(SA)_2(MA)_1$	-1775.280179	0.127282	-1775.152897
$(NA)_2(SA)_1(MA)_1$	-1356.344711	0.114497	-1356.230214
$(NA)_2(SA)_1(MA)_2$	-1452.095375	0.180389	-1451.914986
$(NA)_1(SA)_2(MA)_2$	-1871.036314	0.192662	-1870.843652
$(NA)_1(SA)_2(MA)_3$	-1966.794457	0.261848	-1966.532609
$(NA)_2(SA)_1(MA)_3$	-1547.85172	0.248328	-1547.603392
$(NA)_1(MA)_1$	-376.2721918	0.061153	-376.2110388
$(NA)_1(MA)_2$	-471.9934427	0.120294	-471.8731487
$(NA)_1(MA)_3$	-567.7236542	0.184261	-567.5393932
$(NA)_2(MA)_1$	-656.8366666	0.082008	-656.7546586
$(NA)_2(MA)_2$	-752.5852841	0.148447	-752.4368371
$(NA)_2(MA)_3$	-848.3150413	0.208378	-848.1066633
$(NA)_3(MA)_1$	-937.4045633	0.103340	-937.3012233
$(NA)_3(MA)_2$	-1033.153882	0.167825	-1032.986057
$(NA)_3(MA)_3$	-1128.896614	0.229390	-1128.667224
$(SA)_1(MA)_1$	-795.197688	0.072625	-795.125063
$(SA)_1(MA)_2$	-890.927571	0.132992	-890.794579
$(SA)_1(MA)_3$	-986.65875	0.19662	-986.46213
$(SA)_2(MA)_1$	-1494.709149	0.107431	-1494.601718
$(SA)_2(MA)_2$	-1590.454826	0.174314	-1590.280512
$(SA)_2(MA)_3$	-1686.183444	0.230949	-1685.952495
$(SA)_3(MA)_1$	-2194.208579	0.141184	-2194.067395
$(SA)_3(MA)_2$	-2289.963668	0.205543	-2289.758125
$(SA)_3(MA)_3$	-2385.716335	0.272156	-2385.444179
A	-56.48024907	0.015714	-56.46453507
SA	-699.4627499	0.011182	-699.4515679
MA	-95.705457	0.041861	-95.663596
NA	-280.5415393	0.00149	-280.5400493
DMA	-134.9377016	0.067928	-134.8697736
$(NA)_1(DMA)_1$	-415.5057069	0.086285	-415.4194219
$(NA)_2(DMA)_1$	-696.0768686	0.110709	-695.9661596
$(NA)_2(DMA)_2$	-831.0648693	0.203255	-830.8616143
$(NA)_3(DMA)_1$	-976.6455726	0.133587	-976.5119856
$(NA)_3(DMA)_2$	-1111.634636	0.225008	-1111.409628
$(NA)_3(DMA)_3$	-1246.617857	0.317365	-1246.300492

$(NA)_1(SA)_1(DMA)_1$	-1115.014974	0.124942	-1114.890032
$(NA)_1(SA)_1(DMA)_2$	-1250.003162	0.215199	-1249.787963
$(NA)_2(SA)_1(DMA)_1$	-1395.580433	0.145875	-1395.434558
$(NA)_1(SA)_2(DMA)_1$	-1814.520062	0.157029	-1814.363033
$(NA)_2(SA)_1(DMA)_2$	-1530.572935	0.238897	-1530.334038
$(NA)_1(SA)_2(DMA)_2$	-1949.512551	0.252846	-1949.259705
$(NA)_2(SA)_1(DMA)_3$	-1665.560968	0.332443	-1665.228525
$(NA)_1(SA)_2(DMA)_3$	-2084.506775	0.343849	-2084.162926
$(SA)_1(DMA)_1$	-834.4400164	0.097619	-834.3423974
$(SA)_1(DMA)_2$	-969.4026559	0.186603	-969.2160529
$(SA)_1(DMA)_3$	-1104.36721	0.274966	-1104.092244
$(SA)_2(DMA)_1$	-1533.957122	0.133275	-1533.823847
$(SA)_2(DMA)_2$	-1668.942843	0.225894	-1668.716949
$(SA)_2(DMA)_3$	-1803.915673	0.316243	-1803.59943
$(SA)_3(DMA)_1$	-2233.461148	0.168265	-2233.292883
$(SA)_3(DMA)_2$	-2368.455641	0.259809	-2368.195832
$(SA)_3(DMA)_3$	-2503.444982	0.351638	-2503.093344
$(SA)_1(A)_1$	-755.9664372	0.044667	-755.9217702
$(SA)_2(A)_1$	-1455.473432	0.080691	-1455.392741
$(SA)_2(A)_2$	-1511.983413	0.116992	-1511.866421
$(SA)_3(A)_1$	-2154.965927	0.111125	-2154.854802
$(SA)_3(A)_2$	-2211.48869	0.149758	-2211.338932
$(SA)_3(A)_3$	-2268.009283	0.189116	-2267.820167
$(NA)_1(A)_1$	-337.0435125	0.0342	-337.0093125
$(NA)_2(A)_1$	-617.6009034	0.056902	-617.5440014
$(NA)_2(A)_2$	-674.1139883	0.094983	-674.0190053
$(NA)_3(A)_1$	-898.1670092	0.076699	-898.0903102
$(NA)_3(A)_2$	-954.6809968	0.113803	-954.5671938
$(NA)_3(A)_3$	-1011.191101	0.152253	-1011.038848
$(NA)_1(SA)_1(A)_1$	-1036.535387	0.063602	-1036.471785
$(NA)_1(SA)_1(A)_2$	-1093.052076	0.104441	-1092.947635
$(NA)_2(SA)_1(A)_1$	-1317.108675	0.088228	-1317.020447
$(NA)_2(SA)_1(A)_2$	-1373.623326	0.130638	-1373.492688
$(NA)_2(SA)_1(A)_3$	-1430.144519	0.1702	-1429.974319
$(NA)_1(SA)_2(A)_1$	-1736.044683	0.100882	-1735.943801
$(NA)_1(SA)_2(A)_2$	-1792.561856	0.143387	-1792.418469
$(NA)_1(SA)_2(A)_3$	-1849.083343	0.180341	-1848.903002

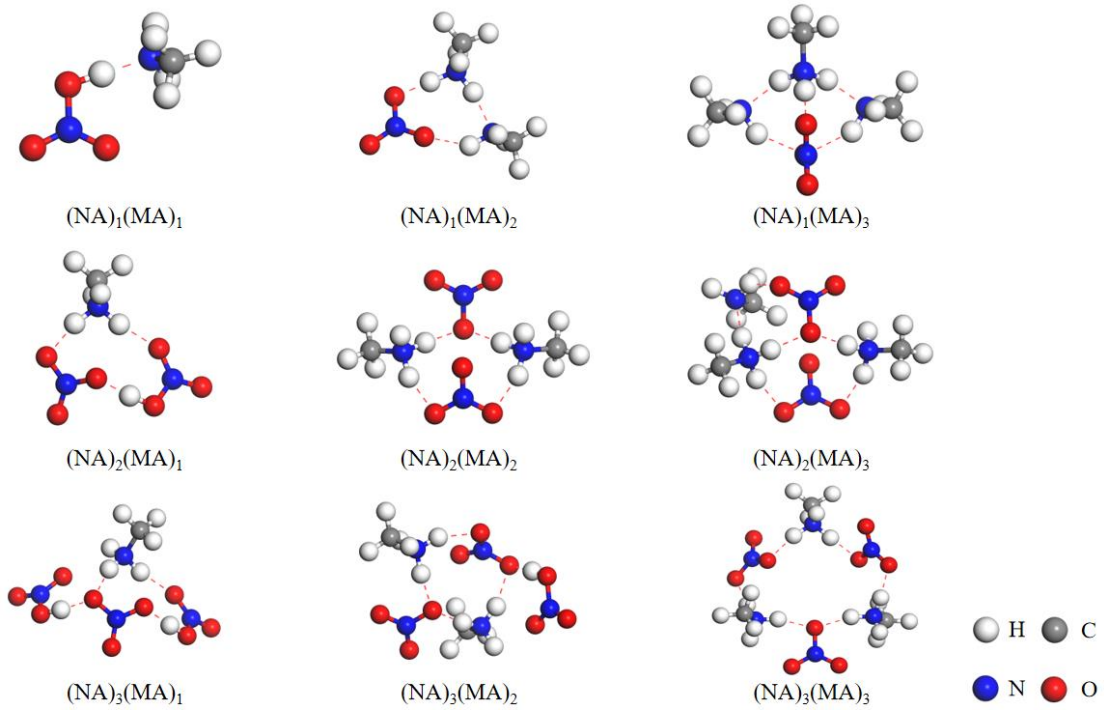

Figure S1. Lowest Gibbs free energy conformations of the $(NA)_{1\text{-}3}(MA)_{1\text{-}3}$ clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, 298.15 K and 1 atm. The dashed red lines indicate hydrogen bonds.

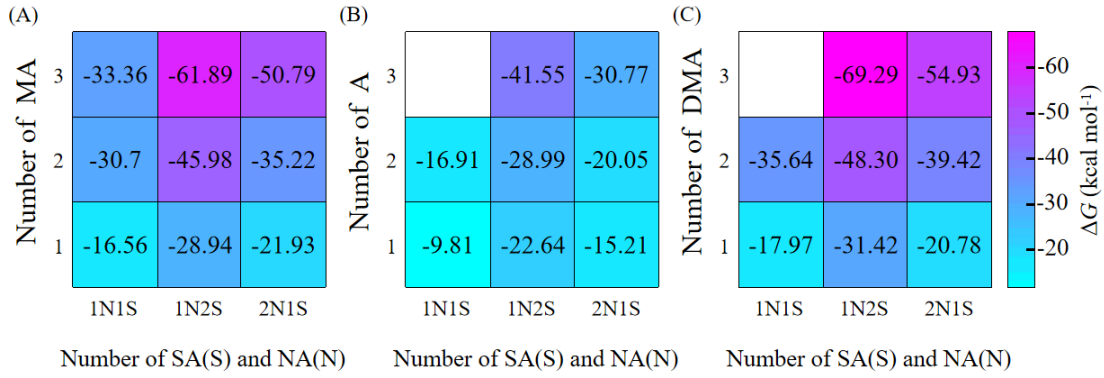

Figure S2. Formation free energy (Δ*G*) of (A) $(NA)_x(SA)_y(MA)_z$ ($1 \le x$, $1 \le y$, $x + y \le 3$, $1 \le z \le 3$), (B) $(NA)_x(SA)_y(A)_z$ ($x \ge 1$, $y \ge 1$, $1 \le z \le x + y \le 3$) and (C) $(NA)_x(SA)_y(DMA)_z$ ($x \ge 1$, $y \ge 1$, $1 \le z \le x + y \le 3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, 298.15 K and 1 atm.

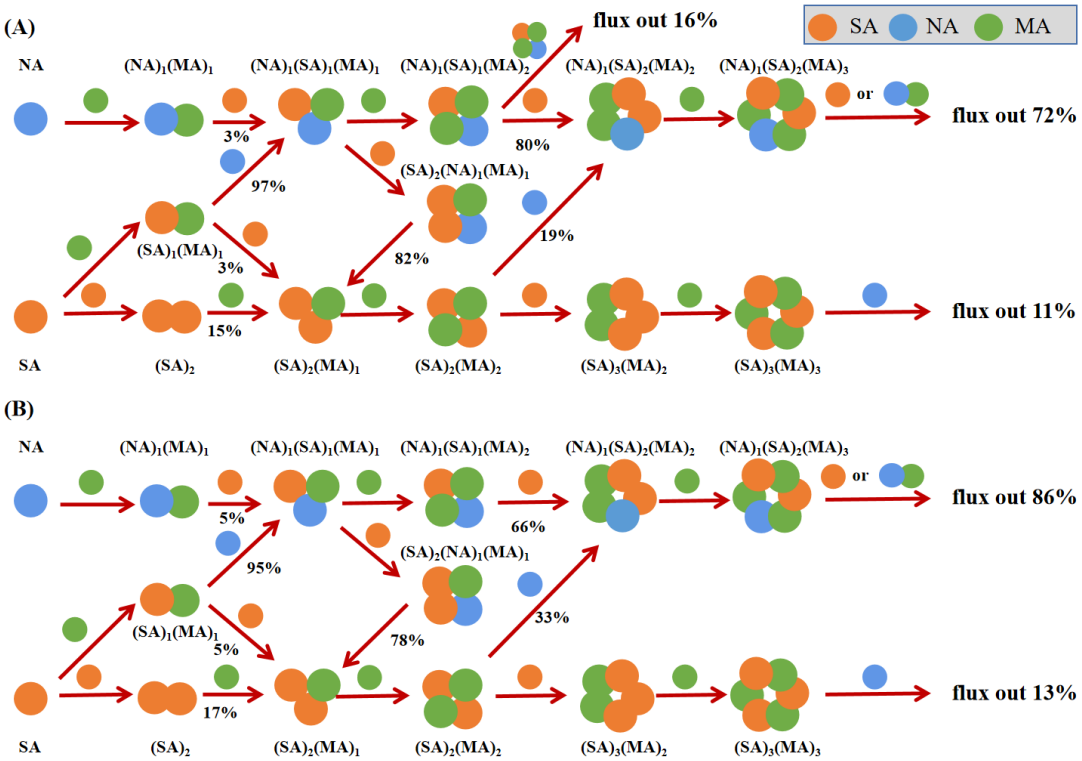

Figure S3. Cluster growth pathways for the NA-SA-MA system at (A) 238.15 K, [NA] = 10^{10} molecules cm^{-3}, [SA] = 10^{6} molecules cm^{-3} and [MA] = 10^{8} molecules cm^{-3}, (B) 278.15 K, [NA] = 10^{12} molecules cm^{-3}, [SA] = 10^{6} molecules cm^{-3} and [MA] = 10^{8} molecules cm^{-3}.