Supporting Information

for

Enhancement of Sulphuric Acid Based New Particle Formation by 3-Aminopropanamide: Mechanistic, Thermodynamic, and Kinetic Insights

Janardhanan Aswathi, Aleena Ann Babu and Deepa Janardanan*

Computational Chemistry & Molecular Modelling Laboratory, Department of Chemistry, School of Physical Sciences, Central University of Kerala, Kasaragod, Kerala-671320, India

*Corresponding Author:

Deepa Janardanan: Email: deepa.j@cukerala.ac.in; ORCID: https://orcid.org/0000-0003-4144-0689

Contents

Boundary condition of ACDC simulations

In ACDC simulations, boundary conditions require that the outgrowing clusters - clusters that grow rather than evaporate - must be stable. In our study, the largest cluster that we included for the simulation is $(APA)_3(SA)_3$. Upon closer examination of the overall evaporation rates (**Figure S4**), it is substantiated that clusters with one additional SA molecule than APA exhibit comparatively lower evaporation rates. Therefore, the cluster $(APA)_3(SA)_4$ is considered to be stable and (which is allowed to leave the simulation box) has been set as the boundary condition.

Table S1: The topological parameters; electron density ($\rho(r)$), Laplacian ($\nabla^2\rho(r)$), Lagrangian kinetic energy (G(r)), Potential energy density (V (r)) and Energy density (H(r)), at the Bond Critical points (BCPs) corresponding to H-bonds in heteromolecular clusters of APA-SA.

Cluster		$\rho(r)$	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
(APA)(SA)	N-H--N	0.026	0.108	-0.022	0.024	0.002
	N-H--O	0.025	0.085	-0.018	0.019	0.002
(APA)(SA)$_2$	N-H--O	0.016	0.06	-0.011	0.013	0.002
	O-H--O	0.049	0.151	-0.051	0.044	-0.006
	N-H-O	0.02	0.081	-0.015	0.018	0.002
	O-H--O	0.035	0.136	-0.034	0.034	0.0002
	N-H--O	0.016	0.06	-0.011	0.013	0.002
(APA)(SA)$_3$	O-H--O	0.042	0.143	-0.042	0.039	-0.003
	O-H--O	0.057	0.165	-0.064	0.053	-0.011
	O-H--O	0.02	0.077	-0.016	0.017	0.002
	O-H--O	0.063	0.167	-0.071	0.056	-0.015
	N-H--O	0.021	0.084	-0.016	0.018	0.002
	N-H--O	0.015	0.057	-0.01	0.012	0.002
	N-H--O	0.057	0.158	-0.061	0.05	-0.011
	O-H--O	0.062	0.157	-0.068	0.053	-0.014
	N-H--O	0.014	0.055	-0.01	0.012	0.002
(APA)$_2$ (SA)	N-H--O	0.019	0.076	-0.014	0.017	0.003
	N-H--N	0.034	0.091	-0.026	0.024	-0.002
	N-H--O	0.018	0.071	-0.013	0.016	0.002
	N-H--O	0.064	0.158	-0.07	0.055	-0.015
	O-H--O	0.036	0.134	-0.034	0.034	-0.0003
	N-H--O	0.021	0.084	-0.016	0.019	0.002
	N-H--O	0.026	0.101	-0.021	0.023	0.002
(APA)$_2$(SA)$_2$	N-H--O	0.015	0.058	-0.01	0.012	0.002
	N-H--O	0.009	0.036	-0.007	0.008	0.001
	N-H--O	0.012	0.049	-0.009	0.01	0.002
	N-H--O	0.028	0.112	-0.024	0.026	0.002
	O-H--O	0.045	0.155	-0.046	0.043	-0.004
	O-H--O	0.029	0.115	-0.026	0.027	0.001
	N-H--O	0.017	0.063	-0.012	0.014	0.002
	N-H--O	0.017	0.065	-0.012	0.014	0.002
	N-H--O	0.021	0.085	-0.016	0.019	0.003
	N-H--O	0.025	0.095	-0.019	0.022	0.002
(APA)$_2$(SA)$_3$	N-H--O	0.013	0.05	-0.009	0.011	0.002
	N-H--O	0.01	0.033	-0.007	0.007	0.001
	N-H--O	0.007	0.024	-0.005	0.005	0.001
	N-H--O	0.015	0.06	-0.011	0.013	0.002
	N-H--O	0.051	0.15	-0.052	0.045	-0.007

|						
	N-H--O	0.021	0.083	-0.016	0.018	0.002
	O-H--O	0.06	0.163	-0.066	0.053	-0.013
	N-H--O	0.026	0.1	-0.021	0.023	0.002
(APA)$_3$(SA)	N-H--O	0.036	0.125	-0.032	0.032	-0.0003
	O-H--N	0.065	0.091	-0.063	0.043	-0.02
	N-H--O	0.022	0.087	-0.017	0.019	0.002
	N-H--O	0.023	0.089	-0.018	0.02	0.002
	N-H--O	0.012	0.043	-0.009	0.01	0.001
	N-H--O	0.028	0.119	-0.024	0.027	0.003
	N-H--O	0.064	0.148	-0.068	0.052	-0.015
	N-H--O	0.023	0.09	-0.017	0.02	0.003
(APA)$_3$(SA)$_2$	N-H--O	0.011	0.037	-0.007	0.008	0.001
	N-H--O	0.037	0.098	-0.03	0.027	-0.003
	N-H--O	0.035	0.132	-0.032	0.033	0.0005
	O-H--O	0.033	0.123	-0.03	0.03	-0.005
	N-H--O	0.048	0.153	-0.049	0.044	-0.006
	N-H--O	0.027	0.108	-0.023	0.025	0.002
	N-H--O	0.012	0.048	-0.009	0.01	0.002
	N-H--O	0.017	0.069	-0.013	0.015	0.002
	O-H--O	0.058	0.16	-0.063	0.052	-0.012
	N-H--O	0.038	0.092	-0.03	0.026	-0.003
	N-H--O	0.031	0.12	-0.027	0.029	0.002
(APA)$_3$(SA)$_3$	O-H--O	0.397	0.123	-0.034	0.016	-0.005
	N-H--O	0.015	0.053	-0.011	0.012	0.001
	N-H--N	0.027	0.082	-0.019	0.02	0.001
	N-H--O	0.033	0.123	-0.03	0.03	0.001
	N-H--O	0.027	0.106	-0.022	0.024	0.002
	N-H--O	0.028	0.112	-0.024	0.026	0.026
	O-H--O	0.025	0.108	-0.022	0.024	0.003
	N-H--O	0.025	0.1	-0.02	0.023	0.002
	N-H--O	0.018	0.074	-0.013	0.016	0.002
	N-H--O	0.014	0.052	-0.01	0.011	0.002
	N-H--O	0.013	0.05	-0.01	0.011	0.001

Table S2. The evaporation coefficients of different pathways for APA-SA clusters obtained by kinetic simulation at 298.15 K and 1 atm.
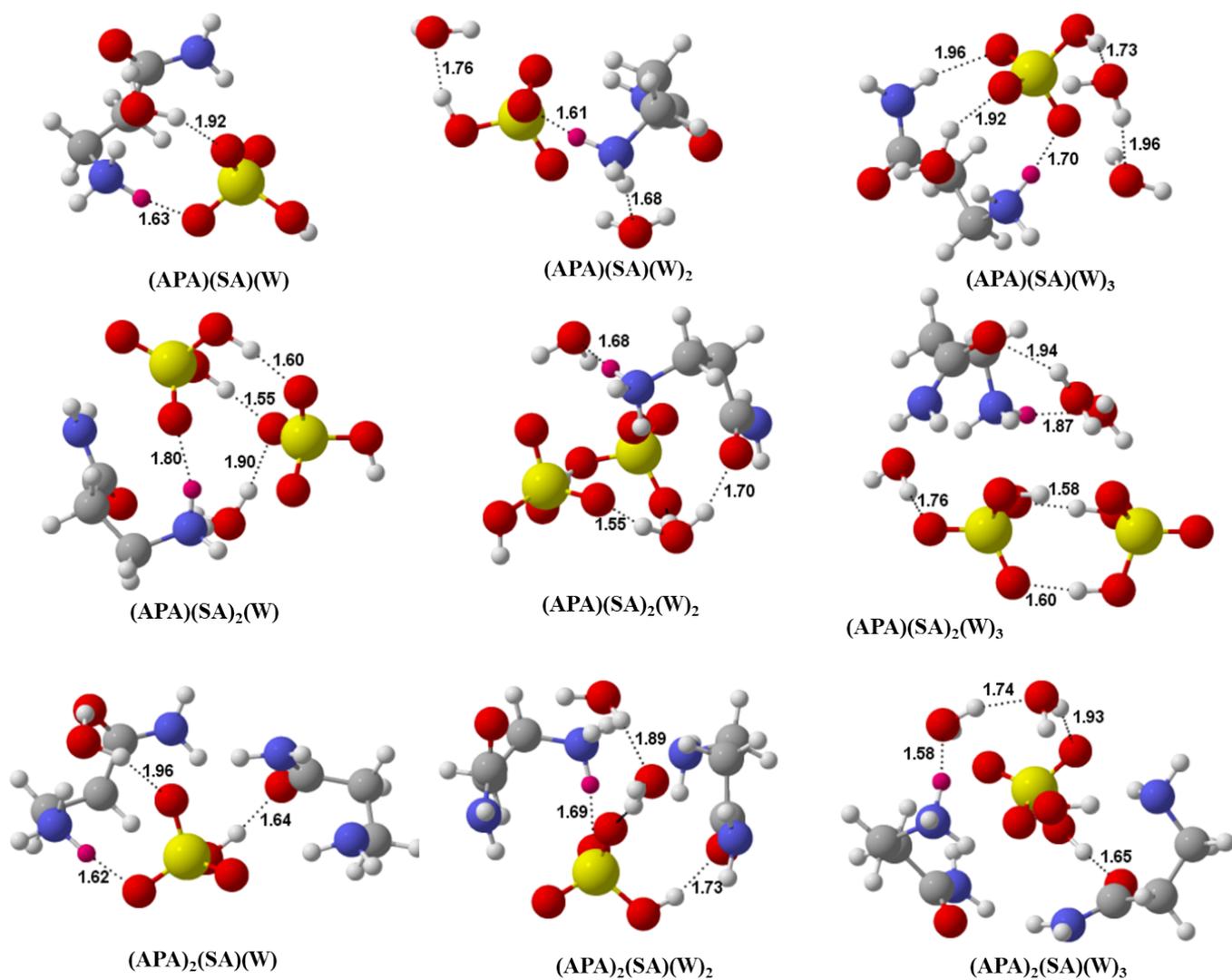
			Evaporation Coefficients (s^{-1})
$(SA)_2$	$\longrightarrow$	$SA + SA$	3.40E+04
$(SA)_3$	$\longrightarrow$	$(SA)_2 + SA$	1.04E+06
$(APA)_2$	$\longrightarrow$	$APA + APA$	2.80E+08
$(APA)_3$	$\longrightarrow$	$(APA)_2 + APA$	6.27E+08
$(APA)(SA)$	$\longrightarrow$	$APA + SA$	5.99E+01
$(APA)_2(SA)$	$\longrightarrow$	$(APA)_2 + SA$	5.82E-05
$(APA)_2(SA)$	$\longrightarrow$	$(APA)(SA) + APA$	5.13E+02
$(APA)_3(SA)$	$\longrightarrow$	$(APA)_3 + SA$	4.26E-06
$(APA)_3(SA)$	$\longrightarrow$	$(APA)2(SA) + (APA)$	4.28E+07
$(APA)_3(SA)$	$\longrightarrow$	$(APA)_2 + (APA)(SA)$	3.38E+01
$(APA)(SA)_2$	$\longrightarrow$	$(APA)(SA) + SA$	1.02E+00
$(APA)(SA)_2$	$\longrightarrow$	$(SA)_2 + APA$	7.96E-04
$(APA)_2(SA)_2$	$\longrightarrow$	$(APA)_2(SA) + SA$	4.02E-07
$(APA)_2(SA)_2$	$\longrightarrow$	$(APA)_2 + (SA)_2$	2.46E-16
$(APA)_2(SA)_2$	$\longrightarrow$	$(APA)(SA)_2+(APA)$	1.83E-04
$(APA)_2(SA)_2$	$\longrightarrow$	$(APA)(SA) + (APA)(SA)$	1.39E-06
$(APA)_3(SA)_2$	$\longrightarrow$	$(APA)_3(SA) + SA$	5.04E-07
$(APA)_3(SA)_2$	$\longrightarrow$	$(APA)_3 +(SA)_2$	1.93E-17
$(APA)_3(SA)_2$	$\longrightarrow$	$(APA)_2(SA)_2 +APA$	5.10E+07
$(APA)_3(SA)_2$	$\longrightarrow$	$(APA)(SA)_2 +(APA)_2$	1.33E-05
$(APA)_3(SA)_2$	$\longrightarrow$	$(APA)_2(SA) + (APA)(SA)$	2.50E-01
$(APA)(SA)_3$	$\longrightarrow$	$(APA)(SA)2 + SA$	2.34E+03
$(APA)(SA)_3$	$\longrightarrow$	$(APA)(SA) + (SA)_2$	2.69E-02
$(APA)(SA)_3$	$\longrightarrow$	$(SA)_3 +APA$	1.64E-06
$(APA)_2(SA)_3$	$\longrightarrow$	$(APA)_2(SA)_2 +SA$	1.22E+01
$(APA)_2(SA)_3$	$\longrightarrow$	$(APA)_2(SA) + (SA)_2$	4.65E-11
$(APA)_2(SA)_3$	$\longrightarrow$	$(APA)_2 +(SA)_3$	2.23E-21
$(APA)_2(SA)_3$	$\longrightarrow$	$(APA)(SA)_3 + APA$	9.25E-07
$(APA)_2(SA)_3$	$\longrightarrow$	$(APA)(SA)_2 + (APA)(SA)$	2.80E-05
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)_3(SA)_2 + SA$	1.99E-01
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)_3(SA) + (SA)_2$	8.36E-13
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)_3 + (SA)_3$	2.52E-24
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)_2(SA)_3 +APA$	7.96E+05
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)(SA)_3 +(APA)_2$	9.47E-10
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)_2(SA)_2 +(APA)(SA)$	1.09E+05
$(APA)_3(SA)_3$	$\longrightarrow$	$(APA)(SA)_2 + (APA)_2(SA)$	3.60E-02

Table S3. The enthalpy ($\Delta H_{298.15}$) and Gibbs free energy ($\Delta G_{298.15}$) of the hydrated clusters used for finding new particle formation rate in ACDC simulation program

Clusters	$\Delta H_{298.15K}$ (Kcal/mol)	$\Delta G_{298.15K}$ (Kcal/mol)
(APA)(SA)(W)	-16.91	-40.67
(APA)(SA)(W)$_2$	-17.25	-50.19
(APA)(SA)(W)$_3$	-16.37	-59.68
(APA)$_2$(SA)(W)	-21.14	-57.64
(APA)$_2$(SA)(W)$_2$	-23.46	-71.21
(APA)$_2$(SA)(W)$_3$	-18.97	-77.98
(APA)(SA)$_2$(W)	-29.89	-65.46
(APA)(SA)$_2$(W)$_2$	-28.33	-76.19
(APA)(SA)$_2$(W)$_3$	-28.53	-85.20
(APA)$_2$(SA)$_2$(W)	-47.14	-97.42
(APA)$_2$(SA)$_2$(W)$_2$	-44.09	-104.88
(APA)$_2$(SA)$_2$(W)$_3$	-43.28	-113.98
(APA)(W)	0.34	-9.57
(APA)(W)$_2$	0.10	-19.54
(APA)(W)$_3$	4.03	-26.76
(APA)$_2$(W)	-0.77	-24.08
(APA)$_2$(W)$_2$	-0.48	-33.15
(APA)$_2$(W)$_3$	0.07	-44.48

ΔG = 0   ΔG = 0.4
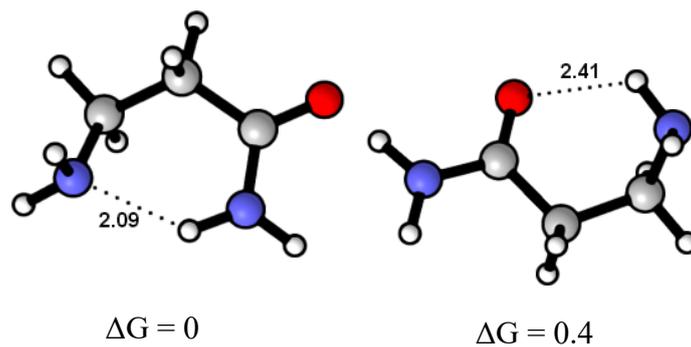
Figure S1. The optimised geometries of two minimum configurations of 3-amino propanamide obtained at the M06-2X / 6-311++G (3df, 3pd) level of theory (relative energies in kcal/mol).

(APA)(SA)(W)

(APA)(SA)(W)$_2$

(APA)(SA)(W)$_3$

(APA)(SA)$_2$(W)

(APA)(SA)$_2$(W)$_2$

(APA)(SA)$_2$(W)$_3$

(APA)$_2$(SA)(W)

(APA)$_2$(SA)(W)$_2$

(APA)$_2$(SA)(W)$_3$

S8
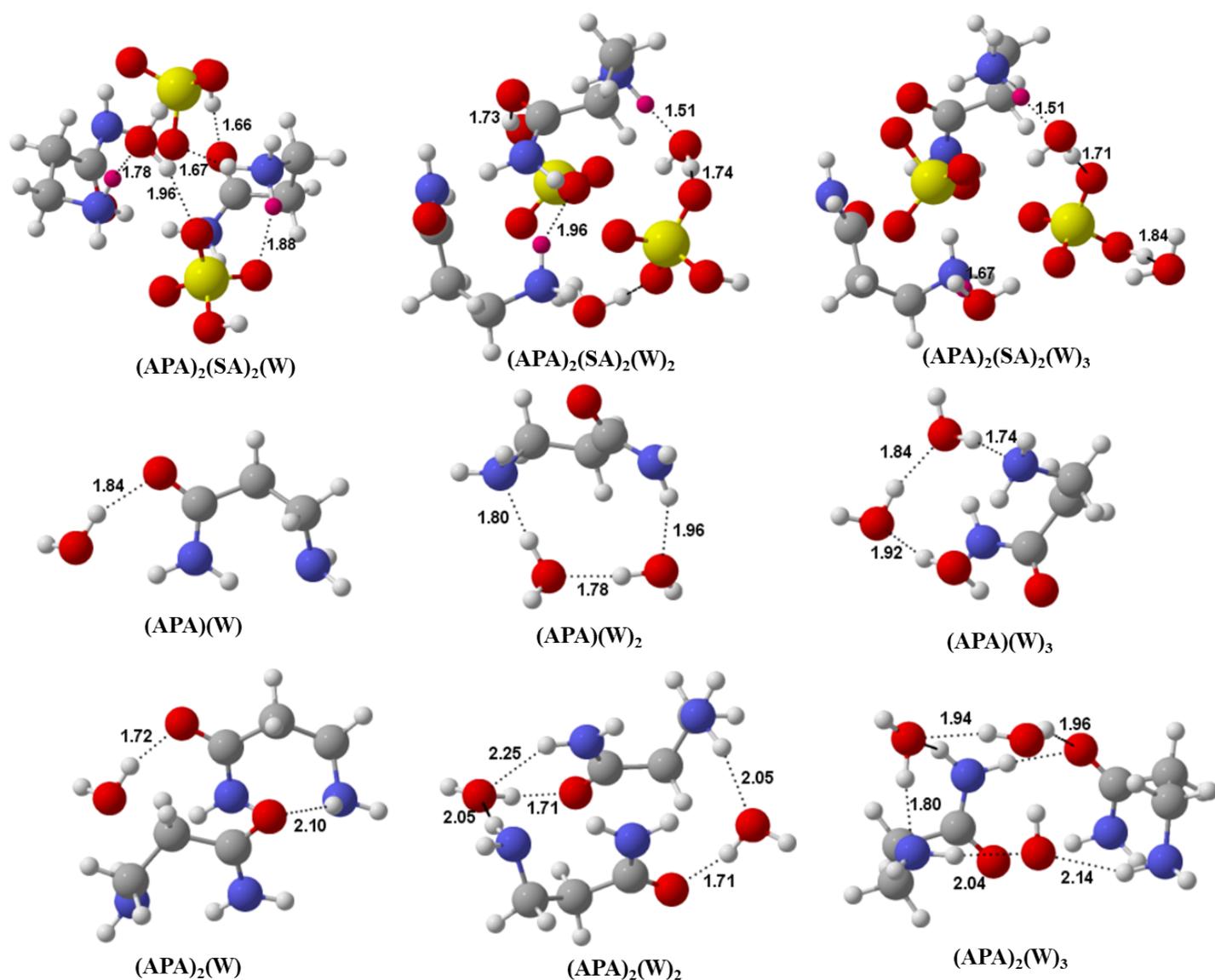
Figure S2. The optimised structures of the hydrated APA-SA system used for kinetic simulation at M062X/6-311++G(3df,3pd)//DLPNO-CCSD(T)/aug-cc-pVTZ level of theory (the transferred proton in the structures of APA is indicated in pink colour).

(PA)(SA)
[1, 0]

(PA)(SA)$_2$
[3, 0]

(PA)(SA)$_3$
[8, 1]

(PA)$_2$(SA)
[2, 0]

(PA)$_2$(SA)$_2$
[9, 2]

(PA)$_2$(SA)$_3$
[10, 1]

(PA)$_3$(SA)
[5, 0]

(PA)$_3$(SA)$_2$
[19, 5]

(PA)$_3$(SA)$_3$
[21, 4]
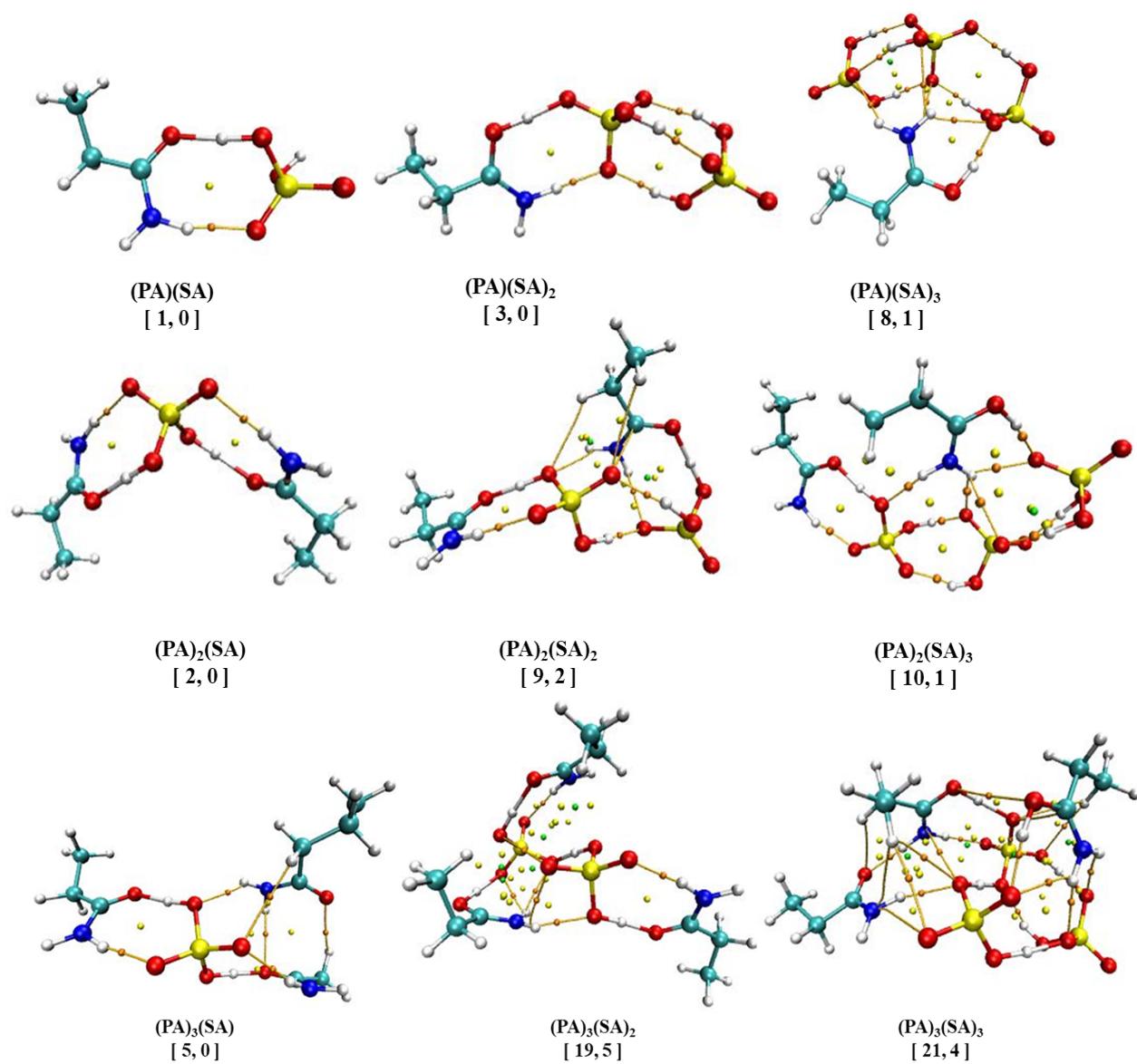
Figure S3. The AIM plots for heteromolecular PA-SA clusters showing the BCP (orange balls), RCP (yellow balls), CCP(green balls). In the parenthesis, indicated are the number of RCPs and CCPs in the structure ([RCP, CCP]).
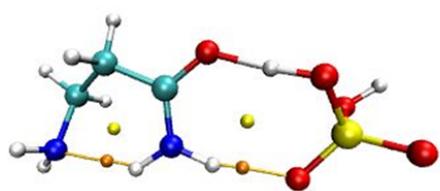
(APA)(SA)
[2, 0]
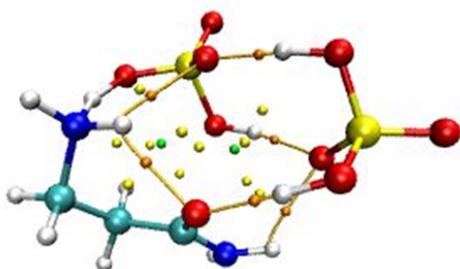
(APA)(SA)$_2$
[11, 2]
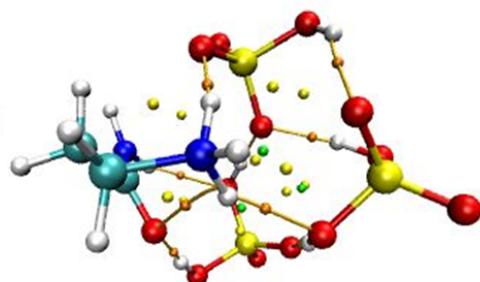
(APA)(SA)$_3$
[13, 4]
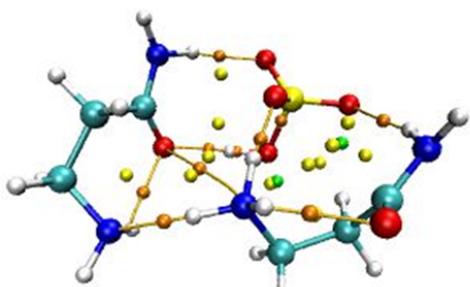
(APA)$_2$(SA)
[12, 2]
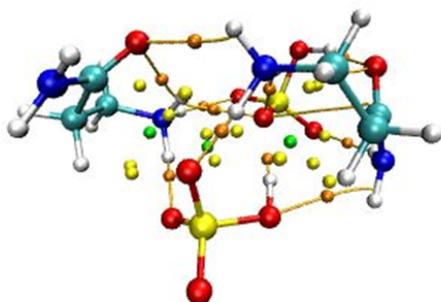
(APA)$_2$(SA)$_2$
[16, 3]
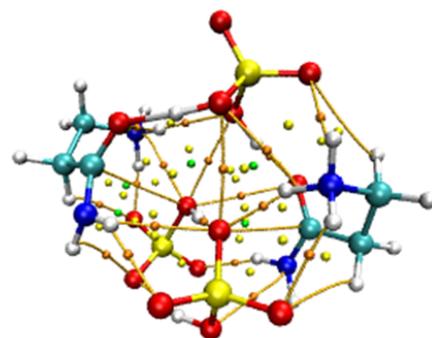
(APA)$_2$(SA)$_3$
[25, 6]
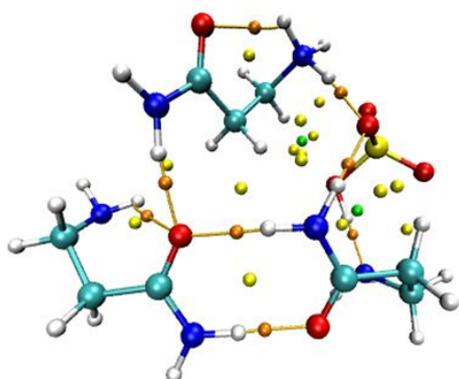
(APA)$_3$(SA)
[16, 2]
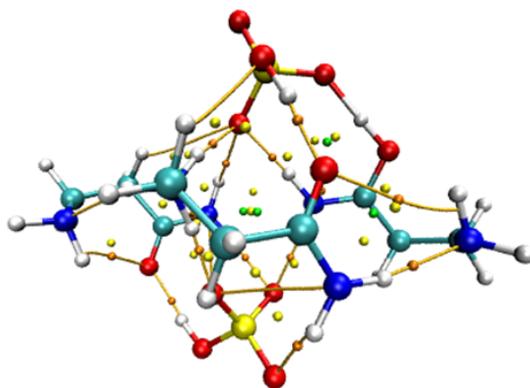
(APA)$_3$(SA)$_2$
[22, 5]
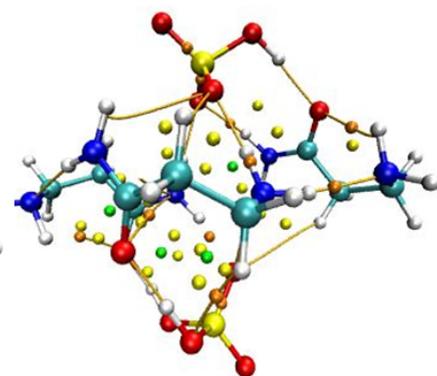
(APA)$_3$(SA)$_3$
[28, 6]

Figure S4. AIM plots of APA-SA clusters indicating the Ring critical points (RCP, yellow balls), Bond Critical points (BCP, orange balls) and the Cage critical points (CCP, green balls) for the APA-SA system. In the square brackets are given the number of RCPs and the CCPs for the corresponding clusters.
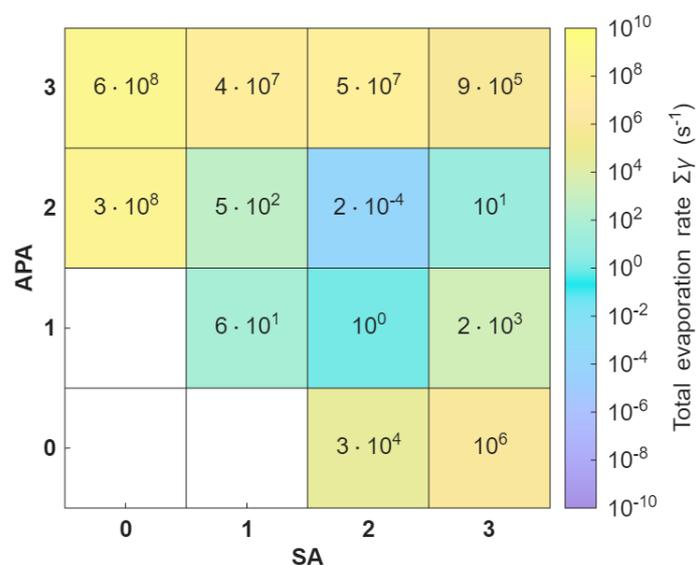
Figure S5. The overall evaporation rate of $(APA)_m(SA)_n$ (m = 0-3, n = 0-3) clusters obtained at 298.15 K and 1 atm and vapour concentration 10^6 molecules cm^{-3} of SA and 10 ppt of APA.
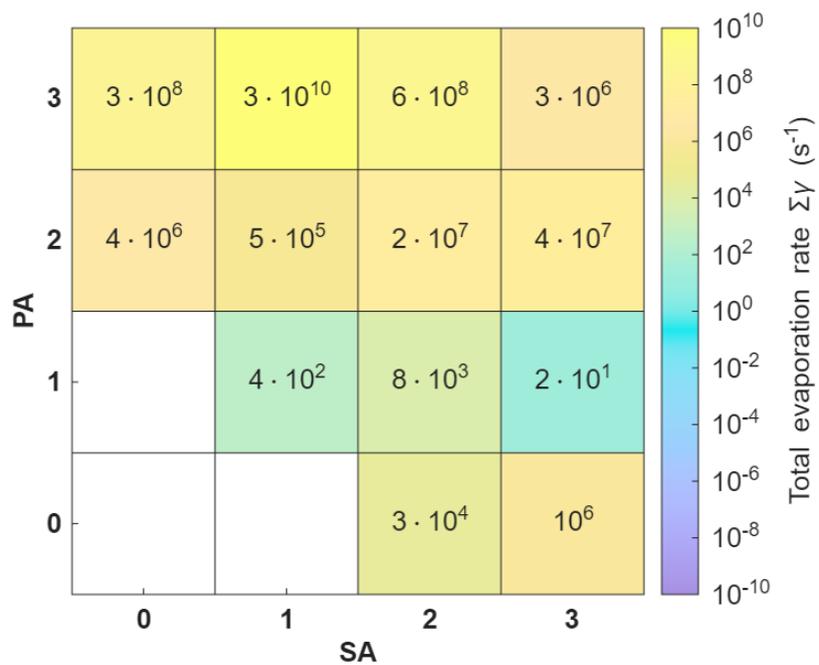
Figure S6. The overall evaporation rate of $(PA)_m(SA)_n$ (m = 0-3, n = 0-3) clusters obtained at 298.15 K and 1 atm and vapour concentration 10^6 molecules cm^{-3} of SA and 10 ppt of PA.
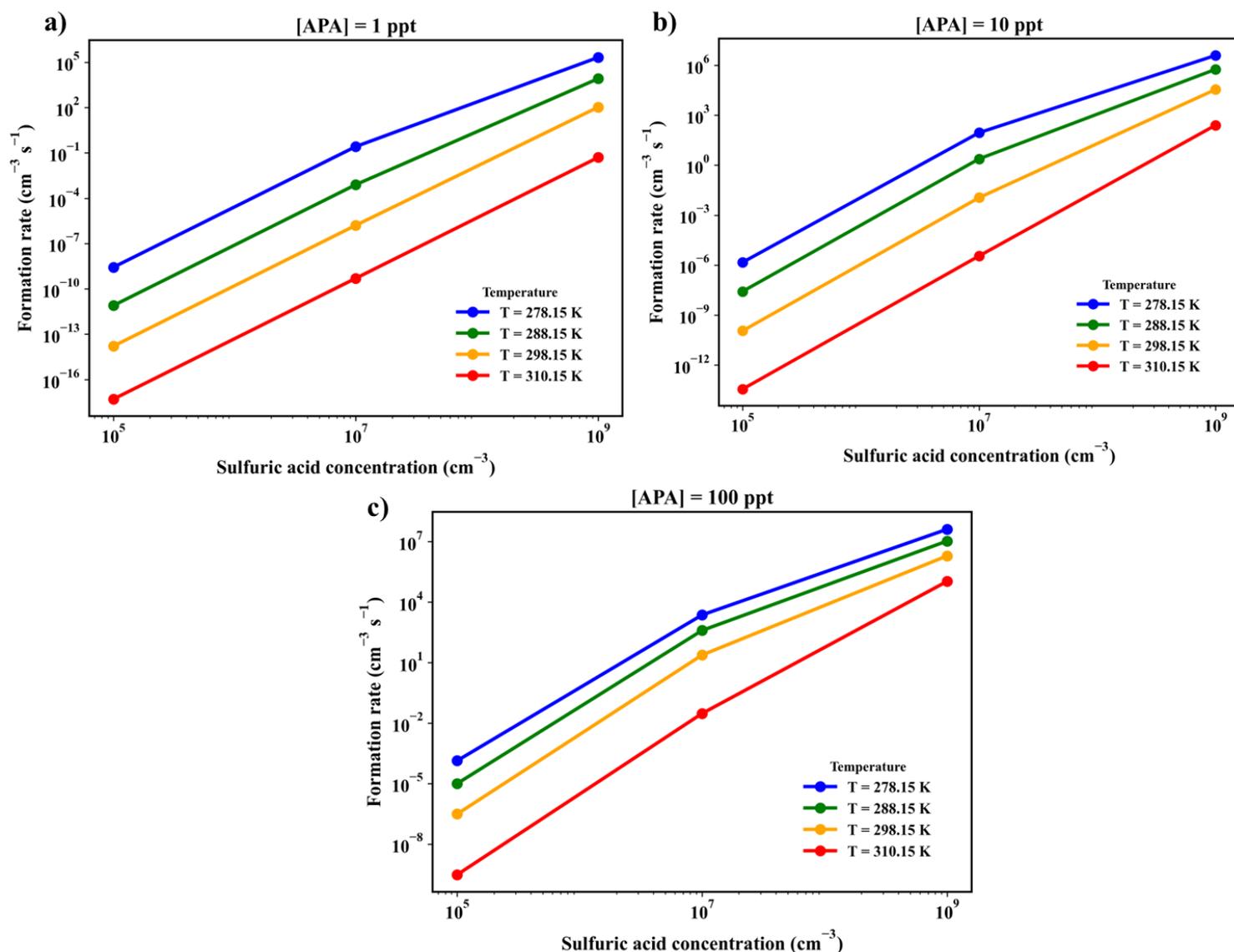
Figure S7. The formation rates of clusters at concentration of (a) APA = 1 ppt, (b) APA = 10 ppt and (c) APA =100 ppt as a function of temperature and SA monomer concentration.

Cartesian coordinates of the optimised geometries of APA-SA clusters computed at the M06-2X/ 6-311++G (3df, 3pd) level of theory

(APA)(SA)

C	1.52392900	0.51989400	-0.15717000
O	0.61707600	1.36741500	-0.15167700
N	1.30837100	-0.78531600	-0.19929100
H	2.11036100	-1.40322800	-0.24324000
H	0.35403300	-1.13672500	-0.19288600
S	-2.43737700	-0.20888900	-0.05502900
O	-1.77020500	1.02526800	-0.64216800
H	-0.74000600	1.11681000	-0.40240600
O	-2.61740600	0.15690800	1.47727600
H	-3.39005700	0.72718200	1.57483300

O	-1.52607900	-1.30933800	-0.04163600
O	-3.72492500	-0.35234400	-0.62901900
C	2.95791500	1.00298400	-0.12546900
C	3.95590500	0.09096300	0.58076100
H	2.93999200	1.98289000	0.34573200
H	3.26640700	1.16031300	-1.16289100
H	4.88527600	0.64744100	0.72712700
H	3.57328400	-0.16460500	1.56937600
N	4.14856000	-1.15793200	-0.16162100
H	4.60072300	-0.97679200	-1.05039500
H	4.74530900	-1.79465700	0.35066800

(APA)(SA)$_2$

C	0.89074600	-1.90491800	0.53274900
C	2.38857400	-1.69535500	0.61188700
C	3.02899200	-1.64680300	-0.76524200
H	2.84051000	-2.49960000	1.19201500
H	2.56114300	-0.75810600	1.14677800
H	2.80100400	-2.54573900	-1.33256300
O	0.32247200	-1.88642300	-0.55932800
N	0.25014700	-2.11422100	1.68444700
H	-0.75424200	-1.98666200	1.68536400
H	0.73028800	-1.94404800	2.55247500
N	2.52232100	-0.47383700	-1.52509900
H	2.97669000	-0.36954700	-2.42735200
H	4.10678100	-1.54301600	-0.67346200
H	1.50819400	-0.56354300	-1.66107000
S	-2.64253800	-0.14951100	-0.13713100
O	-1.81856900	-0.16198200	1.05523100
O	-4.04439300	-0.16768200	0.00149100
O	-2.24602200	1.05820000	-0.99409100
O	-2.22841200	-1.38916700	-0.97711900
H	-1.23827300	1.19964200	-0.99778200
H	-1.26930400	-1.61254000	-0.83211900
S	1.01484300	1.82084100	0.19911700
O	0.29269000	1.20531500	-0.93305200
O	0.65351000	3.16284600	0.48055900
O	0.64220700	0.90812200	1.44102100
O	2.45257200	1.56885900	0.04851100
H	-0.30848100	0.66187900	1.39403600
H	2.62322000	0.43414400	-0.93569000

(APA)(SA)$_3$

C	0.77981200	2.33469700	-0.91689000
C	-0.34977800	3.17940900	-1.46688800
C	-1.19744400	2.37909400	-2.44586700
H	0.09716100	4.02014800	-1.99950300
H	-0.95484100	3.57178200	-0.65360600

H	-0.63388900	2.13483600	-3.34109600
O	1.19427300	1.38311800	-1.58754100
N	1.28995600	2.68269300	0.25995500
H	1.99943300	2.09803700	0.68477600
H	0.80584700	3.33750800	0.85261000
N	-1.63809300	1.10257700	-1.81979600
H	-2.45582200	0.68602600	-2.25885200
H	-2.08202500	2.94547500	-2.72195900
H	-0.89304000	0.39443100	-1.84031400
S	-1.64456700	-2.15523300	-0.63586400
O	-2.58006400	-1.07490000	-0.43451500
O	-2.10952800	-3.34081300	-1.23798800
O	-0.47439600	-1.53923600	-1.47007800
O	-0.97424800	-2.51000100	0.70797100
H	0.43211500	-1.64452300	-1.03986800
H	-0.61697400	-1.67494900	1.11369400
S	2.88417400	-0.92881000	0.16558600
O	1.78530700	-1.75061900	-0.28507400
O	4.04866900	-1.56134100	0.63745100
O	3.28725900	0.04094400	-0.96219600
O	2.32494900	0.02545300	1.25843000
H	2.48429200	0.57022000	-1.26797600
H	1.31416900	-0.00761600	1.30433800
S	-1.20083200	0.90555700	1.77433700
O	-0.21835300	-0.04624500	1.18671000
O	-0.71876900	1.58282500	2.92366900
O	-1.72987300	1.77005000	0.72216200
O	-2.39150400	-0.00929000	2.23392600
H	-1.84655300	1.24761300	-0.79164100
H	-2.77863600	-0.43888400	1.44781700

(APA)₂(SA)

C	2.55787500	0.66298500	-0.24118900
C	3.18921300	-0.46151000	-1.03719300
C	3.73051200	-1.59463200	-0.17715200
H	3.98255000	-0.06457000	-1.67108500
H	2.40972100	-0.84089300	-1.70537600
H	4.52859600	-1.21022100	0.46275000
O	2.15967800	0.46878700	0.90793800
N	2.44141400	1.84015100	-0.86111000
H	1.74828600	2.49985200	-0.50335400
H	2.64549200	1.89213000	-1.84434600
N	2.67153400	-2.24906500	0.60648900
H	2.99810900	-3.14599600	0.94426800
H	4.17155000	-2.34011500	-0.83682600
H	2.47819700	-1.66727500	1.41493000
C	-2.85477700	-1.42101200	-0.45895500
C	-2.30736100	-1.28777000	0.95124100

C	-0.95221100	-1.97354300	1.08141000
H	-3.01516200	-1.77805800	1.62051700
H	-2.24721700	-0.24416300	1.24515600
H	-1.05935300	-3.05039000	1.18033800
O	-2.63770000	-2.42872700	-1.11800100
N	-3.58325000	-0.37932400	-0.89121200
H	-3.87394500	-0.40448200	-1.85560100
H	-3.42133100	0.53108200	-0.47036900
N	-0.11572700	-1.71991300	-0.12473800
H	0.87065300	-2.01347600	0.02225700
H	-0.41599500	-1.57882600	1.94086300
H	-0.53904800	-2.22900000	-0.90397100
S	-0.81814900	1.81798900	0.13992900
O	-0.04823500	3.02243100	-0.04863900
O	-2.23909900	1.98088600	0.28753500
O	-0.45965200	0.78059700	-0.84505900
O	-0.36223800	1.19787900	1.53931200
H	-0.16071200	-0.68301600	-0.37885200
H	0.61067600	1.07470600	1.50018000

$(APA)_2(SA)_2$

C	-3.10793300	0.35939600	1.46712000
C	-3.59295500	1.17142300	0.28061000
C	-2.72649200	2.38963000	0.01367000
H	-4.61977700	1.48590100	0.46736800
H	-3.59693300	0.51780500	-0.59498600
H	-2.63758800	3.01035000	0.90166100
O	-2.10022800	0.64843600	2.09465300
N	-3.89917500	-0.67959100	1.80332000
H	-3.54894200	-1.33373200	2.48336400
H	-4.57539700	-1.02527100	1.14375800
N	-1.37369700	1.94937800	-0.38221500
H	-0.69102300	2.69558000	-0.57333800
H	-3.14475000	2.98115800	-0.79604600
H	-0.95390000	1.39898600	0.37089900
C	2.79747300	-1.47750300	0.53318300
C	1.82604800	-2.60092000	0.87063700
C	1.00227700	-2.24105400	2.09436300
H	2.40473800	-3.49989400	1.08594900
H	1.18141800	-2.81321400	0.01742400
H	1.64997100	-2.02131000	2.93787000
O	3.16655800	-0.70568300	1.41221000
N	3.20428600	-1.40130800	-0.73795300
H	3.63770200	-0.53051000	-1.02899600
H	2.69699400	-1.91175900	-1.44377300
N	0.18683100	-1.03220600	1.81125000
H	-0.37516400	-0.70947800	2.59804600
H	0.32332500	-3.04963400	2.35179800

H	0.78199100	-0.25059800	1.50140400
S	1.94743100	1.83265700	-0.29683900
O	3.00478900	1.52010100	-1.21556300
O	1.23691800	3.06792600	-0.49885000
O	0.99639600	0.69550900	-0.15850800
O	2.58240600	1.96866200	1.14341100
H	0.68951600	-0.48377200	-1.30455700
H	3.06308300	1.13664000	1.33067800
S	-1.25158700	-1.26493900	-1.63534500
O	0.32922400	-1.29476700	-1.74640300
O	-1.70419400	-2.43667600	-2.30064200
O	-1.52824000	-1.25068300	-0.18161000
O	-1.67479600	0.00639100	-2.21715700
H	-0.48780500	-1.18162100	0.99860200
H	-1.41983200	1.28741300	-1.20282100

$(APA)_2(SA)_3$

C	2.16891300	-0.77723700	-1.77412300
C	3.58573900	-0.89608500	-1.23179500
C	3.99653600	0.38253100	-0.53019600
H	4.25005000	-1.05020900	-2.08333500
H	3.66984900	-1.75973700	-0.57385500
H	3.79126900	1.24613300	-1.15499500
O	1.69673200	0.34014300	-1.98921800
N	1.53435600	-1.91226500	-2.02756500
H	0.55742400	-1.91747300	-2.31866100
H	1.89718700	-2.77939700	-1.66593400
N	3.19888300	0.57261000	0.71732500
H	3.45772100	-0.10958000	1.43637600
H	5.04659800	0.36432600	-0.25212400
H	3.26282400	1.53422100	1.05224400
C	-2.29803500	0.66858600	1.63534800
C	-3.68243400	0.60139900	1.02282900
C	-3.89976000	1.70584900	0.00530300
H	-4.40848800	0.72678900	1.82712100
H	-3.84617400	-0.38074800	0.57931500
H	-3.72125100	2.68227900	0.44604300
O	-1.63957300	1.70975000	1.51143900
N	-1.89919900	-0.39576000	2.30939200
H	-0.94864000	-0.47247400	2.65580000
H	-2.36368000	-1.27740700	2.14696700
N	-2.96359800	1.54566000	-1.14507800
H	-3.14275900	2.22906500	-1.87588500
H	-4.91018700	1.65848100	-0.39165500
H	-1.98308600	1.64824200	-0.84709600
S	1.11420600	-1.90555400	1.54698000
O	0.74873500	-0.65308000	0.82428500
O	0.56032100	-3.07498100	0.65936900

O	2.54676700	-2.07744600	1.53675300
O	0.46725400	-1.95770900	2.82795700
H	2.18683600	0.37924800	0.56679700
H	-0.41521800	-2.97622600	0.52065900
S	0.88761200	3.03615900	-0.06647300
O	0.10966500	2.14985500	-1.08949100
O	0.80643800	2.22367100	1.24963500
O	2.27834500	3.04854000	-0.39811100
O	0.15735500	4.24514000	0.03511600
H	0.66829200	1.39590300	-1.45376600
H	-0.15731800	1.97017800	1.47310200
S	-1.94404300	-1.69035100	-1.20878300
O	-3.20882000	-1.08725300	-1.61847000
O	-1.05858400	-0.40254200	-0.93484000
O	-2.02089700	-2.38412600	0.07351700
O	-1.28553600	-2.44695300	-2.23871400
H	-3.06016700	0.56253600	-1.52303100
H	-0.33996700	-0.56424300	-0.24820000

(APA)₃(SA)

C	1.48275200	2.77622500	-0.65709100
C	0.64294400	2.06586200	0.39379700
C	-0.48726300	2.94212000	0.89637800
H	1.27814400	1.77933900	1.23198100
H	0.24063800	1.13554900	-0.01230400
H	-0.10639000	3.85846500	1.34025400
O	1.18840900	3.89455400	-1.05599700
N	2.55264900	2.09804000	-1.10106200
H	3.08241300	2.51143300	-1.85051900
H	2.70411900	1.12399400	-0.85296300
N	-1.37337900	3.32073400	-0.24082000
H	-2.23264600	3.74710500	0.10194300
H	-1.10319800	2.40401300	1.61073900
H	-0.84759400	3.92749400	-0.87209700
C	-0.70687700	-2.36333800	-0.98342100
C	-2.19627500	-2.55504200	-1.15327600
C	-2.80555600	-3.21892800	0.07816600
H	-2.34661200	-3.19576800	-2.02337200
H	-2.68423200	-1.60229100	-1.34417700
H	-2.61633700	-4.29270900	0.05860500
O	0.00394200	-3.27521600	-0.55374100
N	-0.22961200	-1.16164800	-1.32033900
H	0.74609800	-0.95996100	-1.12566700
H	-0.88360500	-0.39689300	-1.45102900
N	-2.26884400	-2.61326800	1.31105300
H	-2.85130900	-2.85538400	2.10352000
H	-3.87893500	-3.04808100	0.06169500
H	-1.34347100	-2.99253800	1.48676600

C	3.24304400	-1.64262400	-0.02723800
C	4.72047800	-1.50828500	0.28982700
C	5.14979600	-0.06195400	0.46686500
H	5.27037300	-1.97019000	-0.53340100
H	4.94328900	-2.07271300	1.19592700
H	4.96003500	0.48399900	-0.46417700
O	2.57337300	-0.66877000	-0.38379100
N	2.71616700	-2.86113500	0.07691200
H	1.72900600	-3.02941800	-0.16439800
H	3.29068400	-3.63099900	0.37066000
N	4.48860900	0.51762800	1.63020400
H	4.86491800	1.43344500	1.83765500
H	6.22495200	-0.04023900	0.63991400
H	3.50232900	0.63844900	1.43356800
S	-3.06196100	0.68865100	0.27208300
O	-2.25590400	0.95473100	-0.95540200
O	-2.03708000	0.03317400	1.27083000
O	-3.43943300	1.94329600	0.88281000
O	-4.10386300	-0.27122800	0.04475200
H	-1.69810100	2.41820600	-0.71860200
H	-2.14613700	-0.98372500	1.27477500

(APA)$_3$(SA)$_2$

C	1.20483800	-0.46278200	2.08766700
C	0.01042100	-0.29120200	3.00779100
C	-0.81752900	0.94882200	2.71641800
H	0.41812400	-0.19621600	4.01626400
H	-0.60890900	-1.18416100	2.97875700
H	-0.23631100	1.85734000	2.84071300
O	1.83701400	0.51416100	1.66678200
N	1.57482400	-1.71174100	1.82548700
H	2.45412500	-1.86626100	1.32756200
H	0.94565000	-2.48838000	1.97472700
N	-1.36017500	0.93572200	1.32790600
H	-2.37329000	1.18021100	1.30689500
H	-1.66051200	0.98590800	3.40224500
H	-0.83564000	1.54946900	0.68051900
C	-3.02825300	0.08624200	-1.45770000
C	-3.64449700	1.45281500	-1.22025900
C	-4.74685700	1.39907400	-0.17554900
H	-4.04992800	1.80031800	-2.17247400
H	-2.86262100	2.15975000	-0.93355400
H	-5.57757700	0.80257000	-0.55530400
O	-3.63814200	-0.94280200	-1.18116700
N	-1.79840800	0.08897600	-1.98508000
H	-1.32258700	-0.79874700	-2.10931500
H	-1.28756500	0.95312800	-2.08694300
N	-4.22397900	0.85838700	1.09015700

H	-4.87847600	1.03494800	1.84221400
H	-5.11012600	2.40891200	0.00512000
H	-4.15105600	-0.15184900	0.99480200
C	2.59038300	-0.36699600	-1.33923300
C	3.19904200	-1.71944800	-1.55160300
C	4.51594100	-1.86331100	-0.79756600
H	3.36637900	-1.83053000	-2.62517800
H	2.47774100	-2.47787400	-1.24651400
H	5.26775300	-1.21152700	-1.24666600
O	3.39588900	0.62370200	-1.24356100
N	1.30234400	-0.24368100	-1.27211600
H	0.86487700	0.67007400	-1.11018500
H	0.70856400	-1.09263300	-1.27933300
N	4.30210200	-1.58655900	0.62391600
H	5.07542700	-1.92923000	1.17896900
H	4.85747400	-2.89069200	-0.90390000
H	4.24499200	-0.58433600	0.78145200
S	1.01255000	3.19869400	-0.34739800
O	-0.01378800	2.20726300	-0.74438000
O	0.63646000	4.54933200	-0.55403200
O	1.15612800	3.01581200	1.21004200
O	2.30494400	2.81820600	-0.92626300
H	1.48733800	2.10321800	1.42666800
H	2.91948800	1.54118800	-1.08433800
S	-1.01975500	-2.80170800	-0.11601200
O	-0.33097900	-2.40112600	-1.34911900
O	-0.37599000	-3.86302000	0.59464500
O	-1.30171200	-1.63144600	0.72133500
O	-2.42338500	-3.33762800	-0.56128500
H	-1.31567600	-0.03466800	0.93471800
H	-2.95179300	-2.56835400	-0.87902400

(APA)₃(SA)₃

C	1.40348500	1.94922600	1.58069200
C	0.22999600	2.70957300	2.15628100
C	-0.03461100	4.02242100	1.44076700
H	0.43995400	2.88762200	3.21162300
H	-0.64075100	2.05165200	2.14230400
H	0.87550000	4.62509400	1.44223900
O	2.02520400	2.40467200	0.60765800
N	1.72755800	0.81483000	2.18683300
H	2.57229200	0.33529400	1.89643000
H	1.13750800	0.46105800	2.93772300
N	-0.52827000	3.77987700	0.07989300
H	-0.73760400	4.65785900	-0.38164300
H	-0.79961200	4.57057900	1.98938800
H	0.19932700	3.33311800	-0.47128300
C	-3.35186000	1.49017400	-0.80779100

C	-4.52443700	0.60928100	-0.49246700
C	-4.91179600	-0.30074300	-1.64938600
H	-5.36043100	1.25869700	-0.22381500
H	-4.26377700	0.02434200	0.39181000
H	-5.26036200	0.30571200	-2.48843900
O	-3.08421300	1.70805600	-2.04885400
N	-2.64949200	2.01149000	0.14573300
H	-1.82378500	2.68260900	0.01303600
H	-2.81273900	1.65818300	1.08000400
N	-3.79317800	-1.17230000	-2.01099600
H	-4.11331700	-1.91747600	-2.61780600
H	-5.74426100	-0.92044600	-1.32182400
H	-3.09871200	-0.64814400	-2.53544500
C	-0.73529100	-3.03633600	-0.79468100
C	0.18462800	-3.93242700	0.00517200
C	1.58981200	-3.35145400	0.03049000
H	0.21843500	-4.89548900	-0.50415400
H	-0.19491500	-4.07867000	1.01345600
H	1.99507000	-3.25163600	-0.97250500
O	-0.37710000	-2.68550400	-1.93076400
N	-1.87543200	-2.66647400	-0.23728000
H	-2.54224900	-2.07974200	-0.75096600
H	-2.01472900	-2.82170300	0.75096600
N	1.56811900	-1.99582500	0.63923500
H	2.51870300	-1.63789100	0.81377600
H	2.24983000	-3.97455800	0.62727800
H	1.13369400	-1.30739800	0.00514400
S	0.03253000	0.61155600	-1.95760800
O	0.07921500	0.19776100	-0.55222700
O	1.33762500	0.55215400	-2.58174300
O	-0.92249200	-0.36977200	-2.68475200
O	-0.60301800	1.91356400	-2.14968700
H	-0.72407400	-1.35158700	-2.42562300
H	-2.08280400	1.93110200	-2.17225800
S	-1.30980500	-0.96593000	2.89810400
O	-0.54675500	-0.01798100	3.67917700
O	-2.55466000	-1.39330100	3.44695000
O	-1.76610000	-0.16373100	1.56591800
O	-0.47434800	-2.05597300	2.37867900
H	-1.04326800	-0.08144000	0.91419300
H	0.97656000	-1.98126600	1.49925700
S	4.20184700	-0.06884800	-0.57971200
O	3.94523400	-0.49980200	0.78424400
O	5.48973700	-0.31728200	-1.10155100
O	3.13519100	-0.80237000	-1.44256900
O	3.85910600	1.40612600	-0.72345600
H	2.48193000	-0.19754900	-1.93397400
H	3.07972800	1.76122400	-0.11600100

(APA)₂

C	-2.00109300	0.49090400	-0.31443300
C	-3.45549700	0.92478100	-0.35576800
C	-4.40662900	-0.22865500	-0.08797200
H	-3.64140500	1.35425600	-1.34296900
H	-3.61106700	1.71123100	0.38418700
H	-4.24895200	-0.99912300	-0.84873700
O	-1.68745500	-0.69475800	-0.29636800
N	-1.09151700	1.47605500	-0.31976700
H	-0.09437100	1.25329900	-0.30977700
H	-1.38643700	2.43547400	-0.31891800
N	-4.22520000	-0.71537400	1.27626800
H	-4.95107600	-1.37744200	1.51685600
H	-5.42852200	0.13545800	-0.18967100
H	-3.34160900	-1.20847400	1.33272200
C	2.00108300	-0.49091000	-0.31436600
C	3.45548500	-0.92479000	-0.35571500
C	4.40662700	0.22865200	-0.08797300
H	3.64137600	-1.35429700	-1.34290600
H	3.61106500	-1.71121800	0.38426100
H	4.24893000	0.99910400	-0.84875100
O	1.68744500	0.69475300	-0.29638600
N	1.09150500	-1.47606000	-0.31965500
H	0.09435700	-1.25330100	-0.30971200
H	1.38642100	-2.43547900	-0.31879400
N	4.22524400	0.71540000	1.27626300
H	4.95113000	1.37747000	1.51681300
H	5.42851600	-0.13546600	-0.18969400
H	3.34165600	1.20850400	1.33273400

(APA)₃

C	2.44383700	-1.33805600	0.61518100
C	3.83057100	-0.91818700	0.17639400
C	3.81362700	0.57335500	-0.15797700
H	4.50418100	-1.10393500	1.01253900
H	4.17406900	-1.49332300	-0.68410600
H	3.33847900	1.09803500	0.66947800
O	1.96654400	-0.88163500	1.64465400
N	1.77619800	-2.19827900	-0.17320400
H	0.81737500	-2.46134000	0.06072200
H	2.18071500	-2.50767500	-1.03735900
N	3.02813000	0.81890200	-1.36780000
H	3.61260500	0.82039800	-2.19317900
H	4.83941300	0.94066900	-0.23833100
H	2.55455400	1.71459300	-1.30159600
C	-0.18581200	1.81751800	-0.81059900
C	-1.62786200	2.27660700	-0.67493200

C	-1.82289000	3.10692700	0.58370000
H	-1.86120700	2.87945800	-1.55506600
H	-2.29023300	1.41182300	-0.68742400
H	-1.28717000	4.05210800	0.47215100
O	0.73636600	2.52039500	-0.41618600
N	-0.01365100	0.62507100	-1.40194700
H	0.93114800	0.25879300	-1.46268600
H	-0.81629500	0.03838400	-1.59829500
N	-1.37615700	2.35319900	1.76147200
H	-1.66537300	2.82455400	2.60949400
H	-2.88225200	3.33262200	0.70041300
H	-0.35969800	2.35080100	1.76466300
C	-1.55415200	-1.54350500	0.83328400
C	-3.00075900	-1.19783500	0.53031000
C	-3.41980700	-1.73028200	-0.83284600
H	-3.61876600	-1.64490000	1.31160500
H	-3.13552500	-0.11794200	0.59052400
H	-3.54427300	-2.81322000	-0.77217800
O	-1.04846000	-2.56593900	0.36772000
N	-0.90375400	-0.69112600	1.62535400
H	0.09579800	-0.83052900	1.78032300
H	-1.29161700	0.22900100	1.80829100
N	-2.43787300	-1.35007200	-1.85841400
H	-2.84452000	-1.42787200	-2.78183900
H	-4.38425800	-1.30021400	-1.09941400
H	-1.67352000	-2.01597400	-1.81156000