Uptake of ammonia by mixed sodium sulfate–bisulfate cluster cations

Supplementary information

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Table S1. Product-to-reactant ratio for ammonia uptake by mass-selected mixed sodium sulfate–bisulfate cluster ions at final conversion as a function of NH_3 concentration (0.1, 1, 5, and 10% NH_3 in He buffer gas).

Cluster (*m*/*z*)	Conversion in % / v/v NH_3			
$Na^+[Na_2SO_4][NaHSO_4]_2$ (404.8)	31	46	23	/ 10%
	39	44	17	/ 5%
	46	41	13	/ 1%
	83	17	0	/ 0.1%
$Na^+[Na_2SO_4]_2[NaHSO_4]$ (426.8)	61	39	0	/ 10%
	45	44	11	/ 5%
	34	56	10	/ 1%
	62	38	0	/ 0.1%
$Na^+[Na_2SO_4][NaHSO_4]_3$ (524.7)	61	39	0	/ 10%
	56	44	0	/ 5%
	58	35	7	/ 1%
	88	12	0	/ 0.1%
$Na^+[Na_2SO_4]_2[NaHSO_4]_2$ (546.8)	54	39	7	/ 10%
	51	38	11	/ 5%
	57	35	8	/ 1%
	90	10	0	/ 0.1%
$Na^+[Na_2SO_4]_3[NaHSO_4]$ (568.7)	26	58	16	/ 10%
	17	76	7	/ 5%
	21	69	10	/ 1%
	32	59	9	/ 0.1%
$Na^+[Na_2SO_4][NaHSO_4]_4$ (644.7)	56	34	10	/ 10%
	53	37	10	/ 5%
	67	33	0	/ 1%
	90	10	0	/ 0.1%
$Na^+[Na_2SO_4]_2[NaHSO_4]_3$ (666.7)	52	33	12	3 / 10%
	73	22	5	0 / 5%
	71	25	4	0 / 1%
	95	5	0	0 / 0.1%
$Na^+[Na_2SO_4]_3[NaHSO_4]_2$ (688.7)	49	41	10	/ 10%
	54	33	13	/ 5%
	71	21	8	/ 1%
	90	10	0	/ 0.1%

$Na^+[Na_2SO_4][NaHSO_4]_5$ (764.7)	0	0	0	16	35	49	/ 10%
	0	10	6	6	14	64	/ 5%
	36	42	8	6	0	8	/ 1%
	76	24	0	0	0	0	/ 0.1%
$Na^+[Na_2SO_4]_2[NaHSO_4]_4$ (786.6)	3	0	7	21	69	/ 10%	
	4	2	0	8	86	/ 5%	
	8	2	0	2	88	/ 1%	
	97	3	0	0	0	/ 0.1%	
$Na^+[Na_2SO_4]_3[NaHSO_4]_3$ (808.6)	0	0	16	84	/ 10%		
	0	0	15	85	/ 5%		
	0	0	12	88	/ 1%		
	9	0	0	91	/ 0.1%		
$Na^+[Na_2SO_4]_4[NaHSO_4]_2$ (830.6)	9	18	73	/ 10%			
	0	18	82	/ 5%			
	5	13	82	/ 1%			
	9	19	72	/ 0.1%			
$Na^+[Na_2SO_4][NaHSO_4]_6$ (884.6)	0	0	0	30	46	24	/ 10%
	0	0	19	21	60	0	/ 5%
	0	0	38	0	62	0	/ 1%
	69	31	0	0	0	0	/ 0.1%
$Na^+[Na_2SO_4]_2[NaHSO_4]_5$ (906.6)	0	0	17	56	27	/ 10%	
	5	9	5	37	44	/ 5%	
	0	0	0	25	75	/ 1%	
	72	28	0	0	0	/ 0.1%	
$Na^+[Na_2SO_4]_3[NaHSO_4]_4$ (928.6)	0	11	43	46	/ 10%		
	15	5	19	61	/ 5%		
	0	0	17	83	/ 1%		
	38	0	18	44	/ 0.1%		
$Na^+[Na_2SO_4]_4[NaHSO_4]_3$ (950.6)	0	30	70	/ 10%			
	6	18	76	/ 5%			
	0	0	100	/ 1%			
	0	23	77	/ 1%			

Table S2. Bimolecular rate coefficients (in $cm^3\ s^{-1}$) for ammonia uptake and the corresponding unimolecular evaporation rate coefficients (s^{-1}) for mass-selected mixed sodium sulfate–bisulfate cluster ions.

Cluster (*m*/*z*)	$k_{attachment}$ $cm^3\ s^{-1}$	$k_{evaporation}$ s^{-1}
$Na^+[Na_2SO_4]_3[NaHSO_4]$ (568.7)	0.05% NH_3	0.05% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	1.4×10^{-10}	23
$Na^+[Na_2SO_4]_2[NaHSO_4]_4$ (786.6)	1% NH_3	1% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	3.5×10^{-11}	130
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 < k_1$	$k_{-2} < k_{-1}$
$[M+2NH_3]^+ + NH_3 \rightleftharpoons [M+3NH_3]^+$	$k_3 >> k_1$	$k_{-3} >> k_{-1}$
$[M+3NH_3]^+ + NH_3 \rightleftharpoons [M+4NH_3]^+$	$k_4 >> k_3$	$k_{-4} < k_{-1}$
	0.5% NH_3	0.5% NH_3
	1.0×10^{-11}	200
	$k_2 \approx k_1$	$k_{-2} < k_{-1}$
	$k_3 > k_2$	$k_{-3} < k_{-1}$
	$k_4 \approx k_3$	$k_{-4} < k_{-1}$
$Na^+[Na_2SO_4]_3[NaHSO_4]_3$ (808.6)	0.5% NH_3	0.5% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	1.4×10^{-11}	130
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 > k_1$	$k_{-2} << k_{-1}$
$[M+2NH_3]^+ + NH_3 \rightleftharpoons [M+3NH_3]^+$	$k_3 > k_2$	$k_{-3} < k_{-1}$
	0.1% NH_3	0.1% NH_3
	1.6×10^{-10}	630
	$k_2 \approx k_1$	$k_{-2} << k_{-1}$
	$k_3 \approx k_1$	$k_{-3} << k_{-1}$
	0.05% NH_3	0.05% NH_3
	4.5×10^{-12}	4.8
	$k_2 >> k_1$	$k_{-2} >> k_{-1}$
	$k_3 >> k_2$	$k_{-3} \approx k_{-1}$
$Na^+[Na_2SO_4]_4[NaHSO_4]_2$ (830.6)	0.01% NH_3	0.01% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	3.4×10^{-10}	170
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 > k_1$	$k_{-2} < k_{-1}$

$Na^+[Na_2SO_4]_2[NaHSO_4]_5$ (906.6)	0.5% NH_3	0.5% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	6.8×10^{-11}	25
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 >> k_1$	$k_{-2} >> k_{-1}$
$[M+2NH_3]^+ + NH_3 \rightleftharpoons [M+3NH_3]^+$	$k_3 > k_1$	$k_{-3} \approx k_{-1}$
$[M+3NH_3]^+ + NH_3 \rightleftharpoons [M+4NH_3]^+$	$k_4 > k_2$	$k_{-4} >> k_{-1}$
$Na^+[Na_2SO_4]_3[NaHSO_4]_4$ (928.6)	0.5% NH_3	0.5% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	3.6×10^{-11}	~0
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 >> k_1$	$k_{-2} \approx k_{-1}$
$[M+2NH_3]^+ + NH_3 \rightleftharpoons [M+3NH_3]^+$	$k_3 >> k_1$	$k_{-3} \approx k_{-1}$
	0.1% NH_3	0.1% NH_3
	1.8×10^{-10}	20
	$k_2 \approx k_1$	$k_{-2} \approx k_{-1}$
	$k_3 \approx k_1$	$k_{-3} \approx k_{-1}$
	0.05% NH_3	0.05% NH_3
	5.1×10^{-11}	180
	$k_2 >> k_1$	$k_{-2} > k_{-1}$
	$k_3 > k_1$	$k_{-3} < k_{-1}$
$Na^+[Na_2SO_4]_4[NaHSO_4]_3$ (950.6)	0.01% NH_3	0.01% NH_3
$M^+ + NH_3 \rightleftharpoons [M+NH_3]^+$	5.7×10^{-10}	67
$[M+NH_3]^+ + NH_3 \rightleftharpoons [M+2NH_3]^+$	$k_2 >> k_1$	$k_{-2} >> k_{-1}$

Table S3. Calculated standard Gibbs energies (in kcal/mol) for adsorption of ammonia molecules on $Na^+[Na_2SO_4]_m[NaHSO_4]_n$ clusters as calculated using different methods. For all methods but r2SCAN-3c, the def2TZVP basis set was used. Mean absolute errors are provided with respect to the values calculated through r2SCAN-3c. Global minimum structures were selected based on energies from r2SCAN-3c and directly reoptimized with the respective methods.

m	*n*	#(NH_3)	r2SCAN-3c	B3PW91	*ω*B97X-D4	B3LYP	B3PW91-D4	B3LYP-D4	CAMB3LYP-D4
1	1	1	-10.3	-9.8	-12.1	-11.0	-10.8	-12.0	-12.7
1	1	2	-8.2	-8.2	-9.3	-8.3	-10.3	-10.1	-10.9
1	2	1	-7.1	-7.3	-8.5	-8.3	-8.3	-10.0	-10.0
1	2	2	-8.0	-7.2	-9.2	-8.4	-8.9	-8.3	-10.3
1	3	1	-8.0	-7.3	-8.9	-8.3	-8.7	-9.8	-10.2
1	3	2	-7.1	-7.0	-8.5	-7.2	-8.9	-8.7	-9.5
1	3	3	-6.8	-6.0	-8.1	-6.9	-6.8	-8.1	-8.7
1	4	1	-8.2	-3.5	-10.4	-3.6	-7.9	-8.3	-8.5
1	4	2	-7.1	-6.4	-8.5	-7.4	-7.7	-8.4	-8.9
1	4	3	-10.5	-2.7	-9.4	-3.4	-12.1	-12.5	-15.8
1	4	4	-6.6	-4.9	-7.7	-6.0	-7.2	-8.2	-8.7
2	1	1	-9.4	-9.0	-11.0	-10.8	-9.8	-13.2	-11.2
2	1	2	-7.1	-6.4	-8.7	-7.0	-7.5	-5.8	-9.9
2	2	1	-7.5	-6.7	-6.6	-7.6	-6.4	-7.4	-8.8
2	2	2	-10.3	-3.2	-7.9	-1.2	-10.7	-8.2	-9.4
2	3	1	-12.2	-9.1	-15.0	-8.4	-15.2	-14.4	-17.2
2	3	2	-9.1	-7.5	-11.0	-9.2	-10.5	-11.3	-13.0
2	3	3	-9.4	-5.1	-8.5	-6.1	-7.8	-8.9	-10.6
2	4	1	-6.6	-4.9	-7.2	-5.3	-6.3	-6.9	-7.9
2	4	2	-7.3	-3.7	-10.0	-2.4	-13.7	-11.8	-13.5
2	4	3	-11.4	-11.2	-15.7	-12.5	-13.8	-14.6	-14.2
2	4	4	-15.6	-7.2	-13.8	-8.4	-14.3	-15.2	-18.4
3	1	1	-12.8	-9.7	-15.2	-10.1	-12.9	-12.7	-15.7
3	1	2	-6.1	-5.0	-7.2	-5.6	-6.2	-7.1	-7.7
3	2	1	-9.0	-6.8	-7.5	-8.1	-8.2	-9.5	-11.1
3	2	2	-8.5	-1.6	-8.3	-2.2	-9.6	-9.9	-11.8
3	3	1	-11.3	-8.3	-13.6	-7.3	-14.7	-14.5	-15.3
3	3	2	-8.7	-8.5	-12.5	-10.0	-11.5	-11.8	-11.5
3	3	3	-11.2	-5.7	-11.9	-7.7	-11.0	-12.7	-14.7
3	4	1	-9.6	-6.6	-7.6	-7.2	-8.5	-8.4	-10.0
3	4	2	-10.8	-8.0	-12.6	-8.6	-11.7	-12.3	-13.4
3	4	3	-5.9	1.8	-7.3	0.5	-7.6	-8.4	-10.1
3	4	4	-7.9	-7.9	-9.7	-7.6	-11.0	-10.9	-11.9
Mean absolute error				2.6	1.7	2.4	1.3	1.7	2.6

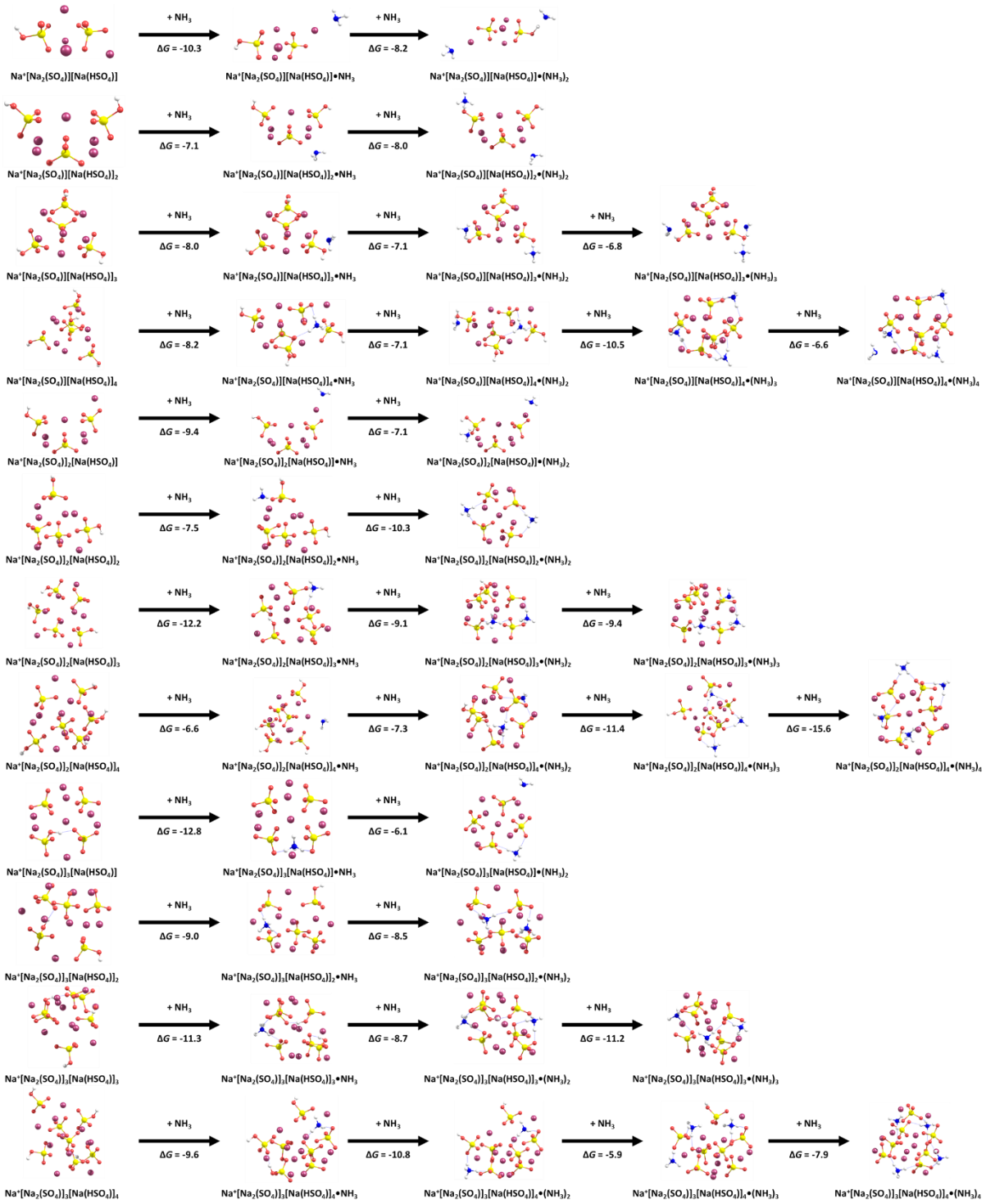

Figure S1. The most stable structures obtained through quantum chemical calculations, along with the respective Gibbs energy values for NH_3 adsorption in kca/mol.

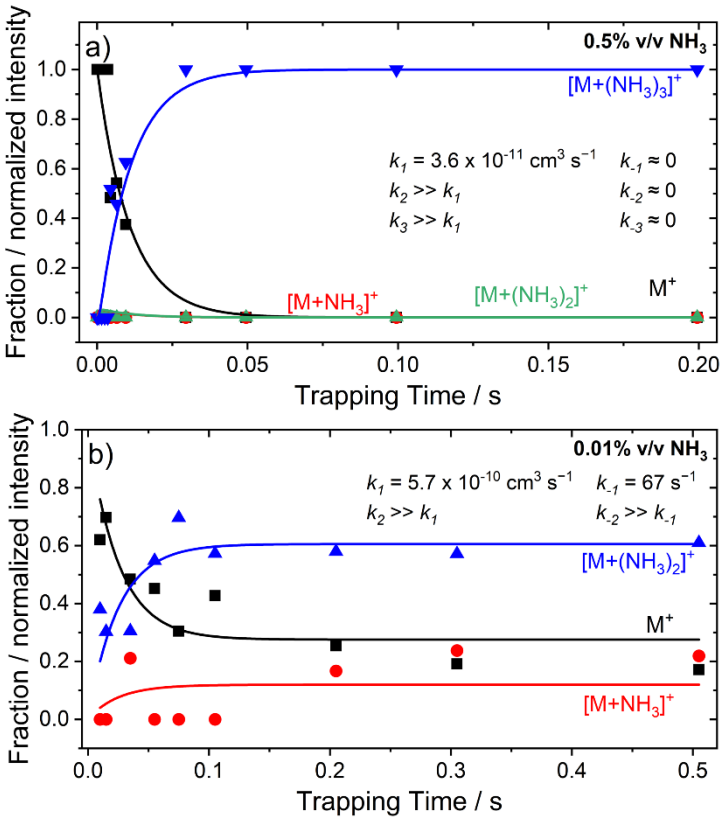

Figure S2. Kinetic measurements of ammonia uptake by mixed sulfate–bisulfate cluster ions: (a) $Na^+[Na_2(SO_4)]_3[Na(HSO_4)]_4$; and (b) $Na^+[Na_2(SO_4)]_4[Na(HSO_4)]_3$. The kinetic model assumes reversible NH_3 uptake.

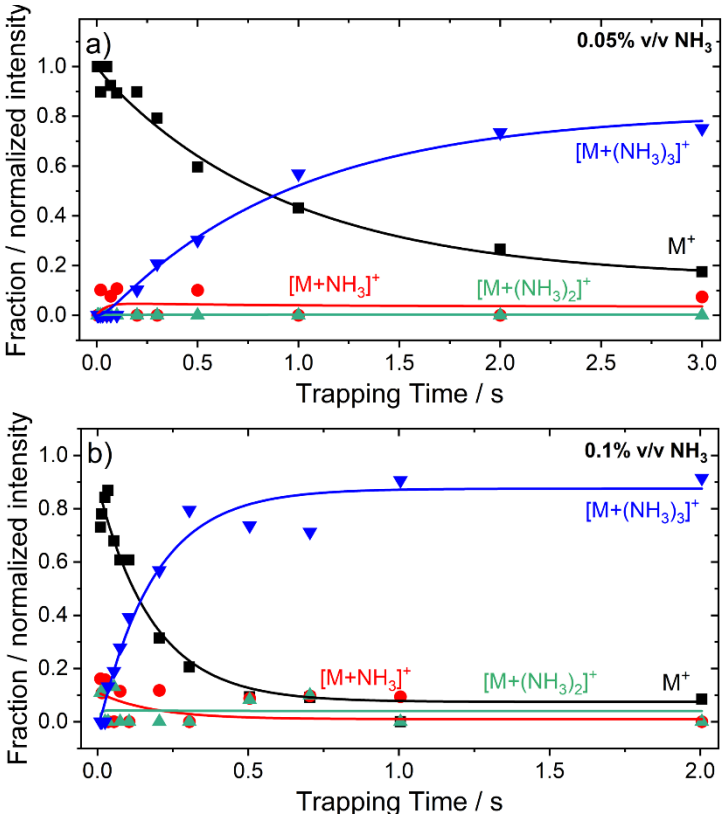

Figure S3. Kinetics of NH_3 uptake by $Na^+[Na_2SO_4]_3[NaHSO_4]_3$ cluster ions (*m/z* = 808.6) exposed to NH_3/He gas mixtures (2.1 Pa) containing (a) 0.05% and (b) 0.1% (v/v) ammonia. The kinetic model assumes reversible NH_3 uptake.

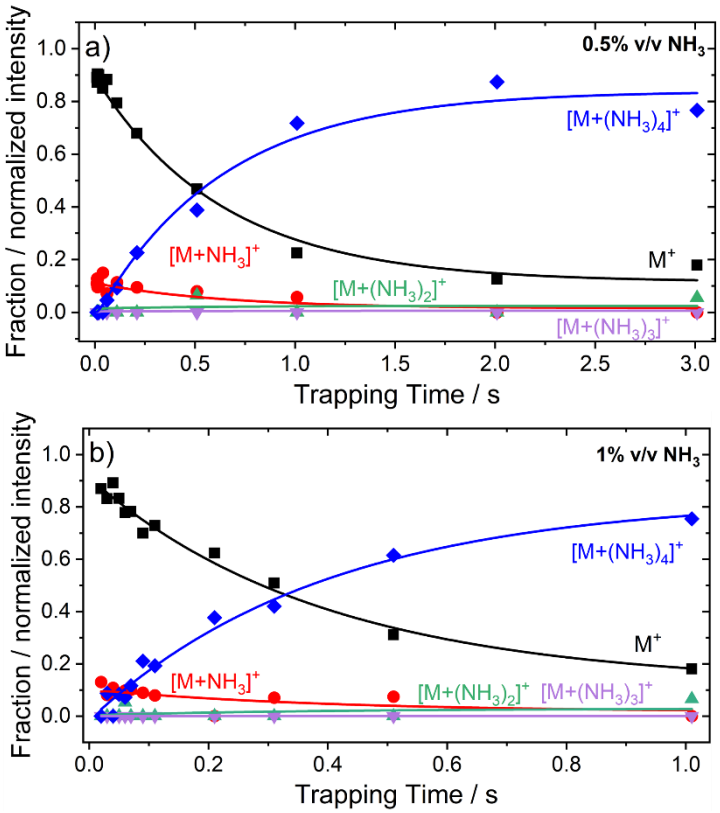

Figure S4. Kinetics of NH_3 uptake by $Na^+[Na_2SO_4]_2[NaHSO_4]_4$ cluster ions (*m/z* = 786.6) exposed to NH_3/He gas mixtures (2.1 Pa) containing (a) 0.5% and (b)1.0% (v/v) ammonia. The kinetic model assumes reversible NH_3 uptake.

Calculated Gibbs energies and Cartesian coordinates of optimized clusters

NH_3

Final Gibbs free energy ... -56.52551615 Eh

N	1.14702696018563	1.00554661981032	1.43887649524083
H	0.15671900211907	0.85053998012559	1.28386985526031
H	1.30203360001661	1.99585457790846	1.28386985548877
H	1.30203360020452	0.85053998016615	2.42918445335640

$Na^+(Na_2SO_4)(NaHSO_4)$

Final Gibbs free energy ... -2047.86671755 Eh

S	-3.39985808817083	-0.42264008323417	-5.01876254639175
O	-3.51643357445839	0.44344321614970	-6.38176622653281
O	-4.77189197656024	-0.67476441337114	-4.48306710131827
O	-2.55928062719843	0.32421292393815	-4.03468233855317
O	-2.73733529636470	-1.68160754748640	-5.47489652971882
H	-3.94585840096515	1.29645602462531	-6.19495291631586
Na	-4.29104160820465	-3.13638717876055	-4.42189605184532
Na	-1.69959467589834	-5.62035543408873	-1.72969311980749
Na	-1.08863073913350	-1.65957541714280	-3.73523171555692
Na	-4.02065519628494	-0.40000158850170	-2.14735124729102
S	-2.86806294238978	-3.06425688755779	-1.84992737787605
O	-2.69935036217932	-3.96609957013206	-0.67257906134344
O	-2.12944098585850	-1.74591474582473	-1.70303913691422
O	-4.31948639038382	-2.74511718548825	-2.15620194978291
O	-2.27596781295380	-3.79353832712078	-3.09719115273756

$Na^+(Na_2SO_4)(NaHSO_4)(NH_3)$

Final Gibbs free energy ... -2104.40867949 Eh

S	-1.47871643229425	-0.52933287388029	-4.22184428380825
O	-1.76054439401919	0.60836057929166	-5.34150636636851
O	-1.26760278058946	-1.84229327109833	-4.90473354698233
O	-2.73149470437384	-0.51839605080292	-3.40855483114646
O	-0.28225278759708	-0.13479653311812	-3.41876915039385
H	-0.98609266037922	0.69104890470031	-5.92463897681282
Na	-1.61229193117962	-0.45497548886306	-1.29827060042848
Na	-3.14774101728923	-4.08850748953568	0.83637601098949
Na	0.51655008902205	-2.49138722441841	-3.29916367587955
Na	-3.00623571456209	-2.90745808587482	-3.46961280644530
S	-1.26132747062321	-3.35692697236090	-1.16901998113327
O	-0.22258909300362	-2.25063068675056	-1.07747745784946
O	-1.17139472830122	-3.94999840881154	-2.56576261621554
O	-2.66308959392775	-2.68389634266850	-1.04384100571129
O	-1.13550664309024	-4.37359813217157	-0.08857821969055
N	-4.46730823442400	-4.96472571620857	2.64958215896998
H	-4.77116043998098	-4.28403241835266	3.34080808902482
H	-3.92304219415489	-5.64739397632422	3.17127126163223
H	-5.31243934553705	-5.45650664261569	2.37185667791223

$Na^+(Na_2SO_4)(NaHSO_4)(NH_3)_2$

Final Gibbs free energy ... -2160.94733162 Eh

Na	-5.86972267558443	-4.31751653100634	-0.23877073306948
Na	-1.82913277724979	-4.91997752138115	-2.08159637236837
Na	-5.25068283224768	-7.61796333907634	-1.04987883453443
Na	-5.17995161281749	-6.63634241993787	2.23382616119398
S	-3.35125178645789	-5.74152018896544	0.16082006997470
O	-3.63394595446018	-7.18517391803713	0.53578585145616
O	-3.96573574818763	-5.50342766214802	-1.25452704434472

O	-4.11441139883633	-4.85585947281708	1.13352187938436
O	-1.89632291890935	-5.42307560237994	0.09376014017313
N	-10.35452929378652	-5.72840311274384	2.21017332376325
H	-10.70098268946289	-6.34453161961101	2.93992505945592
H	-11.15051563763523	-5.24157843573646	1.80831470125321
H	-9.63200400915296	-6.39072365008425	1.28117098473328
H	-9.74177204817880	-5.03998622646709	2.63983134048154
N	-0.02315181602036	-4.35412279301544	-3.57536860283020
H	0.19257102884861	-5.05736279414586	-4.27672846021346
H	-0.11587330210798	-3.48283454871242	-4.09016110726985
H	0.82860601043914	-4.25257436012540	-3.02898027683919
S	-7.51590691837415	-6.60518328346105	0.46736588659099
O	-7.25539086154335	-5.48007162407081	1.45087262669898
O	-6.70727709742872	-7.81684135814066	0.84832732009015
O	-9.02415346393958	-6.95594622867176	0.47769170817803
O	-7.12224004090611	-6.16761659626418	-0.92364894295460

$Na^+(Na_2SO_4)(NaHSO_4)_2$

Final Gibbs free energy ... -2909.88002556 Eh

S	1.68430222396876	3.75989454745947	3.22628145400943
O	1.06232208405237	4.93648143114053	4.15302196770277
O	2.92193022768471	3.23139761461451	3.90068041114895
O	2.01692428636199	4.46360161641165	1.95904302106055
O	0.66922942794384	2.68100402415535	3.06634395389314
H	0.70911303276233	4.55401962135549	4.97466100290059
S	0.80955258399311	1.58842081122726	-2.32997911582638
O	-0.15755639162275	1.63470550252740	-3.63138061778154
O	1.41375223454884	2.93776741041722	-2.12387913035252
O	0.01020975601467	1.15166318522756	-1.14765673573645
O	1.83522970395524	0.57222122537442	-2.72328876867024
H	-0.88334667434984	2.26389483772390	-3.47695802234355
Na	1.73418551522623	-0.68663264884322	-0.73270353175642
Na	4.35920086619257	3.58532556023107	2.03872107007171
Na	2.45780456200357	0.95265091728884	3.38901366722889
Na	1.06996856563537	2.85688282821534	0.38601501454180
Na	3.71240810742505	1.89366662685846	-2.13781887115425
S	3.55699359901211	1.12391602871266	0.68200885311523
O	2.11777812868107	0.74945144332188	1.08022832215194
O	4.39177222717689	1.13940495130268	1.93407073983031
O	3.99772498023812	0.18241627140214	-0.40471698702172
O	3.53364575509593	2.54634047787583	0.10367426598726

$Na^+(Na_2SO_4)(NaHSO_4)_2(NH_3)$

Final Gibbs free energy ... -2966.41688163 Eh

S	2.33373159534559	6.90050836254347	0.78994295407185
O	1.29046443138655	7.94100727367208	1.48346885453450
O	3.72117938817432	7.34537288725753	1.08197782233744
O	2.02184405156956	5.62366507446548	1.51502665526082
O	2.01044343072430	6.85048236079374	-0.66081998864167
H	1.36619551280265	8.80403217249140	1.04212495820460
Na	4.41367056180932	5.21433758070782	1.83229078615248
Na	1.54151161449991	3.74019256916849	0.41555517485102
Na	3.96049256141792	2.62736002397514	-3.29559784958359
Na	6.87172142035407	4.08714650516064	-1.80924230093576
Na	3.72338255152871	6.10135434216409	-1.98726577377399
S	4.25761043288885	3.47574328429447	-0.52312865058714

O	3.80432246134748	3.08951016369648	0.86205945708306
O	3.01207833228057	3.72578830490442	-1.38951643903366
O	5.04256472348253	4.79066567972019	-0.42238071563159
O	5.11901287733720	2.45922774230314	-1.22180160125386
S	5.38138206547214	4.99346744545273	-4.19678863539731
O	3.89623775849731	4.91357040629914	-4.12170425810609
O	5.96456772931904	5.95193238675627	-3.21233270070894
O	6.01269873829647	3.63914952378039	-4.07841408856649
O	5.64872572933070	5.56249824796163	-5.69306695209877
N	8.99055021727083	3.05543269612674	-1.28395580288618
H	6.59424913113962	5.76296507478044	-5.80013455275090
H	8.79234671936252	2.10645522682952	-0.97772225550689
H	9.61171944890162	2.95978074121178	-2.08227821856440
H	9.55685718247047	3.46670004548145	-0.54779445446592

$Na^+(Na_2SO_4)(NaHSO_4)_2(NH_3)_2$

Final Gibbs free energy ... -3022.95511068 Eh

S	2.04526063280751	6.88269416876669	0.67055688755233
O	1.15088277816839	8.05944435675938	1.14390859219431
O	3.42184662934541	7.41221822459409	0.32233332048023
O	2.15340365098171	5.87566463050372	1.79166115327678
O	1.42356954697374	6.22100359209857	-0.52811213838188
H	1.63945877943399	9.08245252102431	1.02731386742142
Na	4.43956134276701	5.53421616530054	1.58852071763658
Na	1.57480972683498	4.01949213797085	0.46006633094704
Na	3.96482433634265	2.75770607322257	-3.27455204715036
Na	6.93872401339720	3.95216952325236	-1.80048519410867
Na	3.46011866166027	6.10359095189818	-1.82106137029732
S	4.29172364476995	3.51404718272462	-0.51213521588540
O	3.86194314612959	3.27440484661762	0.91099928989006
O	3.02903574660563	3.70211764417840	-1.36732145590901
O	5.09041989429405	4.82983587449604	-0.55015007665674
O	5.13363437201179	2.43765243147042	-1.13863334133602
S	5.56239059196431	5.08627615812952	-4.10836498566196
O	4.09330919731349	5.22149214277520	-3.88935195084596
O	6.42048841576348	5.94122992194133	-3.25591245061757
O	5.97483007486829	3.64131665648793	-4.02693000071740
O	5.73048649643047	5.56838642950058	-5.65661815161457
N	9.06054148740396	2.89198401889825	-1.33671700663863
H	6.67539471695905	5.69932499257973	-5.84276540077022
H	8.90089298131468	2.05732938377165	-0.77912779672873
H	9.50426590907553	2.56672243930147	-2.19106981976375
H	9.77558225050799	3.41877832453568	-0.84417217095250
N	2.22698396708006	10.31741073155542	0.89750469211052
H	1.74605867174779	10.91049893741136	0.22755153671989
H	3.17546490747226	10.16572219649578	0.56420556028187
H	2.27717509251092	10.81992984293573	1.77884856010483

$Na^+(Na_2SO_4)(NaHSO_4)_3$

Final Gibbs free energy ... -3771.89464810 Eh

S	-0.48813550452024	-3.01768810143584	-2.86695916003805
O	0.03304565222283	-4.17190100428915	-3.88260911944489
O	0.63888801158412	-2.86335727030995	-1.91250852490343
O	-1.74472590250817	-3.49978606081574	-2.20822564369301
O	-0.75291292203497	-1.77408949119055	-3.66046877649462
H	-0.64666775641186	-4.34117166059248	-4.55752242020829

S	-3.98512639803126	-1.79386059625342	0.82714805973482
O	-5.43659259047704	-2.26826745641458	1.39059078434534
O	-3.62528167905029	-0.69845687053196	1.78183207365882
O	-3.08935890593252	-2.97135338609569	0.88255725550734
O	-4.19956041498733	-1.23681882258638	-0.54272831725304
H	-5.69328118984448	-3.09663301832571	0.95091060565003
S	-1.77309459468554	2.06682523722776	-2.40644743467814
O	-1.98351234480556	3.17907388708809	-3.57086234423088
O	-2.01201892371792	2.73014140626901	-1.07904971274625
O	-0.33912504882667	1.71081951738686	-2.56330476922044
O	-2.76728966895797	0.98594223769018	-2.63979265004023
H	-2.93257084130718	3.36738159035163	-3.66924218419441
Na	-1.70211558056751	-0.66190756334214	2.97177327986216
Na	0.15098790286694	2.46598836730278	-0.17692141242392
Na	0.65449054907695	-0.39187356878669	-2.32111568435622
Na	-3.07766966994051	0.88919145350271	0.01571136839667
Na	-2.79708173027175	-1.32144407490589	-2.39254452191373
Na	-0.94858542995060	-3.15068337174907	0.02308112494383
S	-0.30517327056688	-0.26774352774168	0.51067415322050
O	0.97801961434591	0.26045265142742	-0.07540497011827
O	-0.11672541176763	-1.43010677998823	1.45450595964496
O	-0.99980886155837	0.87353350013396	1.26656176865915
O	-1.21864283237432	-0.71246300702536	-0.63053676466381

$Na^+(Na_2SO_4)(NaHSO_4)_3(NH_3)$

Final Gibbs free energy ... -3828.43285233 Eh

S	-0.66134054927208	-3.14537122630041	-2.93136613323177
O	-0.25262852164149	-4.28642989469262	-4.01297379293445
O	0.44889555679033	-3.19215965218537	-1.94505932465777
O	-1.98390794565151	-3.51433123599458	-2.33214593626495
O	-0.75121142319738	-1.83069527275740	-3.64391192436979
H	-0.92529130181711	-4.32208436597428	-4.71451062166942
S	-4.08770088732093	-1.77672875208148	0.77244160147691
O	-5.59968415304262	-2.12956145712144	1.26402875556406
O	-3.65419664578004	-0.77797693036942	1.79996747688330
O	-3.31677537634805	-3.04084194984524	0.79146121115997
O	-4.19628561198150	-1.12930334132218	-0.56910817711680
H	-5.92601537925206	-2.89487372891489	0.76086067665757
S	-1.38226975148543	1.99274636645236	-2.17354171739708
O	-1.43898588933570	3.22573099396900	-3.24006037659932
O	-1.57930414901360	2.57012104999277	-0.80271179376977
O	-0.00132391914668	1.48351151291947	-2.35675700989224
O	-2.49488675865933	1.06683514564091	-2.51953146621993
H	-2.36419169738148	3.50035986813903	-3.35636859128192
Na	-1.76168649782270	-1.04579449302742	3.01695562499976
Na	0.57198255921042	2.10532309454469	0.15396626154475
Na	0.75068951946461	-0.71557833671129	-2.15812759874306
Na	-2.86966573293315	0.84868375733721	0.17788340245667
Na	-2.76158865649538	-1.21819992274031	-2.38423294788727
Na	-1.18939942095587	-3.37566998232293	-0.06536852783304
S	-0.25319912665994	-0.63075963194902	0.63804713015588
O	1.09565285691210	-0.21626046747539	0.11735606257834
O	-0.22080476271729	-1.87234229258810	1.49879147775902
O	-0.84600631604895	0.51898715477466	1.45934610726405
O	-1.17645577121441	-0.89878023500553	-0.55339386953017

N	1.58535678654533	4.14219105369572	-0.62255520098133
H	0.86662337600487	4.86032212925853	-0.65043380605229
H	1.84460453123285	3.98707807873760	-1.59325903139285
H	2.39268923842940	4.57610288240837	-0.18572735744595

$Na^+(Na_2SO_4)(NaHSO_4)_3(NH_3)_2$

Final Gibbs free energy ... -3884.96968264 Eh

S	-0.44298101173413	-3.04309135525907	-2.91038641636588
O	0.10948795391805	-4.20838882890324	-3.90209695076589
O	0.64589579772138	-2.89287383066544	-1.91354792911805
O	-1.72993650857157	-3.51259504290623	-2.30528884954888
O	-0.66451918011898	-1.80381080562304	-3.72438300539655
H	-0.55324923629635	-4.38220359317765	-4.59191984679558
S	-4.09558767904197	-1.76705515674203	0.59528837962075
O	-5.57965999214295	-2.22735760564408	1.09771231885874
O	-3.77013032269866	-0.66527965561895	1.55012809594713
O	-3.22246776739076	-2.95862557223478	0.70126648476523
O	-4.24905875309236	-1.22812521482281	-0.79052039758178
H	-5.80162905921543	-3.07421719912113	0.67579154154144
S	-1.76652327299248	2.11271762008200	-2.55490978564191
O	-1.93998818306810	3.17623965500328	-3.69134469722759
O	-2.05093466185969	2.75797162551168	-1.21836808387685
O	-0.32684871402838	1.69746903202042	-2.59552939361652
O	-2.75078186167217	1.00231226453769	-2.79237961326436
H	-2.93466824387776	3.17899696240418	-4.12980907140362
Na	-1.90813437341628	-0.62059991123093	2.89927968514914
Na	0.06466085044396	2.44131622276619	-0.28153485706144
Na	0.63589412816834	-0.38385183562725	-2.31964570543841
Na	-3.10094078411025	0.90754123106196	-0.18497952943390
Na	-2.71839129103590	-1.27845436979418	-2.52765338011332
Na	-1.03252456526501	-3.11714962484115	-0.03516051070568
S	-0.38247799145106	-0.27122070977703	0.47614049200527
O	0.92700179346401	0.24283515154391	-0.06441860839217
O	-0.23857569719819	-1.42266154309927	1.43879681266349
O	-1.10714216780116	0.88336953760655	1.17425270722992
O	-1.24574529351304	-0.73599334679962	-0.70123572148668
N	-4.24530023316534	3.20967819893707	-4.80759548960884
H	-4.76421401351657	2.36815736529454	-4.57516495247872
H	-4.14151621142012	3.23669600951368	-5.81755454550851
H	-4.81331586412968	4.00724864207153	-4.53859305850520
N	-1.63674241000694	-0.47956818841251	5.29852896428973
H	-2.16685180661747	0.26536841583209	5.74179147296662
H	-0.66686190276320	-0.30826498717224	5.54828233240976
H	-1.89796336982662	-1.32662288153011	5.79547840698518

$Na^+(Na_2SO_4)(NaHSO_4)_3(NH_3)_3$

Final Gibbs free energy ... -3941.50604584 Eh

S	-0.45965784758387	-3.07000328529986	-2.80162960554153
O	-0.02572058522639	-4.26547507196429	-3.81709864393650
O	0.67699689783479	-2.99541434730664	-1.85092521471939
O	-1.74808127551254	-3.45969470843346	-2.14415655981530
O	-0.63518891430748	-1.81629687085168	-3.60371809564405
H	-0.72610358556845	-4.39239182052964	-4.47932490172940
S	-3.88599118623347	-1.64269266993556	0.85889521036504
O	-5.37263604792249	-2.03672060207261	1.41792424117510
O	-3.48264425713223	-0.55496604159360	1.79841042620358

O	-3.06350328695198	-2.87127510010403	0.94260590151090
O	-4.06694957767038	-1.10588670539584	-0.52404218093529
H	-5.66871021297633	-2.84442029227282	0.96586274802795
S	-1.50225028844888	2.12754956780057	-2.38128580867649
O	-1.67437627083584	3.24488144506629	-3.47971265895485
O	-1.68003728941957	2.75261450504376	-1.02131936181754
O	-0.10125048828390	1.63204286360116	-2.53814990980315
O	-2.56864399330545	1.09025821127655	-2.59800627341216
H	-2.68628938635575	3.32460731264040	-3.82733566599579
Na	-1.53740585209515	-0.62269942007034	3.07004921272777
Na	0.49450282585464	2.42335035355794	-0.11882711028603
Na	0.77660957860799	-0.46753959030318	-2.23169543767842
Na	-2.77893264352472	0.97819346213262	0.05066380558188
Na	-2.61788201860955	-1.18406585716212	-2.33116612500479
Na	-0.92097083066746	-3.12349388770522	0.09136468386146
S	-0.10906888007410	-0.31871531065736	0.59336770669670
O	1.19740782533282	0.13379486304548	-0.00023488468350
O	0.01846281899106	-1.48966074569356	1.53689509166559
O	-0.74941968259964	0.85443615384795	1.33855084044814
O	-1.04601917876138	-0.73108442428819	-0.54976914555790
N	-4.08148991279948	3.42570735805998	-4.39724907635026
H	-4.59064311932369	2.58415249673479	-4.14391700392676
H	-4.07164979223612	3.48157558092300	-5.41116079206866
H	-4.61241983185380	4.22068544721709	-4.05548449904567
N	-2.52375472907201	-1.34104605514097	5.14528877094497
H	-2.52973315472659	-0.70394729178191	5.93625235716778
H	-2.18295738100628	-2.22504165163011	5.51171605654356
H	-3.50092218842197	-1.49850012308952	4.91189724655848
N	1.34559130261134	4.35254286181551	-1.27654548818000
H	1.34024757008400	4.00823097117383	-2.23372080687270
H	2.23750401643191	4.81796119461850	-1.14481658102690
H	0.63950320587368	5.08275757060904	-1.25351683058679

$Na^{+}(Na_2SO_4)(NaHSO_4)_4$

Final Gibbs free energy ... -4633.88888739 Eh

S	-1.09485226207224	-4.50884867641395	-4.31743885865103
O	-1.62282650435432	-5.49800514582444	-5.49544632975237
O	0.16857145468484	-5.10205137704741	-3.77148276252502
O	-0.91162630378597	-3.17117917633270	-4.92209339253979
O	-2.19449762399689	-4.62312829719816	-3.31310001033637
H	-1.09194035322926	-5.35619410238666	-6.29760729553154
S	-2.44757944254356	-3.68057805658019	1.01269616141449
O	-3.54821613529228	-4.31072174435782	2.03119123094289
O	-1.17556510702745	-3.56874452671727	1.76010449920060
O	-2.98365381122978	-2.36475711157698	0.53551678375587
O	-2.46232327072148	-4.67723531167575	-0.09951220049155
H	-3.49910849800431	-3.84898903644548	2.88554255968754
S	-0.45828103982213	1.72017757554519	-2.18647593506289
O	-0.69067806170440	3.28151464122463	-2.60634722576747
O	0.97270234754582	1.59306518322362	-1.79647147738214
O	-1.38825078414035	1.44580708776291	-1.05407990363881
O	-0.81389667051399	1.01746292588421	-3.44088959145683
H	-0.45182199824710	3.84426205005931	-1.85157293935123
S	3.94103597906482	-3.06070457284477	-0.36605156873723
O	5.51601471196475	-3.16811221092971	0.05272285345091

O	3.76756175858214	-3.91323792028009	-1.57678248717334
O	3.15748122387300	-3.56334020313571	0.79833847693631
O	3.79048760034072	-1.61014392517713	-0.61514926607348
H	5.72453222945425	-4.09853153170381	0.23761340164731
Na	-3.15896335967793	-3.18868197489694	-1.81613239448272
Na	-0.89608505711997	-5.50765568318294	-1.54077706611797
Na	-1.73519096482559	-0.44629607979463	0.02440837083526
Na	2.03914592891197	-3.95987655020650	-2.94692136282827
Na	1.01941541080385	-3.19527353640066	1.21064264707874
Na	-0.56512570783864	-1.05419225375706	-4.11839888043689
Na	2.29546128708281	-0.10905546931834	-1.24927129441135
S	0.15484843139656	-2.19907769214383	-1.46193663144096
O	1.10263081203278	-1.80777378546303	-2.58117021503744
O	0.43782627187791	-1.37383201720241	-0.22008576449878
O	-1.26578201129285	-1.92785339819313	-1.91984284550765
O	0.37246411082775	-3.66195778751265	-1.12359848571702

$Na^+(Na_2SO_4)(NaHSO_4)_4(NH_3)$

Final Gibbs free energy ... -4690.42743191 Eh

S	0.78177782593791	-0.38813542470217	-4.58529635207778
O	1.16826289658258	-1.25425497533000	-5.91543189714662
O	1.55869483248844	-0.95962666512118	-3.46507130040107
O	1.12151097935922	1.04386680175881	-4.88992405436252
O	-0.70076042050103	-0.56731133774082	-4.52673096987445
H	2.12544946708097	-1.42229748835550	-5.91230215506039
S	2.74329920271529	1.06105875666139	1.00343637285262
O	1.96068631866733	0.98295520018446	2.27347578695361
O	4.18638233235292	1.73767579892709	1.35903456636265
O	3.01554029252866	-0.25449799489037	0.37782763015208
O	2.14762633751873	2.06945050583876	0.07058795210718
H	4.73874434968247	1.07797360279685	1.81105670425216
S	-2.42090565964304	1.10650540625096	3.29018496634096
O	-3.02770689965713	1.68867643340066	4.68484174177480
O	-1.58422006991734	2.17309139017984	2.69614898834403
O	-1.69437494312205	-0.11194739258643	3.74611217227314
O	-3.58545098253679	0.72966822348219	2.41916265550260
H	-3.35163818194243	2.59319915515340	4.53682236721400
Na	-1.17960739147461	1.80609470086812	-4.96992913949128
Na	-3.16043585023326	1.13591885960633	0.12331078066595
Na	-0.00051229765163	2.12254109541321	1.04437450318986
Na	1.33587464178251	-0.69785581733341	-1.16386405431104
Na	-3.09413421018372	-1.63101772131005	2.41410730017736
Na	-1.67986002033571	-1.02799942996621	-2.42597237166842
Na	0.41703709495165	-0.71256445017132	2.89565575523501
S	-1.28965990401691	1.92319134434639	-1.95162117649342
O	-0.14059761191561	0.93757342044795	-1.91346042399851
O	-0.96889420950460	2.97123312417655	-3.01177223562835
O	-2.55973003721279	1.17084664313547	-2.31948365685427
O	-1.48313249095445	2.57544418214476	-0.60220503163549
S	-1.05119792684829	-1.46276881324179	0.44149640470153
O	-1.02864362843515	-2.34147506569515	1.67071313588469
O	-0.24835580228986	-0.20645340185836	0.76330701445391
O	-2.50296797093989	-1.08253022702532	0.13361669523552
O	-0.45575895816467	-2.11812697679117	-0.77680229491173
N	1.82959044154321	2.81283615167022	-2.73744492584678

H	1.86235098625330	2.04420467235784	-3.43032355029943
H	2.48633551311942	3.55058962424420	-2.98032227711938
H	0.83759750194420	3.14453423325338	-2.77666502655874
H	2.02367582696858	2.45472424582212	-1.78645193093790

$Na^+(Na_2SO_4)(NaHSO_4)_4(NH_3)_2$

Final Gibbs free energy ... -4746.96421451 Eh

S	0.95916894948781	-0.20730108943990	-4.70440804229957
O	1.41600588786468	-0.99802047622293	-6.06011627210777
O	1.66731317435496	-0.85266318417141	-3.57850794249885
O	1.32429150652745	1.23652803645420	-4.90350363432574
O	-0.52539773639596	-0.37744601417404	-4.73913054725520
H	2.37025115257730	-1.17485483165001	-6.01081785231330
S	2.60254487960704	0.91167566549909	1.06009956060186
O	1.75828031908972	0.74461737095969	2.28050559569743
O	4.02292558268174	1.56528836891707	1.53459741573864
O	2.91460536662425	-0.35808933923552	0.36187724379418
O	2.05038574855363	1.97959920339166	0.16801073682031
H	4.55120534475864	0.87818954164371	1.97423365641502
S	-2.60931723042858	0.84775595265818	3.08898801304357
O	-3.38050926806816	1.29721156904200	4.46228904837758
O	-1.71787362261669	1.96545737079197	2.70685036757402
O	-1.93053293864499	-0.40488903790477	3.51776357796477
O	-3.67517709654823	0.56923283214871	2.07243714979168
H	-3.68811843365091	2.21355132281543	4.36256948902905
Na	-0.99289683615294	2.01625793078251	-5.05318239668743
Na	-3.22743766606006	1.01674229168250	-0.17485701604666
Na	-0.14654759356085	1.97159087390900	1.04090623392906
Na	1.31790933077441	-0.71306279790367	-1.28116843273637
Na	-3.33314282445789	-1.87679247178947	2.01234817758740
Na	-1.61578631759251	-0.96882271791266	-2.71491858119197
Na	0.18293403993460	-0.97973506759656	2.69124198959039
S	-1.24322153920592	1.95760056481564	-2.05514751876423
O	-0.09880307610762	0.96729808708057	-2.02247130086739
O	-0.86468894954018	3.07239609529310	-3.02487038584398
O	-2.49123251995657	1.23559381371763	-2.54428423752862
O	-1.51392983866644	2.52029037071514	-0.67956614837942
S	-1.16281206041374	-1.57109574715336	0.13859558809752
O	-1.19515895357492	-2.51438729422272	1.31555252664275
O	-0.41116842941184	-0.31588981800571	0.57804676819559
O	-2.59461711184949	-1.19921112135086	-0.25279249956091
O	-0.47111212567454	-2.14758760696024	-1.07092572050646
N	1.90940703648604	2.87748770517340	-2.61029637743654
H	1.97860672396881	2.14176377790769	-3.33492642275460
H	2.57772724520394	3.62403505178699	-2.78471112374698
H	0.92021763587449	3.21303053649641	-2.68623558796242
H	2.05153425350368	2.47610430616838	-1.66733754194294
N	-4.72252236662734	-2.36487816245069	3.92282985809578
H	-4.46344619394026	-1.61899260087758	4.56426655903155
H	-4.54201177538308	-3.23103795496246	4.42157269933835
H	-5.73185737965439	-2.30758761259918	3.82827151695787

$Na^+(Na_2SO_4)(NaHSO_4)_4(NH_3)_3$

Final Gibbs free energy ... -4803.50654074 Eh

S	0.45707894811488	2.69454916309547	3.10654612501230
O	1.60293325579351	3.50780708598215	3.94782216646385

O	-0.14366688908793	3.66385018958297	2.15684903156252
O	-0.50212723088979	2.14451849316581	4.09538784937259
O	1.28018805999051	1.63714203673571	2.44206250790231
H	1.17925243093453	4.25891647806383	4.39526262976295
Na	1.02901445848279	-2.69529562487223	2.84311827243743
Na	-2.36213132212939	-1.01921924704328	-0.06037861491972
Na	-4.64211463875666	-1.24733750519325	2.55808488412760
Na	-2.10897086771745	0.56196270167260	3.92176167832327
Na	-1.52655481812901	3.11119471070205	0.43918702847630
Na	0.28863112918234	-1.13952902650776	-2.59409465039646
Na	-0.03382009489477	0.11475270212209	1.30794487075200
S	-0.79814569947359	1.35311961874447	-1.89420422985315
O	-0.02234006881821	1.45094841842281	-0.56579718552616
O	-1.69916945264087	0.12368121978244	-1.88044064360556
O	0.18353095367942	1.21078531800205	-3.00753500287176
O	-1.68064590937413	2.59223968691372	-1.95355317442780
S	1.17648400316755	-2.31243995416323	-0.04966245342422
O	-0.27033828026264	-1.90920443584438	-0.32621717634868
O	1.92757555565689	-2.27434234723743	-1.33724340786140
O	1.76541994218507	-1.32658460320029	0.96786706711208
O	1.18448344366203	-3.67474281377642	0.63807045604728
S	-3.65900962485935	1.23403388328892	1.40566798824829
O	-3.86247337286454	2.61617169444805	0.87586823892969
O	-2.15606015626021	0.93626642803700	1.42495379233725
O	-4.18882134209594	1.00518531210996	2.80058209590570
O	-4.31528637250274	0.19378140659583	0.47359120984000
S	-1.93518197182835	-2.29785247768623	3.02552196610919
O	-2.71006674987167	-2.42661350845647	1.71215141701059
O	-2.90138667474886	-1.80280609706252	4.06853394298042
O	-1.27710504392709	-3.62656550694002	3.34779734607976
O	-0.80557863269003	-1.27645211984057	2.90842515283895
N	-1.16328707385416	-4.90778050805703	0.95316832740239
H	-0.22922510765400	-4.48370399098376	0.65848846252939
H	-1.30174353763297	-4.61809036601622	1.95793022255125
H	-1.18004563758864	-5.91663614354656	0.83133673358634
H	-1.91379154717437	-4.46613413647414	0.42671583682147
N	-4.28507711700329	1.90133969652857	-1.84948192513935
H	-4.79770965799507	2.69581941807812	-1.46967133374293
H	-4.67413436807614	1.61409777126616	-2.74373948672426
H	-4.35204976933805	1.13993064381868	-1.14221291492815
H	-3.25479553623145	2.16987510139307	-1.95711885170854
N	2.60458181384214	1.21703038087292	0.01075195896882
H	1.69726395541688	1.42717017572443	-0.48308085641017
H	2.55152963062157	1.70575294457263	0.91662552769217
H	3.41729804034223	1.49521086155414	-0.53211392961248
H	2.60334581629773	0.19838845364600	0.21827411931287

$Na^+(Na_2SO_4)(NaHSO_4)_4(NH_3)_4$

Final Gibbs free energy ... -4860.04264792 Eh

S	0.75339066783522	2.48397825371685	3.01316701336306
O	1.97490077965740	3.24555588597286	3.79643086752825
O	0.04775989984510	3.52078831682802	2.21904382731630
O	-0.09184144117018	1.83965865647883	4.04921202372188
O	1.50683744828724	1.49695809406974	2.18169390668643
H	1.59645337614456	3.97546113740560	4.31386129760614

Na	1.47795484591923	-2.70762984892926	2.41995592221015
Na	-2.36934324563827	-1.01268387129311	-0.09864612616720
Na	-4.46410053835501	-1.32038482113532	2.63713500163266
Na	-1.80032719211221	0.36305565245280	3.90371037107149
Na	-1.43050831255869	3.09191072587393	0.54413138783750
Na	0.04161968904937	-1.00439809297290	-2.86252910245174
Na	0.05826061036046	0.01934579973482	1.13681684586151
S	-0.94805565563704	1.45608905789595	-1.92743935332272
O	-0.07824398242401	1.47732548183844	-0.65510012561181
O	-1.86440794069146	0.23900768091238	-1.90864186786209
O	-0.04962204812524	1.36173386831692	-3.11479775621344
O	-1.81017941252724	2.70882452170487	-1.86394485216619
S	1.15849765001515	-2.28554916051818	-0.46839617254675
O	-0.30520111512348	-1.86407214357739	-0.57947138245718
O	1.77030803469834	-2.20905980750828	-1.82671134794792
O	1.86005534609167	-1.32673787367881	0.50580470926037
O	1.23448886317609	-3.66356115815791	0.17471847922944
S	-3.51762953729611	1.19283177107032	1.57085757664145
O	-3.71073556110378	2.60181838799112	1.11001718054406
O	-2.02511459156622	0.85006621669800	1.48853115847267
O	-3.97064450407949	0.92451228859781	2.98345488064805
O	-4.25914138437916	0.21293345705851	0.63721217335768
S	-1.76636038753367	-2.46414109607879	2.87576354857127
O	-2.62917173545955	-2.49635030793237	1.61051970245294
O	-2.61669992616307	-1.88731100256398	3.98301086190045
O	-1.27210040189588	-3.86253783406803	3.16974496267353
O	-0.55627494047308	-1.55481108112962	2.68651066556002
N	-1.06576417797622	-4.93207922915011	0.69538767407851
H	-0.16623187992675	-4.46642608774248	0.36012671826545
H	-1.18310013237552	-4.68096314461885	1.71986240273946
H	-1.04352807425599	-5.93668191551144	0.54369008897458
H	-1.85719814347819	-4.51443517037125	0.21108801286661
N	-4.40627050978929	2.04457268910307	-1.58268028503732
H	-4.86186524480508	2.82206444109205	-1.10735809589849
H	-4.88235335018396	1.82132497249921	-2.45264871987579
H	-4.42435772158566	1.24190830912612	-0.91964395747266
H	-3.38382161647462	2.30221434796809	-1.76570311771330
N	2.59872680269901	1.21775629525546	-0.39393561868889
H	1.63240502840124	1.44087176700857	-0.75310425395050
H	2.67479447647537	1.68237309647416	0.51979110304075
H	3.32959533610580	1.50733883298371	-1.03750945634763
H	2.61263445867729	0.19112397932075	-0.21451206292031
N	1.58029702778767	-3.76334719714487	4.56719151288193
H	1.77559826199603	-3.15864223101853	5.35911882494412
H	2.08845615454969	-4.62336659299316	4.74637862697522
H	0.58923709881248	-3.99410093493022	4.62431769524763

$Na^+(Na_2SO_4)_2(NaHSO_4)$

Final Gibbs free energy ... -3071.64908432 Eh

S	-2.13190068586754	-0.37557974453286	2.76696790566730
O	-2.83721738251901	-1.03431512990847	4.07658866667203
O	-2.93337380770927	-0.96015537981936	1.64524531098278
O	-0.70636537842288	-0.81455723789660	2.72462128627989
O	-2.26567963824542	1.10671751066917	2.83862437064006
H	-2.35943271593764	-0.75172770352543	4.87489680398701

Na	2.26703688055469	0.97483017369762	-0.97581718618616
Na	-3.23632342858646	1.07799783409986	0.49333944317588
Na	-1.15754576063787	-1.74690043125152	0.33382182709279
Na	0.19762245974522	3.64860867551573	-0.84038422170729
Na	2.40488105938379	5.30698806358046	2.71080494358375
Na	0.26934301509736	1.34826589744924	1.97851261680133
S	2.47160427701657	3.17178294929441	0.91680744050562
O	2.42841063787790	3.26258190840275	-0.60118892578909
O	2.46427866248911	1.70460921199766	1.29103880413380
O	3.62179629201940	3.92312372168225	1.50903080888115
O	1.15881897040073	3.81268251160019	1.45761129804916
S	-0.66516482222477	0.85792898181436	-0.86973781090319
O	0.32634503039094	-0.04503748100200	-0.12365754017456
O	-1.11564083828582	1.96861185657072	0.10147264396925
O	0.05097983285269	1.51077324932846	-2.01568329686829
O	-1.87945082038981	0.03522429923445	-1.21456918577977

$Na^+(Na_2SO_4)_2(NaHSO_4)(NH_3)$

Final Gibbs free energy ... -3128.18952330 Eh

S	-1.80350767127860	3.09655838039395	-2.42659340152475
O	-2.79780537381580	4.27193705098447	-2.95801173254607
O	-1.65114827228821	3.43097984824710	-0.98535083440223
O	-2.51297183199842	1.77783793792144	-2.59926281800782
O	-0.56274641964003	3.12920498794137	-3.23905691014199
H	-2.84026597265084	4.23344622100803	-3.92850182029277
Na	4.45392366814135	4.85799036117235	0.88314317616793
Na	-2.61393848441491	1.02386047509915	-0.41790516634464
Na	0.94616529133541	0.65056957825129	2.50703868983018
Na	0.43647054634309	3.14447765877565	0.04319888224649
Na	3.00429530775044	0.72393451580442	-0.17600835498484
S	2.77792171341658	2.79761720793017	1.85121733608893
O	3.12061747379871	1.32340933804846	2.01938998050213
O	2.93852472985503	3.13512408982238	0.33724055221088
O	3.68229008000812	3.69593272100442	2.62611019457094
O	1.31279484846547	2.97218565615142	2.20144753169545
S	0.13477756744336	0.15887464440904	-0.28168044307772
O	-0.87556798180619	-0.55988986214871	-1.13910740064422
O	1.12083560694698	-0.70720769599785	0.44789468058650
O	0.92457901271303	1.11463364167680	-1.19897493587388
O	-0.62342967574751	1.00554789389900	0.74897555232006
Na	-0.40393291948953	0.69871387964175	-3.10739131684965
N	5.90465038529434	6.77494582298327	0.69899138675747
H	5.45804946823704	7.62491805639039	0.36588555646312
H	6.73140800711557	6.66167803292669	0.11897080316103
H	6.25647441574944	7.00435852111332	1.62507972379951

$Na^+(Na_2SO_4)_2(NaHSO_4)(NH_3)_2$

Final Gibbs free energy ... -3184.72638476 Eh

Na	-1.53404575508451	5.88243131936309	-0.36238608268313
Na	2.16239711840679	0.34665286046705	4.67624166317554
Na	-0.18671786942211	3.24392944617342	2.37590696350535
Na	2.72122313655769	4.62192215503192	0.93941294852277
Na	1.95447363666328	1.39805349483138	0.30065668636836
Na	-2.21848751637418	2.50769118480656	-1.11515541383432
S	-3.34500138698563	3.48100658892588	1.32074862379282
O	-4.78503484533400	3.86514207330718	1.99284797832672

O	-3.16091923666604	4.38936582291688	0.13201794707645
O	-3.42842395566776	2.07031112423216	0.85622121648210
O	-2.39992178149988	3.75837704887101	2.41998909452406
S	0.37132760318595	3.70006205431977	-0.56723250499806
O	-0.17635734428661	2.40537311038029	0.05945884164906
O	0.35334436098627	4.79425115903023	0.50678247501373
O	1.79973207402109	3.45509921667810	-0.97196398734063
O	-0.55185231930922	4.10510845315219	-1.68886711953510
S	2.63348621135056	2.49684373218164	2.90240696683812
O	3.45436488551577	2.50720232560622	1.62171287306171
O	1.49374275127340	1.44906704440989	2.70608427956396
O	1.97754889191813	3.85747717952397	3.04011667877538
O	3.42422930030779	2.09841414120556	4.10302355138453
N	1.89911677568509	-1.06838824118673	6.61154582401133
H	0.94182622256522	-1.29168322757203	6.86943980861053
H	2.37777816368718	-1.96328241496868	6.55681063277351
H	2.29486625783862	-0.60441781610566	7.42527413616077
H	-5.49034390764790	3.47656704391993	1.45001155516820
N	-2.24216183730645	8.19731809271325	-0.34459072850832
H	-3.25576908502763	8.24459433751881	-0.40294214344502
H	-1.89787277729488	8.79625572609352	-1.08947556337890
H	-2.00138634754802	8.67331411775771	0.52054251207223

$Na^+(Na_2SO_4)_2(NaHSO_4)_2$

Final Gibbs free energy ... -3933.66253771 Eh

S	-2.17963297125054	1.92076272975912	1.19935946057638
O	-2.09151311746370	2.87052924734661	2.51769280557161
O	-0.85483418104771	2.00763586190429	0.50471025461590
O	-2.49254705430443	0.55141330629187	1.68082320429124
O	-3.24207658799221	2.58876433773587	0.40732719875386
H	-1.51610457573627	2.44983954015897	3.17861767988177
S	-3.07964509599235	4.29579614977856	-3.78660259012793
O	-3.53164862331445	5.77799016982367	-4.29041700930206
O	-3.42841257539042	3.34759785876372	-4.87321664234825
O	-1.61442805483689	4.47339971986961	-3.55801928807727
O	-3.78239311991002	4.02233518089689	-2.49759015948341
H	-4.41185735161555	5.71882029147265	-4.69823617926003
Na	-1.62864234338774	3.12798909656590	-1.51208868397072
Na	-3.14044286269793	-1.21808352693043	0.50478080997708
Na	-4.62552197424403	2.14358125952567	-1.35049923643222
Na	-2.67802928817033	1.18995150994349	-4.76122566572105
Na	0.53789894681153	3.91813965941533	-4.20610833885326
Na	0.17910588428694	0.53427251833370	-0.90263482039150
Na	-0.66665675325571	-1.38609297805216	-3.61762546226339
S	0.64784535582031	1.18903073917902	-3.66832780881744
O	0.15175546805139	2.17898747027299	-2.59088539533771
O	-0.51805441360934	0.74826130427291	-4.54723744599751
O	1.13392110090168	-0.05323149251748	-2.93737500876830
O	1.67180445150864	1.90198126049639	-4.48153045721719
S	-2.94424260943426	-0.20561568709757	-2.17475388462032
O	-1.74534141471271	-0.76519847820005	-1.38906111973073
O	-4.19130133992612	-0.40174911266444	-1.34040156185900
O	-2.77983772990884	1.28849960728892	-2.40487783286828
O	-2.99161242017603	-0.88668141463422	-3.51660103322037

$Na^+(Na_2SO_4)_2(NaHSO_4)_2(NH_3)$

Final Gibbs free energy ... -3990.20004983 Eh

S	-2.44782142409501	1.66894957419431	1.30760752315907
O	-2.45706208584291	2.53358157574133	2.68745951535256
O	-1.08204719352719	1.81296283877255	0.70936596756311
O	-2.77105883200466	0.26848562947371	1.68176645483440
O	-3.46629105602379	2.37465157040799	0.49233917807380
H	-1.93098073581739	2.06831443354908	3.35928888482873
S	-3.04776585088639	4.35272275720170	-3.55388013791924
O	-3.45365837071431	5.87251060154298	-3.98838715264840
O	-3.35434866224982	3.48073908994271	-4.71528194397575
O	-1.59739933249912	4.48831473845003	-3.23660379139136
O	-3.82898898730827	4.01394854184842	-2.32592620999277
H	-4.31414315251738	5.84992926173761	-4.43924735142127
Na	-1.70120602754402	3.05596988126777	-1.28643023030206
Na	-3.36598207878084	-1.40073850086003	0.33521946322393
Na	-4.71087316084638	2.05433563191995	-1.39125657324769
Na	-2.49168346760178	1.36021729039119	-4.70253337370563
Na	0.67510269534836	4.05198334216430	-3.69964000987735
Na	0.06742689086035	0.43548931880988	-0.70735085975948
Na	-0.57607394732397	-1.30564272060012	-3.59517395767796
S	0.73518774275019	1.25683386974619	-3.37794238286120
O	0.15352674835777	2.17520950482833	-2.28073581968641
O	-0.36023248760129	0.87763974448555	-4.37075924568396
O	1.15736028953075	-0.03589911324391	-2.68954499155962
O	1.82452277187875	2.00455929484758	-4.05801436954821
S	-2.95999346984987	-0.22267102281764	-2.24910636437758
O	-1.82680119267828	-0.83351433309108	-1.40702161091251
O	-4.26951994458746	-0.47062219590827	-1.52964626047218
O	-2.78585545531857	1.28265798689531	-2.36830581017669
O	-2.89945365219555	-0.81517198240201	-3.63141792113148
N	2.05171884967564	5.91293265328737	-4.37476296198320
H	2.60789618739308	6.32331058994762	-3.63040267749316
H	1.56889096357287	6.69060756033639	-4.81505153704943
H	2.72310416148562	5.57921947717196	-5.06095207477778

$Na^{+}(Na_2SO_4)_2(NaHSO_4)_2(NH_3)_2$

Final Gibbs free energy ... -4046.74204935 Eh

Na	4.81428487263424	-1.31320623832738	-2.28646003393338
Na	2.47141526723765	-0.43932138556129	0.41901235301336
Na	4.35924673408480	1.89431883341954	-1.68877700388117
Na	0.52607248865693	-2.75570095219923	2.50563389821848
Na	-0.20808041490178	1.16580502495478	-1.41601806157680
Na	0.18688588138897	0.44507437532204	3.17407087093977
Na	5.10405407537232	-2.06614202228463	2.27797117849623
S	5.47479727874675	-0.01224472833278	0.22673937592035
O	6.14305416260228	0.33242188743212	-1.08536081097742
O	4.83354430665571	-1.39449703525899	0.07594056584656
O	6.39397951875136	-0.07310000112657	1.43479834992705
O	4.39319856330798	1.02524367577534	0.48644710098329
S	2.26281835680932	0.08659199535972	-2.56118358016400
O	2.51164206698413	-1.24714690303648	-1.87370153301293
O	0.94884817436520	0.00957262489152	-3.32022303148751
O	2.11052150452942	1.18667760081357	-1.50706822635700
O	3.48122238001508	0.41332350235245	-3.39561526878817
S	-0.61259052655479	-0.81778092978165	0.65390810679587

O	-1.59496941829169	-0.57517087449548	-0.45227043051529
O	0.30151281729346	-1.99896117125089	0.27323105991570
O	-1.19027870882758	-1.13158483773315	2.01541499997636
O	0.25845846472951	0.43622863124178	0.80273887672837
N	-0.16826099153123	-2.35390321734531	-2.38799346088169
H	0.20327286361161	-3.19713031487637	-2.81655658544402
H	-1.18485871389470	-2.34020193136891	-2.44616447321993
H	0.23629640455259	-1.50654215690003	-2.86456807128571
H	0.09970888442090	-2.29968370390462	-1.36173081848703
S	2.68082729012743	-1.01768980445041	3.46942835857465
O	2.73472446369448	-1.94761269173445	2.24869259440820
O	1.42173273310965	-1.35312046767914	4.23558018267132
O	2.53066991764906	0.43012868312931	2.97005728897136
O	3.97558005575744	-1.15800118707803	4.21405911070953
N	5.05434931557216	1.44137680797246	3.32685386958405
H	5.19825448531171	2.44600280545149	3.27632642918360
H	5.24400410544574	1.09488181484415	4.26601713014259
H	4.05485424824648	1.18470118381258	3.09432465660938
H	5.67296909233899	0.95087767995252	2.62860585239454

$Na^{+}(Na_2SO_4)_2(NaHSO_4)_3$

Final Gibbs free energy ... -4795.66343694 Eh

S	-2.24302145887175	-3.54658757755395	-1.61287058366655
O	-3.59924682086114	-4.44461329430700	-1.74826022516065
O	-1.22988302753374	-4.57938740763410	-1.28744032816079
O	-2.04732151646368	-2.85023543286658	-2.90696386560100
O	-2.48976097562369	-2.58243832799140	-0.49118726581777
H	-4.31176240661545	-3.89426069032782	-2.11491778906588
Na	1.06755878576756	-4.27615726169015	-1.02988795649612
Na	-1.12714399519913	-0.68195487634571	-0.33274375286537
Na	-2.16831940760253	1.51678598073737	2.42900997092216
Na	-2.32203594629280	-3.06601717119219	1.77325704451026
Na	1.01793856357569	-1.27841879396540	1.76501433531022
Na	-0.11613445792840	-3.46515515629410	4.48012063395234
Na	1.98779403334333	1.38320758677801	-1.64819605764471
Na	-0.31157756241617	-1.92349627938018	-3.94955105395643
S	0.10148455339808	-4.98532090456910	1.94081670419041
O	-1.46240948284181	-5.37300689679359	1.50064079780413
O	0.97133735057495	-5.55186253869923	0.89053823396992
O	0.08141601355991	-3.47997589536533	1.95185476743843
O	0.22779645338206	-5.51256771082251	3.31090511514432
S	-1.32078642101248	-1.00270414236511	3.56316999754617
O	-1.43327495001671	-0.81167275233885	2.01871043098552
O	0.14954321462882	-1.18754778451480	3.90056200887855
O	-1.91075416494785	0.20398602979797	4.20891431730933
O	-2.05026646119749	-2.28558070205121	3.91772254973470
S	1.42916418882273	-1.44126899351487	-1.73304050393637
O	1.46897611609256	-2.61206135525923	-2.69827678559048
O	2.73931615144617	-0.74661539494070	-1.58801989930296
O	0.92201610797555	-1.98827576291217	-0.39936712717630
O	0.37754874620111	-0.42849270899923	-2.24753463440429
S	0.02617707238704	2.04438625353055	0.40625837436793
O	0.60669077968069	2.98181950301222	-0.57440295378401
O	-0.16133430894334	2.83927396029304	1.85494406966856
O	0.93818851780320	0.88761927597107	0.66014673920182

O	-1.38774435379571	1.64163986303371	0.17868689153635
H	-1.46870729947167	-5.48161640881766	0.52619122260564
H	0.69697457492812	3.14881629507639	2.18844676646987

$Na^+(Na_2SO_4)_2(NaHSO_4)_3(NH_3)$

Final Gibbs free energy ... -4852.20837087 Eh

S	-3.39636813525390	-0.95755054477149	-3.26152565533011
O	-1.93668538799610	-1.09244607506188	-4.02853292064256
O	-4.02840026754939	0.18859266726583	-3.93969143489564
O	-4.05147236953721	-2.27690393105474	-3.37896350063428
O	-3.06030525380071	-0.68173962027029	-1.81423684759349
H	-1.34062168255534	-1.63703534551817	-3.43969629767337
S	-2.57689772882248	3.51876425456899	0.17878621702218
O	-3.66099363086260	3.83444927893195	1.35136752735698
O	-1.94565353710602	2.21060857351085	0.49452741191696
O	-3.42061412375876	3.56740387905793	-1.04530635141600
O	-1.55656253152113	4.61877673688863	0.17955287946948
H	-3.23226441983595	3.73465423691554	2.21813140672976
Na	-3.54318205289457	2.19957767583009	-2.96756419374904
Na	0.40764009906654	3.17610683143357	-0.30121525644264
Na	-3.17686329367490	-3.09553275169461	-1.33094243499042
Na	0.03476273352446	0.29446361189571	-3.74869821308098
Na	1.40696328717833	-1.14004967507901	0.84076021382465
Na	-1.97317565556560	5.32216544973593	-2.06328228823455
Na	2.49604917842898	-1.73389958569288	-2.19319349951377
Na	-1.33569158719492	0.33857009629192	-0.76536510131424
S	2.18809740527985	0.93707212435543	-1.14210522597641
O	3.08339353434757	-0.10515835726529	-0.51583685544169
O	2.01263849831506	0.57727205229920	-2.61111665691904
O	2.70705000706856	2.35895278672860	-1.04878205902097
O	0.86257229325856	0.90228710004374	-0.37925258859975
S	-0.74652444182033	3.08543290186556	-3.33712502328329
O	-1.97461272476390	3.79843333801422	-3.84921904200334
O	0.17931692471858	2.61653807956665	-4.43871926742001
O	0.00319588721962	4.03213574822415	-2.40672131746400
O	-1.21069854812854	1.85352340006604	-2.56056222296999
S	-0.12708025009170	-2.56368473422526	-1.11395347644299
O	1.28067713692773	-2.95054105282278	-0.69915314424586
O	0.03199249334613	-1.67839308585578	-2.37683025765966
O	-0.72189972161303	-1.72158704468886	0.00840549926532
O	-1.01844665724302	-3.71534367897826	-1.42842684487384
N	2.70778395266640	3.34349582866581	-3.59941842792797
H	1.76641682599007	3.07081147684981	-3.99015202390767
H	2.75377671212561	3.00106402709558	-2.59715113218917
H	2.80316566848968	4.35550188169086	-3.63178987155994
H	3.45328111463820	2.91024500518915	-4.13858936916689

$Na^+(Na_2SO_4)_2(NaHSO_4)_3(NH_3)_2$

Final Gibbs free energy ... -4908.74845768 Eh

Na	-2.19122724827909	1.19494727608390	-0.22297199041299
Na	1.79083471894666	0.35806727449384	-0.57957976095609
Na	4.51752609812908	-1.01010139395958	0.89116030311020
Na	1.27534575990810	-3.02562516401159	-1.17084978777797
Na	-0.74276335458856	-3.28185456007733	1.52061182069876
Na	3.17994025340490	3.41812557224425	-0.21494962230839
Na	0.45382980351964	-0.06430690242332	1.96805152684751

Na	3.07754641510137	-1.07368392705132	3.96776618854857
S	3.44396675143014	1.39236224024529	2.38366627754109
O	3.30847105240574	1.31807270205285	0.86096538387094
O	3.76111979776138	2.82345992708647	2.74781738385947
O	4.50320299944808	0.40408109595407	2.80952057801382
O	2.13856478753330	0.97587038102012	3.06722000294062
S	0.18614523517331	2.90637027134226	-0.27399365154281
O	-0.00069582769262	1.71749634298216	0.66891954060545
O	0.79111477262931	4.07242700113993	0.49396454823414
O	1.22901874091972	2.51034094297504	-1.33443514688706
O	-1.13143052462764	3.20098832143054	-0.90582000917066
S	3.81455967607617	-1.22145071573553	-2.45461168440974
O	4.79189762162827	-1.22733848542391	-1.33890264840501
O	4.67296829185346	-1.14079478435780	-3.84657398058072
O	2.98593939529655	-2.45033520949553	-2.53567735995714
O	3.01923857035907	0.04322047041207	-2.52665748853855
S	2.06571977261947	-2.58030333804039	1.73796219825932
O	1.51518464852949	-3.82169183674824	1.08896341887480
O	2.12197162748758	-1.47708203597989	0.67680494312185
O	1.09757794669874	-2.12562035962367	2.83918195071335
O	3.44408550360370	-2.71981985159972	2.32383488005801
S	-1.20600168185812	-1.43975536082136	-0.73007299582605
O	-1.19601971050024	-1.02574437197550	0.75098136956296
O	-2.39200555289731	-0.81867372245133	-1.38782609247866
O	0.06884267619409	-0.90787887018100	-1.41614921367934
O	-1.12776643509788	-2.94651777198379	-0.77115260243139
N	0.47845229055435	0.81549591887412	-3.44806009807485
H	5.19812783040828	-1.95399531935639	-3.93027366024157
H	1.43108037951303	0.49350016029725	-3.66919261451632
H	-0.08015366674641	0.97568333263014	-4.28153843441122
H	0.06459985996089	0.07897534232112	-2.81733191942317
H	0.58190925852361	1.67417837251189	-2.86846629076907
N	1.31206135817305	3.88149142051770	3.13524862258783
H	0.97417929010866	3.95994381984845	2.13087469644475
H	0.80996703347909	3.12967500944487	3.60198364860873
H	2.33244226090971	3.58071711822584	3.10084379620898
H	1.18437840495520	4.75744013610165	3.63507503872216

$Na^+(Na_2SO_4)_2(NaHSO_4)_3(NH_3)_3$

Final Gibbs free energy ... -4965.28898640 Eh

Na	-2.30068480296320	1.01103583336857	-0.07373486554719
Na	1.70133822187632	0.43737863708375	-0.64361975393128
Na	4.53367829681025	-0.76116812369087	0.77122846792444
Na	1.38603422484464	-2.98065135358951	-1.19814417811220
Na	-0.52938056470321	-3.35754761907720	1.55487162604411
Na	2.87465810882783	3.50071714099581	-0.14243287193372
Na	0.49645605825019	-0.08483998919931	1.96535602151569
Na	3.21889251671458	-0.92794319871286	3.89197325441342
S	3.36231506088364	1.54058524199902	2.28360343919140
O	3.17594313095620	1.35957010423686	0.78215280136003
O	3.57443483356109	3.01602947964283	2.53843044958386
O	4.51473923815568	0.66500578575153	2.71622626815165
O	2.12441855749200	1.06672989025557	3.05197098309563
S	-0.04063733446966	2.86504914454092	-0.22693946167164
O	-0.11820314468593	1.66335020575113	0.71634823287153

O	0.55092876178855	4.04996623591202	0.51916213229572
O	0.95971142635050	2.52719264059332	-1.34186566247552
O	-1.40582603596532	3.09547416751642	-0.78150178499531
S	3.76747814524171	-0.97793150889630	-2.56859746371651
O	4.77635897151763	-0.82249953976112	-1.49022135823758
O	4.57088537105126	-0.87281313502318	-3.99255741118097
O	3.06952650708074	-2.28569939648646	-2.56404871062415
O	2.84606956767592	0.19739250471303	-2.66716178602098
S	2.23454905963528	-2.50430768623023	1.67663099566024
O	1.74701127293302	-3.79094546987406	1.06674714274493
O	2.17079501376450	-1.42045983328316	0.59699808868066
O	1.28188239115049	-2.10096278735208	2.81116036749108
O	3.64113989933418	-2.53501315983127	2.21212271236998
S	-1.17965737202823	-1.55015412275518	-0.67504453492903
O	-1.14140791259086	-1.14032705917239	0.80710747510819
O	-2.42395202686894	-0.99662416948753	-1.28422884849113
O	0.03335083584627	-0.94252359520175	-1.40810178787017
O	-1.01159529168577	-3.04944965836212	-0.72431329775064
N	0.16339762275933	0.86361092846978	-3.40704291543011
H	5.16204889246478	-1.64014856755091	-4.06963033141400
H	1.07486665393741	0.60639291268076	-3.79841321932466
H	-0.52060861052263	1.05783339652255	-4.13311294181803
H	-0.13095138068405	0.06954879722189	-2.77806170394450
H	0.31753615834181	1.68730989429353	-2.77734468342042
N	1.11183324189805	3.91488405591867	3.14621772420653
H	0.73046799216030	3.97867743923255	2.15630949545016
H	0.68030427570168	3.12922393317955	3.62744704731842
H	2.14314548735470	3.67630267003461	3.05204630683480
H	0.95777544885202	4.77788745998430	3.66060127218830
N	4.49906136597314	2.95196603027752	-1.83008555345903
H	4.77138739909743	3.56344253299795	-2.59304199702623
H	4.08608736423412	2.12628665738629	-2.26264350707091
H	5.36632210265033	2.62695225297669	-1.41274067410487

$Na^{+}(Na_2SO_4)_2(NaHSO_4)_4$

Final Gibbs free energy ... -5657.67622398 Eh

S	-0.35219324046001	1.70524983174389	0.33863837106255
O	0.79727620469711	0.78224826759403	0.20261834107085
O	0.20408217266085	3.04881639292402	1.08181209355260
O	-0.92004346186971	2.14795811506866	-0.97968347400511
O	-1.42973791398379	1.26108071708653	1.26331265833521
H	1.01737620852208	3.33774735606779	0.63505372112612
S	1.35333938414858	-0.60200278814523	-4.32781990439391
O	1.83461740677605	0.66352204084997	-5.25626399544291
O	1.51531489638604	-0.03172586879453	-2.96092736044932
O	-0.08910152280430	-0.82365990510588	-4.64929808770721
O	2.24276422584385	-1.73394513839821	-4.67143648835881
H	1.87204011830221	0.37467556233322	-6.18340556056666
S	-3.78753306771844	-3.99253110601516	1.74782282618029
O	-4.43965470800541	-4.76302399546773	3.02983052160790
O	-4.91416201079337	-3.37412823769854	1.01028319906765
O	-2.82956607483096	-3.06082182478101	2.40498953220333
O	-3.05171301999434	-5.02832489198971	0.94836401456412
H	-5.21752189997042	-5.26524040911518	2.73469561118272
Na	-2.07995010128118	-0.79731839216554	2.15621499075853

Na	-0.72965933178089	1.01663659563539	-3.03721338582027
Na	2.41658948604473	-3.74363877636192	-3.73049350257626
Na	-1.46545422780377	-2.39496188426535	-3.54326097035273
Na	-3.09980527049024	1.25616049816010	-0.92957702541271
Na	-0.85648483182501	-4.14780916985338	1.15696045558497
Na	-4.92834890769566	-1.97291061717192	-0.81583145228386
Na	0.88130698212162	-1.17348580084864	-1.02833179009558
Na	-2.49269261591852	-5.13532926350425	-1.31292295084920
S	-3.98822527995868	0.03842645937193	-3.52028714241120
O	-3.39417459883903	-1.16808160009600	-4.13436697822558
O	-4.75895200808031	-0.19201238761677	-2.26275451359815
O	-3.02759315414332	1.17483501900147	-3.33783904731572
O	-5.15206529966367	0.56420186635365	-4.53833593460019
S	0.17771213122992	-4.57302259616399	-2.19974580816873
O	-0.20649065980799	-4.97720506946540	-0.78615737620811
O	-1.07774689437826	-4.66445263534156	-3.05716269937161
O	0.64302156196420	-3.10233446707055	-2.23604410290706
O	1.29180493577188	-5.41050135474064	-2.73640357192079
S	-2.04802989007681	-1.61529795011928	-0.61255507589481
O	-1.42097888481229	-0.76119749417079	-1.68748660681609
O	-0.96747201657582	-1.99435247994501	0.38492221522197
O	-3.12725465050175	-0.82579574599668	0.11707168354668
O	-2.70342334094190	-2.81813636051915	-1.24755450402416
H	-4.79970011792576	0.55618926011976	-5.44388983261039

$Na^+(Na_2SO_4)_2(NaHSO_4)_4(NH_3)$

Final Gibbs free energy ... -5714.21231196 Eh

S	-1.90396399970968	3.28093466882955	-0.29322366638025
O	-2.58939315756533	4.76839495533225	-0.26808138287103
O	-2.29516985672871	2.65794375602505	-1.57798713730527
O	-2.41770820965845	2.54876475224628	0.91177694273649
O	-0.45915905101724	3.60187144558941	-0.14192856912842
H	-3.52717045048271	4.68073462262813	-0.50716070376466
S	-4.19749921874643	-1.62514786022352	-0.76292216915755
O	-5.63475779504205	-1.44131362995669	0.00999539648045
O	-3.91484659047515	-0.22333817634104	-1.17886181995006
O	-3.22661313482817	-2.08093407124028	0.27864468385662
O	-4.43405207920527	-2.59765196424974	-1.85311692230682
H	-5.98252285916336	-2.32019403119099	0.23598066737319
S	-0.32459627906821	-0.85341999768229	2.99290680952349
O	-0.25329672611904	-1.32338597275210	4.55619174645672
O	0.95609253506817	-0.10319494631097	2.83713737655049
O	-1.49105645667551	0.07962406269622	2.87392309301943
O	-0.44490883499449	-2.08388322626874	2.18123606637207
H	-0.94511368444512	-1.98769632383854	4.71215187654213
S	4.20492498108527	0.25923595278548	-1.70593233686965
O	5.69425206910171	0.67000124317814	-2.23598255503929
O	4.32597076247575	0.05076263163087	-0.24270559710257
O	3.38439033197125	1.41665985431976	-2.15039473721039
O	3.80918373311701	-0.98451709671966	-2.44857664383099
H	6.34616817313483	0.06972538881052	-1.83736268364448
Na	-1.93040353923916	0.45388758055745	-2.20048601524968
Na	2.68610297049494	-0.23655650590465	1.32713559544852
Na	-3.08216304929847	-3.20646602484127	-3.50885759762220
Na	-0.90384134057284	-2.32839028487154	-0.11241391238730

Na	1.89488410435366	-0.04103043208924	-3.54424176162786
Na	1.58136101200751	2.95822865807093	-1.36826809223269
Na	2.29141203800770	-2.63253912729787	-1.88054867782823
Na	-0.29812455758953	1.91818956488022	1.84646460468692
Na	-2.90854823268866	0.27738120351003	1.05007013827200
S	-0.32215794588147	-2.74239703282088	-3.05857574696142
O	0.17434234141317	-3.50454972506728	-1.83661426218050
O	-1.40121995327713	-1.75373312466479	-2.56791306194209
O	0.86338552221228	-1.99507047973927	-3.64377442657721
O	-0.96099406827728	-3.64548272337673	-4.06273002348313
S	0.57675467501839	0.33636017702851	-0.59440515135029
O	0.47530314747214	0.88391966865593	-2.00627165354852
O	1.31046617983812	-0.98325589496708	-0.53654010373067
O	1.33113607362014	1.33465074582690	0.27002705127990
O	-0.82569585991425	0.14802274211911	-0.05814350576122
N	1.66073432587944	5.30475739704686	-1.91767291728470
H	1.58940987736751	5.60366859296328	-2.88536939833211
H	2.41067312200893	5.86062171415859	-1.51780488301098
H	0.80551582041177	5.61898858598966	-1.46491974570513

$Na^+(Na_2SO_4)_2(NaHSO_4)_4(NH_3)_2$

Final Gibbs free energy ... -5770.74938678 Eh

S	-1.72019291205049	-1.75700193696255	3.46012257970906
O	-1.31938124727233	-1.34159951937866	1.99749992540350
O	-0.83669429541716	-2.93587888283797	3.78459781149656
O	-1.34425534643520	-0.61552535067117	4.38079171794779
O	-3.17462498017494	-2.05408194157638	3.46621254003996
H	-2.33454505722261	-0.78060554900054	1.27447040381543
S	-1.89439069222932	-3.52849913526135	-0.88341844236663
O	-2.27652765760932	-4.84828228863245	-1.76917463844818
O	-1.83376442447405	-2.36984183428548	-1.82806382158910
O	-2.97115894030300	-3.51592043722597	0.11461481262075
O	-0.51817955405420	-3.76654847916049	-0.32471542874975
H	-1.66232804817262	-4.92093759060752	-2.51783957278132
Na	0.11211861271604	0.28435312885387	1.25495793829836
Na	0.25899082792126	-3.37135091615870	1.79958944602031
Na	-2.12641425184168	1.47666358284032	3.86775811729196
Na	3.53681924265880	-0.39189573442294	-0.38067512479871
Na	0.53989314747919	-1.85703055234825	-1.29375606802184
Na	0.62479091587065	3.85463946935268	-0.70389830213041
Na	-3.46216720167503	3.36596562665657	1.07135371949512
Na	0.88429608290089	-1.58770378225789	4.62011127403066
Na	-4.35698633128696	-2.42545345729432	1.55883809893862
S	1.22578315680923	0.99490669750339	-1.44124139817581
O	2.05300464018621	-0.09300609464718	-2.09773322010416
O	0.97771752758455	2.19118518185102	-2.29583681922603
O	-0.11007287078096	0.34149581185450	-1.04069205725447
O	1.93524677408892	1.41885341937793	-0.14539141760442
S	-0.71621515307990	3.32206904475483	1.86583713876369
O	-0.34358060151465	2.02947885531761	2.57798669325900
O	0.55505666797079	4.15170836709552	1.71943405627991
O	-1.22538451115869	3.02198612489866	0.45128022353577
O	-1.81905567889329	3.99295886055689	2.63613048419316
S	-4.21245270128083	0.55523769377204	1.06443463881515
O	-5.37013269116722	-0.31325370861258	1.35374989194618

O	-4.40517777495151	1.50888024086649	-0.08623893875235
O	-3.69625677076325	1.31737113155769	2.25120552618566
O	-3.05152171469811	-0.42925734479216	0.54526073841288
S	2.44142316006022	-1.36297573211914	2.11844621281882
O	2.27603246506921	-2.59794625890364	2.96140238774671
O	3.84967250918020	-0.99192196034205	1.78364835578065
O	1.75980461768743	-0.21112865543277	2.88666753176368
O	1.66475681992792	-1.57423704226185	0.80131002506573
N	2.61884734199838	2.39744613126773	2.45014920898079
H	1.82101158733527	3.07305465091948	2.32913451516455
H	3.28493670843530	2.73100953330533	3.14199426634181
H	2.26306626629724	1.43895872902570	2.70389259540480
H	3.06698268864472	2.30246740738178	1.53886851786479
N	-2.61231285319044	0.44997823794952	-2.08226717436857
H	-2.73214815603888	-0.57005015440406	-2.02242719938128
H	-3.30858853962246	0.90809490864266	-1.46316349577246
H	-2.70692737265587	0.76349744422781	-3.04451534809350
H	-1.64012909581964	0.63087912379126	-1.72296827580883

$Na^+(Na_2SO_4)_2(NaHSO_4)_4(NH_3)_3$

Final Gibbs free energy ... -5827.29300674 Eh

Na	1.23496375803116	0.85125787094244	0.84959186462359
Na	0.21879424745399	4.12518268158332	0.64065603721668
Na	0.61178840050410	1.09232577413732	-4.17948847954574
Na	2.93573456364059	1.78104315249742	-1.71283742424462
Na	3.31630859304939	1.18405675192180	4.21910647925803
Na	-1.07051848813921	0.61800311639394	-1.06429411276363
Na	-0.45471452795888	-3.16415174827753	3.62850952321931
Na	-0.97199598712900	0.42196521177345	3.06540702090367
Na	-0.25105579918030	-3.00984691012097	-2.13487839456341
S	-2.15726767087490	2.43991795035165	1.35446817631072
O	-0.67392964161548	2.13568234862700	1.51730646663638
O	-2.89580455312079	1.81251420860156	2.49756823880992
O	-2.29951183215280	3.94239159610596	1.23056234099685
O	-2.68298561784435	1.82090107315523	0.03851500502920
S	0.26381547483876	3.08216382901279	-2.19106299272647
O	1.41865702029990	3.08021117212582	-3.15940468812720
O	-0.14880542866375	4.47626187290803	-1.75208297843712
O	-0.91667105675791	2.34962525724200	-2.81343329573798
O	0.70443294846944	2.32199875201949	-0.94112914071927
S	1.45233406107271	-0.98287280994024	4.02448090741894
O	1.72391232811259	-2.31289461356605	3.31816909131861
O	0.01667784872078	-1.05523162811249	4.52439310354280
O	2.44486978247259	-0.72198539154858	5.10716749535144
O	1.54900362068492	0.17805074829222	3.01960844720960
S	-1.25891028024211	-2.00173337191379	0.67014722114248
O	-1.89398235767339	-2.39586572157662	1.97915572843422
O	-2.31653975133040	-1.75923025641910	-0.40527989023393
O	-0.33301468636298	-3.10319896856695	0.16732651630114
O	-0.48931762307211	-0.71045518829152	0.87055891638142
N	-2.82636081304994	4.41698088049381	-1.40962964296575
H	-1.82624695347087	4.59450665177855	-1.70326748590355
H	-2.81871314442445	4.34643532984089	-0.35761050546119
H	-3.06653152444349	3.49113844394444	-1.76362155074697
H	-3.46838559670216	5.12468368371118	-1.75397864073383

N	2.38120390317109	-2.58296814231299	0.71456403094255
H	3.10653731382065	-3.25797255954253	0.49194109100976
H	1.44113601190858	-2.94399443852762	0.45868403680809
H	2.50433262613526	-1.72194090004689	0.14028429878068
H	2.33419390443999	-2.37655096738527	1.74465991051599
H	4.86731212156131	4.80056683920047	1.26579110363884
N	-4.25294560240083	-0.25421815960512	0.76445865225708
H	-3.80356997341735	0.65810300504043	0.45997048170649
H	-4.19263702563495	-0.28203042962529	1.78118973263486
H	-3.64749506981791	-1.01164652072689	0.34259993839064
H	-5.22253890516649	-0.33016791300988	0.47107003465922
S	3.46532231075314	3.17839872100548	1.51974257570704
O	4.67810815442861	3.98998356543109	0.76502650258773
O	3.30777807470702	1.99978593562518	0.62156847032712
O	2.29045700022718	4.08343081558106	1.54356672517550
O	3.96260315847735	2.83342318206497	2.87533434969502
S	1.72401138715269	-0.88268311691338	-2.30302504313030
O	2.14991671788325	-0.36236781236985	-0.92795802446949
O	0.20842811584361	-0.66538814253969	-2.50702916825621
O	2.43864308657100	-0.04135669086859	-3.33275778205368
O	1.98247937621520	-2.35638001960125	-2.38933427412131

$Na^+(Na_2SO_4)_2(NaHSO_4)_4(NH_3)_4$

Final Gibbs free energy ... -5883.84333375 Eh

S	2.51012478712366	3.68731698795334	-2.45527281733179
O	2.90294011355673	5.00936022971481	-1.73921340241773
O	3.75421081731603	3.00689202108953	-2.93335823030779
O	1.51472648588608	4.06092917245285	-3.52938314537221
O	1.80622918009198	2.76578796478027	-1.47128592899124
H	6.01368811334997	4.34110409250913	-2.40559621563224
Na	1.34993837113842	-1.26411133108759	3.55636450004173
Na	2.61399660679728	2.07421911063022	3.42813928372901
Na	0.99029846514517	6.15079694419958	-2.58406028974277
Na	0.98881349808047	2.45144253897178	0.63507621988263
Na	-3.03832328876317	4.61493883988374	-0.73963332477183
Na	-0.38617376298318	2.93314970484484	-2.32138405031771
Na	-2.97261105253992	0.74863905618886	2.37404479288572
Na	2.47620169157151	5.46554739955186	0.53162216881651
Na	3.61824142108211	1.29808962565923	-1.04607155907864
S	4.43256420889035	3.44616335803816	1.44092277295776
O	2.91681668344630	3.32413293296692	1.47170788305146
O	4.78060726180300	4.89029600248207	1.23750502560699
O	5.00591374312559	2.62071964368067	0.27548958189432
O	4.95651695179804	2.85432343094139	2.73768192176253
S	-0.43666094873944	5.68961542487757	-0.09771750981455
O	-0.78431635471932	5.01491234029852	-1.43907348022761
O	0.53009572283924	6.81268016386450	-0.39328129309873
O	-1.73010961090227	6.11078715145665	0.53827429038380
O	0.28568974317472	4.70015407638260	0.81469994410362
S	-2.38427221902812	1.82767373627876	-0.33139672814588
O	-2.84964140202925	2.44543384887450	-1.62653083631096
O	-2.95427981142282	0.46051526011371	-0.03419050563760
O	-0.87441621752976	1.72500117366885	-0.38076776759127
O	-2.83712693994352	2.75999390332439	0.81623779852841
S	-0.30527604530407	1.10729933490472	3.63923271476312

O	0.66091865030398	0.66569394673310	4.70543750384954
O	-1.61411789863023	1.66519338647422	4.15094923100582
O	-0.66224744787831	-0.14104772081697	2.79372659543032
O	0.37272156512296	2.16226971456190	2.78862949964790
S	2.82298497242596	-0.57496020412018	1.18811291586577
O	3.05150091740771	0.03538141801263	2.56870935428753
O	4.16709561567337	-0.71490187664218	0.48996230157861
O	2.09730436426643	-1.87673838115081	1.38332994744874
O	1.97870087751351	0.35457048419389	0.31848840136088
N	6.02733171107927	0.43140331844299	2.07957754449200
H	6.90520059445274	0.58178730375072	1.58985086193581
H	5.32106518455010	-0.03913969235267	1.43302787067547
H	5.63344086139918	1.36938824361515	2.37960494891925
H	6.18517771727349	-0.16083472784734	2.89052166342494
N	-0.45448971677175	-1.03117728428180	0.19596825598956
H	0.35827532672623	-0.52173250033287	-0.18668168002498
H	-1.33385116303421	-0.74838153888924	-0.25706606298381
H	-0.50005622329045	-0.70234399095748	1.18779522018541
H	-0.27346292691769	-2.03077604088549	0.16274467639925
N	-1.60680723836402	4.23309633719072	2.80808204863420
H	-0.68797460083631	4.47466139265656	2.39773389813135
H	-2.11934924645052	5.08490050101059	3.01863985261613
H	-1.51467299648551	3.59304789609662	3.60923968116861
H	-2.07882096825615	3.70164899430378	2.04200835456198
N	5.63126216094469	4.60797935896149	-1.50216205705814
H	6.19641014953718	5.31323585792168	-1.03629373525092
H	5.53436332803775	3.77069481843202	-0.86530725100676
H	4.64442998153642	4.94140321543592	-1.63866760431377

$Na^{+}(Na_2SO_4)_3(NaHSO_4)$

Final Gibbs free energy ... -4095.44188777 Eh

Na	4.29922568010299	2.01811523222885	-0.58791686957773
Na	-2.54816743039729	4.46217893133927	-2.54834079172451
Na	1.69259963657441	6.82246806329230	-1.99052535505550
Na	0.20918925645150	0.77303618654341	-4.31241737093968
Na	4.19476839461437	3.21299870973715	-3.65868082400374
Na	1.74362352996088	5.28254568912615	1.03606996701568
Na	1.12058870377559	3.40490716068498	-2.02287265785013
Na	0.44060677202361	-0.32309171239703	-1.13387495264939
S	-1.63706029363084	1.66723078837547	-2.14124958652883
O	-0.86277307780027	2.57971436548312	-3.06658762579584
O	-1.38609201713485	0.23840915825642	-2.51050005937331
O	-0.91069843370449	1.74971798766549	-0.68616791288310
O	-3.02996609303974	2.11945653262318	-2.00476427719082
S	-0.60095991522027	5.46818354173346	-0.73778714000093
O	-0.13316748753464	4.14177271041869	-0.08060631143194
O	0.24565316727861	6.56021479387234	-0.11721229144427
O	-2.07035022836896	5.62954350069105	-0.59768087351936
O	-0.23984469083279	5.38935760308206	-2.22744463640156
S	3.66534673446762	4.79200455198319	-1.25220266220891
O	2.92078121896193	3.85986602801737	-0.28607160329665
O	3.68015142238957	6.16861351930819	-0.65963725610116
O	4.99439990468317	4.13941987553861	-1.55752760382438
O	2.87516747498827	4.85006049166100	-2.57310080639753
S	2.60592265053697	0.89721449602822	-2.71818730613570

O	2.12544989175942	1.99486957024413	-3.67819070625738
O	2.12681039128430	1.23537114356212	-1.30163861206729
O	4.11339439493354	0.92119090906137	-2.71420992926666
O	1.94041224314373	-0.39574914812022	-3.12174650795157
H	-0.75597220540240	2.72472365142642	-0.39030533331367

$Na^+(Na_2SO_4)_3(NaHSO_4)(NH_3)$

Final Gibbs free energy ... -4151.98772662 Eh

Na	4.31535033846359	2.01514748247744	-0.60593314820496
Na	-2.21420172615769	4.45448280301867	-2.74323850830157
Na	1.71363540512332	6.82292907474218	-2.13633109138983
Na	0.21744345794638	0.87655663497891	-4.36583455892673
Na	4.12595220336146	3.20058143679963	-3.67233575796059
Na	1.89687398384307	5.64722984061008	0.93241065639092
Na	1.00818299209093	3.23537160342082	-1.66279739251244
Na	0.38579497348244	-0.36407730548857	-1.31509799082097
S	-1.54518387077888	1.64955442992803	-2.17315411043561
O	-0.87793136064231	2.60295222072014	-3.17073533293420
O	-1.47925403047786	0.25665414319441	-2.75951909873384
O	-0.75217620690349	1.64609653901985	-0.87402040576979
O	-2.94038326080989	2.18494988190725	-1.91123804305447
S	-0.53379713501192	5.66390867440262	-0.67862478449055
O	-0.03839059500474	4.51292062844191	0.18750336541848
O	0.20857267836707	6.91269023340342	-0.25499208508131
O	-2.04525906622880	5.74473448253174	-0.59849409817889
O	-0.17057856382004	5.38559946693327	-2.14093420729178
S	3.62160925831494	4.78074423847765	-1.26404653074868
O	2.93179054499477	3.88362300738346	-0.22958569816686
O	3.63035384494617	6.18735709049783	-0.71648535689858
O	4.95961068917049	4.15654428130755	-1.58547385976013
O	2.79287988204906	4.78917550718166	-2.55205216429138
S	2.63582640813625	0.87565498004749	-2.71113459323731
O	2.09591187468591	2.03068623932148	-3.56158768259337
O	2.23449636916161	1.09945529025218	-1.24970749795053
O	4.14406139666952	0.92422980240865	-2.78546738220705
O	1.96387302908231	-0.39146103775190	-3.18273245507153
N	-2.65826950132474	3.31226112028946	0.60432116408171
H	-1.67179536235788	3.04648364079435	0.70941378549053
H	-2.99919625078242	2.77751863768732	-0.22980976156885
H	-2.64064199330241	4.32916547214166	0.36527067932094
H	-3.19887646627794	3.11624359890683	1.44175030688303

$Na^+(Na_2SO_4)_3(NaHSO_4)(NH_3)_2$

Final Gibbs free energy ... -4208.52301397 Eh

Na	-0.12511793864697	4.16051477247163	1.72440379215764
Na	0.14609670846340	4.70992903214456	-1.89918169444253
Na	-2.72839756295308	6.85836725676611	-0.97480414269174
Na	3.11612785440985	2.71243517446179	-2.70333851130270
Na	0.92184839307580	7.78195261614128	-3.64152391250929
Na	-3.34682191477170	4.14397541554876	-2.89206822860534
Na	3.59047380214066	5.31499968724840	-0.74870937025470
Na	-0.60491430044728	1.54266731387779	-0.21241314738945
S	1.90803457076552	3.03935113128798	-0.05631451264056
O	1.20447316266009	2.58751411442669	-1.34299778049466
O	3.39467817039282	2.91012761620905	-0.28321802910967
O	1.59898490735004	4.51956916432238	0.18819494633989

O	1.31518490370755	2.25187423998245	1.08731245768615
S	-1.63976030778374	6.36746990646290	-3.66606002552853
O	-1.12134747542767	7.10803251397055	-4.88968150194873
O	-0.88151546728725	6.91834289682179	-2.45518829851504
O	-3.11899534061804	6.50984726717964	-3.39476313924877
O	-1.33103435704094	4.88649187262981	-3.82579221298055
S	2.67888549800135	5.48031862025310	-3.52814127448056
O	2.05841759953706	6.19796465527917	-2.32484657848715
O	2.71163242702947	6.44018555590843	-4.67892205191246
O	4.00724736889260	4.91021539699931	-3.07881315807584
O	1.78221470889430	4.27972321062761	-3.89151465723929
S	-2.30315277682090	3.91001368591207	-0.19727513280593
O	-1.81604591974984	3.13005000742504	-1.42268297308318
O	-2.11201645033676	3.02295167230492	1.01547126549482
O	-3.70784040774596	4.37561286838963	-0.47508224543122
O	-1.41009305721443	5.14055578181937	-0.00724196597668
N	0.44569314202465	5.16870095028036	-6.11583805012890
H	-0.21508008073678	5.91708493126891	-5.78005903962604
H	0.87002557154323	4.71660834828553	-5.25744855876443
H	1.20658362733552	5.58219836969362	-6.65220066378974
H	-0.06148771502052	4.48698468802146	-6.67320139822976
N	-4.60151798851530	7.27840866661434	0.47073983723076
H	-4.52675712449826	7.72057655680554	1.38091228875184
H	-4.78377106817199	6.29150603181410	0.64422506033265
H	-5.44625838967846	7.65293387161116	0.05020692569893

$Na^+(Na_2SO_4)_3(NaHSO_4)_2$

Final Gibbs free energy ... -4957.44922884 Eh

S	2.71670488606369	-2.45549462506016	-1.78654994019860
O	3.10338664546092	-4.00825298978637	-1.41829236438984
O	3.77347552076733	-1.70820715924809	-1.04780532845400
O	2.79539836541876	-2.33302514249231	-3.26296953669094
O	1.35744852999474	-2.18835489243897	-1.24850832531013
H	2.62023010091488	-4.61163026537534	-2.00702702315135
Na	-0.20338689624483	-0.60243198134942	3.71122001954639
Na	-0.14355165230088	-1.88450139258088	0.48060321377940
Na	4.51368387700747	-2.29536255559643	1.11872036222106
Na	2.32366582578019	0.17929942044742	-0.31482280379789
Na	2.64806840571892	-0.37182989086289	-4.32019411269643
Na	-0.06869280084947	2.30059871509961	-1.24753752945595
Na	2.44848874220829	1.51513930879241	2.68632269560053
Na	2.15873069274181	5.22757389823899	-1.80313666981884
Na	-0.32861638140333	3.65616101531662	1.98934909975851
S	2.40757332711620	-1.41538169748746	2.81032105137500
O	2.12360781334241	-0.49653319896518	3.98115581701755
O	1.07253919329210	-1.98265710117042	2.34398916639116
O	3.01383619453934	-0.54002417891737	1.68573453075707
O	3.38901231558182	-2.50438321518018	3.09054912503814
S	2.25503712150950	3.80737632605296	0.67440368098319
O	2.04036063711802	3.78093709140327	2.16352580694821
O	3.17988307109813	4.86860244029908	0.18645686530432
O	2.79572572337801	2.42149467785612	0.25373393792200
O	0.88628654958693	4.01297429815428	-0.00693862410630
H	3.42779366887512	2.57648945819756	-1.20358348401319
S	2.39886160763179	2.22086172231828	-3.07760395252972

O	1.78431588837356	0.98352519305684	-2.45310855191345
O	2.91920466052805	1.92856781522812	-4.42723798225119
O	1.44103436124446	3.36850722381368	-2.97908766867030
O	3.68641039441101	2.61386180241594	-2.19517361428468
S	-0.76916125396947	0.88281041049695	1.25390605014010
O	0.11389234709529	0.41231095854933	0.09483788185699
O	0.09803981607588	1.37608640487940	2.42038434298678
O	-1.57617135424215	2.05501820516468	0.75589194801687
O	-1.56560641369320	-0.30087652849721	1.73407262119253

$Na^+(Na_2SO_4)_3(NaHSO_4)_2(NH_3)$

Final Gibbs free energy ... -5013.98915965 Eh

S	2.48822975719621	-2.73398713976128	-1.89727194297418
O	2.71544312423088	-3.19479274937272	-3.46553666560003
O	2.82687646895306	-1.28671590891369	-2.01202487828517
O	1.06128401627117	-2.99719551257073	-1.58156243111701
O	3.42557914349045	-3.52599115362579	-1.06808265401103
H	2.50991736899266	-4.13989357445551	-3.55646070512629
Na	-0.09905322923365	-0.97860884301944	3.30829832429730
Na	-0.02708754484190	-1.97794110701525	0.09770111659489
Na	3.21648172459850	-3.85501836523026	1.15260026553370
Na	2.56755675185029	0.46761539490070	-0.38170427177351
Na	2.68824929100053	-0.00669751769354	-3.97485869550249
Na	-0.00347188952510	2.24165170892491	-1.45101036360492
Na	2.39100519020442	1.48060090247985	2.73363515749907
Na	1.84184862875470	5.15954010363238	-1.73867939882369
Na	-0.48794230286756	3.44113983215499	1.87396427435847
S	2.65707138140484	-1.44873419748170	2.50595095078346
O	1.47335490704297	-2.18956573114902	1.81745714185554
O	2.10580146754809	-0.72605915266763	3.72056571659056
O	3.69032770938230	-2.47310324126521	2.83917102519626
O	3.20565151867441	-0.40251305664540	1.55695727317935
S	2.19878395917111	3.82475868520393	0.84428293792679
O	1.78709329677157	3.90023551139654	2.29271697278073
O	3.01798338629075	4.97778994941667	0.34604057419365
O	2.99772700360359	2.52194911971851	0.67341518930100
O	0.91628067007103	3.77153387009304	-0.00210224892152
N	5.05914637008429	3.38868153304300	-0.92754907997948
H	5.92160083550719	2.87834616532845	-1.09457060172133
H	5.25694912651468	4.32163932682559	-0.56938793724735
H	4.44250440675700	2.92455331594449	-0.21741674155695
H	4.45243293444647	3.47767279743018	-1.81221441209508
S	2.26781910593916	2.77113635229977	-3.30952217107281
O	2.25690652036836	1.59662742646952	-2.31514972749561
O	2.52246025036878	2.19745429627867	-4.66262513474201
O	0.94289208761794	3.49539966419131	-3.18041417476976
O	3.35251645578150	3.77329265678982	-2.89703858689498
S	-0.66882378010753	0.69056467500604	0.99449090622397
O	0.29244223801944	0.32345419355781	-0.13837076691275
O	0.10442745901592	1.17505411881725	2.22504777272895
O	-1.54305630150701	1.81734127943602	0.51502788939952
O	-1.40904618983804	-0.56865036947093	1.38815462178972

$Na^+(Na_2SO_4)_3(NaHSO_4)_2(NH_3)_2$

Final Gibbs free energy ... -5070.52815354 Eh

S	3.40510999250281	-1.94923358543983	-1.88277807823479

O	3.25717099507908	-2.04535981990543	-3.36095326974903
O	4.11699028393993	-0.66016527801688	-1.49412701308463
O	2.02923986770307	-1.96831793138548	-1.19923732147321
O	4.18938173124044	-3.11875869342840	-1.27923868073804
H	4.73602925985776	-1.24348819098153	1.02608344467518
Na	-0.20502126005886	-1.14304428704053	3.29579642959475
Na	-0.01642547585366	-1.74556273342451	-0.18578845409260
Na	2.65168684988196	-3.77461970259115	0.32076811511373
Na	2.34997494006578	0.37650107737428	-0.41519163409419
Na	2.48701709228505	-0.09243809944162	-4.24575546423571
Na	-0.16103988839635	2.37466945536334	-1.31478789857346
Na	2.43490956098590	1.24525154646130	2.75169207131535
Na	2.11828534037004	4.95924212439730	-1.64635033202113
Na	-0.22197983964213	3.44239757889366	2.09425103130527
S	2.47538347172167	-1.79001108951027	2.36333719617253
O	1.18840180940696	-2.27761518129883	1.67563157180824
O	2.09412885154442	-1.21144914788222	3.69937621343559
O	3.43285501702762	-2.94774652689366	2.39788599075996
O	3.11816417083932	-0.66101467241229	1.54220153781880
S	2.42580483231885	3.58555009078894	0.90783381531336
O	2.08478268737050	3.65063879283994	2.38174267607586
O	3.30229187692854	4.67679922315911	0.39366172631270
O	3.10339391486178	2.22493201480020	0.68319781123471
O	1.09597332155820	3.64335563640514	0.13182404464583
N	4.90804090316098	2.12549899157442	-1.44496388697691
H	4.89556291550761	1.12039325531294	-1.66107106426000
H	5.85307801677944	2.49697313591668	-1.45877481406906
H	4.45571100117256	2.26824699791550	-0.51755520267441
H	4.26796276729313	2.64500791812333	-2.15209015242574
S	1.96261877896291	2.61018727134260	-3.36110963176302
O	1.84624507274509	1.37775987490865	-2.44582835931594
O	2.05539584492407	2.12012070238321	-4.76481339191932
O	0.78876946882672	3.52391900100273	-3.07996605080345
O	3.22167109818006	3.40361039667794	-2.96473071348307
S	-0.74696039917229	0.75131049431535	1.16220086181917
O	0.13488279465170	0.48169970434141	-0.05841612804960
O	0.12937378758172	1.06325067726775	2.38536783165399
O	-1.58657271111636	1.95992977531128	0.86076714822325
O	-1.51003512774619	-0.51849389476823	1.44962687977063
N	5.52142223274049	-1.88099926943896	0.75320326580853
H	6.35869040958223	-1.36285984007273	0.50355105874885
H	5.15884877553893	-2.42401328916393	-0.08416989111637
H	5.69045177120071	-2.50241167096866	1.54311123051742

$Na^{+}(Na_2SO_4)_3(NaHSO_4)_3$

Final Gibbs free energy ... -5819.45784419 Eh

S	1.33987709118579	2.29646133420728	0.81806425467938
O	2.62721146798059	3.30812696910577	0.86359342213314
O	0.32272639011136	2.87029473582483	1.76048836240660
O	0.88826383208547	2.24242451013901	-0.58540228577865
O	1.92608897855786	1.04950304327777	1.38385083177147
H	2.41956934321832	4.10636169239996	0.34962836874678
S	-0.84827011874349	-0.23849055697197	3.55359984560924
O	0.58666593166803	-0.61666391250193	3.82278024608730
O	-1.09862063785336	1.19388842001425	4.05628897355439

O	-1.05357062669061	-0.22238855546771	2.04634958663178
O	-1.83610539596945	-1.15593307586576	4.22082999514844
H	0.16353249827421	-2.92813802852917	3.30950258004322
Na	-1.86680782180674	1.93684080136447	1.80628585158197
Na	-3.44665696340954	-2.46081260773213	3.16504710931961
Na	-0.43876241044947	1.02153195451709	-1.92474415593556
Na	-2.19028483975510	-1.15555776954375	0.34999660748408
Na	1.23753625320744	1.63864221782460	3.66675911342327
Na	-1.01482845452593	-4.57855158124075	-1.04569137703579
Na	-3.02733155936300	-0.97807588140042	-3.20609546719636
Na	-5.75402619495663	2.50448253961895	0.97949369271010
Na	-3.29393744123621	0.65190144435094	4.77261332489061
Na	0.97586072826640	-1.13122541768278	1.25739810161978
S	-4.90397682433837	0.13745290504436	2.36676890953892
O	-6.26801708916314	0.54356293107898	1.92333729821004
O	-4.04715861678422	1.41426047875690	2.50777366537663
O	-4.86654490920856	-0.60289494423416	3.68049166707760
O	-4.26965104537682	-0.79215883765602	1.31679814134212
S	-0.56295539387988	-1.89972996620828	-1.98170164469649
O	-0.10187182741764	-1.07057749916064	-0.77667258397146
O	-1.99042072304961	-2.40788068968927	-1.66730295979693
O	-0.68456575784493	-0.94802021014157	-3.15649247452524
O	0.32016879916467	-3.07545524063106	-2.20534291030782
S	-3.50296573865106	1.33301774187168	-1.26813813000998
O	-4.28408051444978	-0.10003379686507	-1.16901835531686
O	-4.44372866476816	2.39428455750470	-0.84787475294596
O	-2.31225096430259	1.21508213330705	-0.35305217291131
O	-3.07519498088986	1.34717512740484	-2.68888947136669
S	-1.18861647953417	-4.11024224546494	2.06278279516554
O	0.19189319728486	-3.20641865768253	2.37525045911842
O	-2.12066898036155	-3.16647357554585	1.35525531201101
O	-0.69033018932130	-5.15341677318078	1.14305478914319
O	-1.71547137882720	-4.50320655544691	3.37879774650119
H	-4.44630562866447	-0.34957361863996	-0.18522675618879

$Na^{+}(Na_2SO_4)_3(NaHSO_4)_3(NH_3)$

Final Gibbs free energy ... -5876.00143876 Eh

S	0.90388836097779	2.57530389367408	-3.39054460426315
O	-0.49575154527438	3.23935092482349	-3.44457498856742
O	1.13401409349619	1.81871208997147	-4.66027303290765
O	0.95563118725342	1.59218377496233	-2.22469849537693
O	1.89496541809977	3.67836883203844	-3.10712365711413
H	-1.21208591882360	2.70491624985195	-4.89910035121987
Na	-2.25154962723378	2.83139756592755	-1.86453040540569
Na	1.71758968005596	-1.02844928087347	3.14858225912434
Na	2.26554849504108	2.94032547607990	-0.78559978082188
Na	0.74913701718039	-0.33686050505848	-3.57440550967864
Na	0.28079374097322	5.25861301526007	-2.46291379764227
Na	1.20376604682652	4.89158091540282	2.19113855851019
Na	-0.17341600341471	0.64881643010150	-0.46971034823082
Na	-0.65598106284139	-4.73725812066911	-0.14899989389674
Na	-2.64169967223044	-1.55817223984852	-0.74272676185618
S	-0.69147791429548	-1.96061664397629	1.71062367801029
O	0.85855482605110	-2.06586588620445	1.14078817621489
O	-1.38590682402592	-3.22431938861553	1.33077768904701

O	-1.30711523571808	-0.78773791283340	1.01792781316638
O	-0.44489148693426	-1.78365674586215	3.15392837665211
S	0.13207637492044	-2.86902116569702	-2.13799285124991
O	0.28197986493619	-2.64668830715817	-3.62187509708092
O	0.92049941728948	-4.01244234314391	-1.59510700386472
O	0.53600553730637	-1.56315154750592	-1.43076161640777
O	-1.36263395348021	-3.14349474485208	-1.85061449649293
H	-0.14460633235208	2.49012628565415	1.70209340949345
Na	-2.02716769890270	-2.48277371687643	-4.04185570553762
S	1.94070581622333	1.89993798149936	2.01485860295328
O	0.46005005030037	2.38593248608018	2.50698386046433
O	1.74620323001468	1.12599884229475	0.74676999618777
O	2.70350293510826	3.16060109072647	1.75713804004034
O	2.45009278290599	1.08665752411756	3.13760610867414
H	0.85995829968418	-1.89633966911090	0.14039764829732
S	-0.67977935642621	4.38581674671212	0.12512573063460
O	0.79971125957436	4.64402497919653	-0.23661078810205
O	-0.95028577135389	5.03571230781937	1.43718415480112
O	-1.53212169034078	4.88631553164702	-1.01547406770366
O	-0.88725519443626	2.86220735794789	0.23263858657978
S	-2.66772433125214	0.19803720850115	-3.11259900879802
O	-1.55829917235878	-0.16148787063608	-4.13304494749299
O	-3.37691457597228	1.43110265582271	-3.57065003012340
O	-2.03654358494728	0.48027819638864	-1.75210150692543
O	-3.52976483275249	-1.03449178757641	-2.96763769568234
N	-1.54009421329830	2.09804805286224	-5.69601503569550
H	-1.53600571129833	1.13378911374631	-5.27755070340124
H	-0.87892329798902	2.16794896904333	-6.46526673006782
H	-2.48750542626628	2.33749737834488	-5.97694077724358

$Na^+(Na_2SO_4)_3(NaHSO_4)_3(NH_3)_2$

Final Gibbs free energy ... -5932.54083633 Eh

S	0.91425892480324	2.52584763564168	-3.32713715450781
O	-0.49523136217358	3.16952490130852	-3.39766056819478
O	1.17297069728321	1.79765333886814	-4.61095565849396
O	0.96286068165564	1.50683944126649	-2.19010798276394
O	1.88381754192441	3.63212986344042	-3.00409340029243
H	-1.13664782754064	2.68100718617832	-4.91072495384799
Na	-2.39122437148263	2.84193013609721	-1.99935881489589
Na	1.95312143216715	-0.94222071057649	2.63977392469944
Na	2.29467686499898	2.76900446787615	-0.69585204275221
Na	0.72179523634608	-0.36475104576481	-3.58902100933644
Na	0.22113010122964	5.15003033126859	-2.28271506765130
Na	1.06218399409654	4.83918677829930	2.32215459811879
Na	-0.27788795476147	0.86054004893282	-0.40580678805925
Na	-0.20259160812053	-4.43817225884811	0.46404180195696
Na	-2.80032152236414	-1.51032616987059	-0.84612746036382
S	-0.75422390965134	-1.81442983318780	1.63099765845159
O	0.61372389013525	-2.19298879561848	0.94837248416943
O	-1.58214261186704	-3.06465760028884	1.64203234482986
O	-1.42905076675724	-0.74987401895092	0.79027680179777
O	-0.41742002844268	-1.26730859785606	2.98468494040608
S	0.05877371434379	-3.03649418874097	-2.19849990095457
O	0.24886158078528	-2.77579445325669	-3.65569825084680
O	0.76794912155760	-4.19799884537888	-1.62089201837079

O	0.67884904641761	-1.69889045615855	-1.52410611966331
O	-1.41272695811905	-3.07315828669768	-1.85851747827405
N	-1.27592924939629	1.67937959663009	2.82524260754473
H	-1.57024743774715	2.01181466315069	1.88835274471757
H	-1.91454900888669	2.02424370992971	3.53604727193408
H	-0.28314779571236	2.07122438573896	2.97814839583855
H	-1.23006550981122	0.65317115858231	2.85109831393114
Na	-2.07926137176636	-2.52284503590940	-4.14324531982657
S	2.19548450641196	1.97705792447357	2.14402288538720
O	1.15376354949082	2.68421842666747	3.03759239836687
O	1.44379797274045	1.18353005754524	1.06227693072109
O	3.02140532336558	3.04823228539800	1.48059881188671
O	2.99415067789717	1.01634294385165	2.96466504357475
H	0.69552074138210	-1.84278358854215	-0.48382913370460
S	-0.95562830217137	4.19138187627838	0.17704650400579
O	0.54416611337611	4.23669703270216	-0.15695734120678
O	-1.15490424805017	4.79568203761476	1.52980449095370
O	-1.68332539933771	4.90164538957730	-0.94890910773495
O	-1.45121326299419	2.73922563180012	0.16934917819524
S	-2.63797254721147	0.16961597152517	-3.26342355285989
O	-1.53864137836184	-0.23027679117321	-4.28302230108379
O	-3.32610983371005	1.40941665795945	-3.73688348594118
O	-1.99662598310193	0.44256486937980	-1.91230223626841
O	-3.53769236670315	-1.03911951194887	-3.11179412789806
N	-1.40268232786026	2.11516861668426	-5.76001355076498
H	-1.44935748895548	1.13425576267486	-5.39506116089931
H	-0.66778854985117	2.20777784968813	-6.45718820903469
H	-2.31381209969419	2.38823427975730	-6.11920677901627

$Na^{+}(Na_2SO_4)_3(NaHSO_4)_3(NH_3)_3$

Final Gibbs free energy ... -5989.08422268 Eh

S	0.84823650146527	2.68172962267928	-3.53386951423182
O	-0.57206796954592	3.31006664875137	-3.49012488130415
O	1.03606839311036	2.00683411284126	-4.85643309113736
O	0.98160554849776	1.63379345408831	-2.43953982426784
O	1.82000115345735	3.79710510175400	-3.22449243377701
H	-1.34970265673903	2.68053324484071	-4.92965294159749
Na	-2.25467187108308	2.73942052719252	-1.97339193397780
Na	1.24287432052825	-0.54552673416889	3.72376301355513
Na	2.41548250386774	2.81258029096818	-1.00596313384483
Na	0.73527874207466	-0.28658235524478	-3.77085416755585
Na	0.21730916949933	5.22250602779898	-2.25968388826212
Na	1.38464175051467	4.10397477957274	2.55392758521808
Na	0.01913224814357	0.61253410815530	-0.61479764046075
Na	-0.30941005044770	-3.98600281206665	0.43432871204631
Na	-2.53960185590304	-1.50683659221953	-0.59352613688373
S	-0.95904354897561	-1.60085312467821	1.97580083120333
O	0.46228833378612	-2.16288027327170	1.78051741757278
O	-1.92648175282785	-2.68835506879058	1.57917619417159
O	-1.20115067892485	-0.42188563612325	1.02687328813470
O	-1.07189527117922	-1.11516722178774	3.39170916170346
S	0.42158268237242	-2.67083491089221	-2.01984354976270
O	0.45670945143643	-2.78099120961888	-3.52794826780929
O	1.29833052155301	-3.65991598149164	-1.29433408931766
O	0.84006230396298	-1.26265730637373	-1.64796170606074

O	-1.03181152871815	-2.93706311199423	-1.57255364928071
N	-1.80295165806597	1.77030760573272	2.62057908718999
H	-1.42534613654987	2.69951900009015	2.32705393847095
H	-2.81463966130269	1.81168040512538	2.71177319603031
H	-1.39467393373298	1.46127478339194	3.49932289725689
H	-1.53885789769381	1.04396274609099	1.90959162055490
Na	-1.85498244042838	-2.65382837363752	-3.81729622567219
S	2.36709941899052	1.39432468654359	1.84363895659426
O	1.04902542516886	1.61412607929860	2.60092207899055
O	2.08123881240311	0.99708304615505	0.38600375241120
O	3.12130907419840	2.69858460730008	1.81923826151421
O	3.09244079545584	0.25377130153802	2.51282828255440
N	2.79026773421684	-1.69255392998447	0.34762029448394
H	2.71668814147731	-0.68814644374262	0.08998266106275
H	3.61727386835662	-1.83011875984685	0.92224349883072
H	2.74806814882307	-2.31252167475866	-0.46744850309357
H	1.92523082016641	-1.86591990899029	0.90343916810806
S	-0.64425943964394	3.99892790627398	0.20563485657300
O	0.81978366402579	4.25873135281562	-0.16058705425947
O	-0.81649439018860	4.29357617034109	1.68983586173722
O	-1.50232499788892	4.86169912249396	-0.69136374117124
O	-1.02431155009001	2.55450899326843	-0.03422388205311
S	-2.63957059331381	0.05663708099676	-3.14246639237410
O	-1.57372415815389	-0.28662584885915	-4.21781233034076
O	-3.41610958248923	1.25571504690184	-3.59520981755566
O	-1.94941158602900	0.40085087222921	-1.83263380936331
O	-3.45282129956339	-1.19745507715220	-2.92104308874411
N	-1.67536483137931	2.05237935102566	-5.70642125030930
H	-1.60600550595344	1.08322390327040	-5.30555186848506
H	-1.05045630457367	2.16635978003989	-6.50077734093248
H	-2.64678849457733	2.23589658819771	-5.94527073573040

$Na^{+}(Na_2SO_4)_3(NaHSO_4)_4$

Final Gibbs free energy ... -6681.46640314 Eh

S	3.26823555224332	1.28555006610366	-2.45683996761824
O	4.21919856187519	0.69633920867920	-3.67649350843020
O	3.69321399615445	0.53820854613306	-1.23673496438821
O	3.54992903256542	2.73686274215465	-2.36395979500369
O	1.91649588317264	0.92396705965150	-2.95049439181053
H	5.01724106175382	1.24442483993623	-3.75045770163353
S	-2.69530624344652	-0.60731054500340	0.09887429948696
O	-4.18373121334633	-0.11862953328884	0.57686075245202
O	-2.90234240011101	-1.71634443188367	-0.85684840714749
O	-2.13136944721595	0.65286369191663	-0.45277562698330
O	-1.96633618456209	-1.01044062101559	1.34595899221690
H	-4.70491233054248	-0.90105803052659	0.82187789327172
S	0.52346058218584	-4.42206611897701	-4.43874358612753
O	0.46943510368163	-5.42207811535281	-5.73576356609569
O	1.34374508755882	-5.12001279730527	-3.41005959344187
O	1.15975292519957	-3.21966984366141	-5.02447361911780
O	-0.88821338447301	-4.22244963755432	-4.00608185147550
H	0.07435042466008	-6.26334365030519	-5.45537423151741
S	1.69765761142484	-0.26040781936754	3.81305765371238
O	3.20747357556332	-0.05886166595622	3.23365482258434
O	0.81328329693949	-0.23775190583679	2.58746694515191

O	1.64176808504124	-1.56124086813407	4.51753436681714
O	1.50841990523504	0.92774586031290	4.67080754313057
H	3.42150879300108	-0.79987144889082	2.55651557436982
Na	2.05796802975449	2.85837993707175	3.66228454281634
Na	-0.87825891895684	1.17370748366521	1.71587818183892
Na	-0.18343971770407	0.97608887397446	-1.68031637970017
Na	1.97153958873704	-4.52100225868533	-1.34971555393781
Na	3.28916638844091	4.14161475402262	-0.60210951404958
Na	4.05438472185333	-1.75058167720723	-1.00670500173494
Na	1.57215541540557	-1.19814666646912	-4.21966779554506
Na	-1.79236945945872	-2.94321531368343	-2.42237580894951
Na	2.38625295670186	0.47142802860112	0.75741365421108
Na	2.58845157921753	-3.55239048514398	4.14271599635890
Na	0.06316548221915	-2.15267503913285	1.38574927281573
S	1.15437140763518	3.19212912676111	0.94332853813103
O	1.16559759276724	4.44839983540188	0.14280497682652
O	0.65917849067610	2.00781560894256	0.12012501474713
O	2.61429186406494	2.85813525131676	1.35208411018735
O	0.32147985274078	3.25135749196331	2.20483189224972
S	3.32087752885898	-3.17159451515484	1.43944116477445
O	4.20997923836512	-3.64931377881607	2.53739328756241
O	3.61428882030328	-3.79274885692064	0.09371476411840
O	1.87720739925763	-3.42510124813870	1.84917772511587
O	3.52905414128819	-1.64207520953412	1.24199455616918
S	0.74892938459568	-1.82246379156927	-1.50412013913002
O	0.11958657796749	-3.08259592744590	-0.94171066833119
O	-0.13618663235185	-1.24335016421052	-2.59898221644717
O	0.87298933008062	-0.80570343149496	-0.39775300004678
O	2.10263747098025	-2.16066102794018	-2.10464980545382

$Na^+(Na_2SO_4)_3(NaHSO_4)_4(NH_3)$

Final Gibbs free energy ... -6738.00717732 Eh

S	-2.00485388056791	-2.16435519163961	-2.94665345172359
O	-2.38058260120325	-2.86202422327581	-4.38902064532439
O	-0.55483706042870	-2.43562581682640	-2.85715221195123
O	-2.81882108495527	-2.85002042595567	-1.89502474789241
O	-2.39360254737048	-0.72733135007743	-3.06384667260342
H	-3.28395328898062	-2.60757638752288	-4.63759896408719
S	4.44097990341130	-2.42260234223466	-4.05425057540437
O	4.66253977068120	-3.58617648403420	-5.17467294229645
O	3.04157244389314	-2.67507216540818	-3.61463475301945
O	5.41289563013793	-2.70194023427637	-2.94408087544344
O	4.67819589008027	-1.12318141243786	-4.72128913796623
H	5.54642460890955	-3.48343469757138	-5.56669912807559
S	2.27115961528615	-2.18134830088403	1.22770198080237
O	3.72989292635995	-2.61765780113769	1.18098794204708
O	1.71964899646815	-2.37453020067463	-0.20698910149891
O	1.43524210476857	-2.90640994424384	2.20289226271865
O	2.29037575121696	-0.65954106724703	1.50260596581860
Na	0.74042702047035	1.00258324683334	1.87683135789099
Na	1.12869554801253	-1.52278409786375	-4.16817724668324
Na	1.64684917566115	-0.14801504161206	-0.79366706749619
Na	-1.17922225083185	1.04996134460767	-2.13915207938132
Na	-4.03886574481103	-1.16851766131349	-0.76029263395163
Na	3.41405302816290	2.92803097376627	-1.42864171502012

Na	-1.93836472383122	3.00308215041002	0.80635895883646
Na	4.60438798773202	-0.54949476117774	1.59753077867538
Na	4.01412118058600	1.01685548610658	-4.40869434184586
Na	0.55698814966361	4.08505316735762	-2.93923329509142
Na	3.74299246686786	-2.92206939743697	-1.19666287387177
S	-1.87911480459755	0.13566721250484	0.67982250069450
O	-1.58205635425642	0.97455231469876	1.90095179734802
O	-2.78583006944595	0.94532229587647	-0.25925014329393
O	-2.59138556489309	-1.15693019939176	1.02310488953384
O	-0.58035340911109	-0.17159389210473	-0.03723423851627
S	5.13125127098551	0.37670068742945	-1.34587327537696
O	3.94229117866459	-0.53522540377883	-1.41542814111826
O	6.41589850948873	-0.51366872450233	-1.71842638740138
O	5.03068495349245	1.48730575186691	-2.34567144252457
O	5.38880646999696	0.89402031718558	0.02205954490658
S	1.21631079082143	1.43337186764990	-3.89463484400726
O	1.76525394382565	0.69860924749544	-5.09134602904389
O	2.28403482511469	2.42040894715445	-3.39999238500389
O	-0.05192796096618	2.20343047481189	-4.14609473396061
O	0.93202503587495	0.37931193351706	-2.82854570086377
S	0.80793513159853	3.25928974959514	-0.16606826803139
O	-0.41308826654664	2.98851563947630	-1.06091623330637
O	1.70904381992104	2.02837609628853	-0.07133004072882
O	0.29903862041055	3.57550159784417	1.21119139387065
O	1.61185471753032	4.35574829439731	-0.83271887157379
N	-0.82025927515948	-3.27997028401463	0.35922418355045
H	-1.45533749922530	-2.51167618547794	0.66025733225911
H	-0.51309771433400	-3.81538902832079	1.17175525233680
H	0.05113777058424	-2.86448160295637	-0.05259441101383
H	-1.30484832955492	-3.85027267100545	-0.33251675236802
H	6.12563942680936	-1.29552788553901	-2.26985649558185

$Na^+(Na_2SO_4)_3(NaHSO_4)_4(NH_3)_2$

Final Gibbs free energy ... -6794.54994755 Eh

S	-2.03216913162667	-2.15729790615622	-2.93259450317865
O	-2.44952057715896	-2.83875373083149	-4.37262267844328
O	-0.58655317572109	-2.46021509218106	-2.87026745936411
O	-2.83393482929594	-2.84065924971036	-1.87043646553905
O	-2.39800436822492	-0.71460683669513	-3.03616374495950
H	-3.34394375550065	-2.54565281965618	-4.61008678011287
S	4.49613088143662	-2.68561673911838	-4.38725704408556
O	4.94460005911782	-3.83262622605478	-5.46519514423012
O	3.02643514859988	-2.54668752225307	-4.48769283896525
O	5.00791406472454	-3.24510255655210	-3.11620756859237
O	5.21898737713392	-1.42815189387691	-4.79127671699595
H	4.57236010501330	-3.60655085211822	-6.33379506316847
S	2.39282914491363	-2.07282590174562	1.22815365048956
O	3.84731139188008	-2.51407010478304	1.23133705138687
O	1.87652758585518	-2.29215705088767	-0.21719375057150
O	1.52075726162422	-2.76379075488051	2.19842208505621
O	2.41603129879506	-0.54484821717506	1.45993015223038
H	6.70285993224291	-1.36621820566546	-3.76061217731050
Na	0.73626282879056	0.91264193474615	1.95389968186931
Na	1.07565838911659	-1.47474703806994	-4.13586169555631
Na	1.68118824445347	-0.03017568679836	-0.78543523343194

Na	-1.21923023481561	1.09481653226164	-2.08746089477806
Na	-4.01946099279746	-1.21204127249977	-0.67880602742213
Na	3.30717065297612	2.87723852449974	-1.15050086497598
Na	-2.06076182001853	2.97302655002908	0.85246228314419
Na	4.77399100888304	-0.40988776686910	1.36210378723593
Na	4.06115033627308	0.56825719123040	-4.23732928619148
Na	0.62027302911999	4.11374697095132	-2.89209968042396
Na	4.04180222473961	-2.65129752496630	-1.11807213523489
S	-1.86374731192574	0.09896502473532	0.71725203213405
O	-1.57356266503112	0.94931391807496	1.93304515054918
O	-2.80952747394922	0.88549409504768	-0.20574000527187
O	-2.53460369278011	-1.21212869046917	1.07211832656316
O	-0.57125077131460	-0.17771355488639	-0.02046780592149
S	5.00346652279307	0.24677830317882	-1.46233200180800
O	3.72121982571764	-0.38176620897518	-1.99273996544665
O	5.84911128544169	-0.88308490735424	-0.84436957683586
O	5.73214614388185	0.91303894574857	-2.59282196730822
O	4.67358711351839	1.21918588927270	-0.34902073492142
S	1.29674087654232	1.44558137813315	-3.82192395595296
O	1.87100085077233	0.67315601864116	-4.98673444003442
O	2.39552023437592	2.32596710658129	-3.21839399611458
O	0.12165416573509	2.31425476259422	-4.17980608854487
O	0.82686245705074	0.40816793474573	-2.80320140396010
S	0.64285954779016	3.36866609544684	-0.09355081486186
O	-0.53000173066593	3.06994839419354	-1.04474696794887
O	1.49516985625366	2.11798257223768	0.11233665536906
O	0.07329595742207	3.79823810547373	1.22237568539084
O	1.52454067836281	4.39847848217131	-0.77480232611294
N	-0.66206448456884	-3.24903210240423	0.29859855538391
H	-1.31505084530385	-2.51055690057356	0.62904768435804
H	-0.37423440333367	-3.82906176404572	1.08635913473941
H	0.21747688865031	-2.80479380296801	-0.06744656883463
H	-1.12454570749085	-3.78329069866647	-0.43613318093170
N	7.42323360665174	-1.40863893622532	-3.00653232574796
H	7.91787433128327	-2.29644752781767	-3.05333569206623
H	6.89941602275800	-1.30668053104818	-2.08942354168705
H	8.06768620532499	-0.62744567321382	-3.10452631678749

$Na^{+}(Na_2SO_4)_3(NaHSO_4)_4(NH_3)_3$

Final Gibbs free energy ... -6851.08489760 Eh

S	-2.04346691229696	-1.55631595037049	-2.92797095635296
O	-2.36601291582506	-2.09893822081529	-4.45156428991489
O	-0.72125051019286	-2.13874560568000	-2.56729563337759
O	-3.13919349389686	-2.03463364303904	-2.04640773809339
O	-2.04703639102118	-0.08707519605711	-3.15285866718374
H	-2.24474145285635	-3.06304992808787	-4.47089410572356
S	3.25933674930795	-2.07909672933419	-4.87690014941897
O	3.22746932334984	-2.98309814217851	-6.01755869930586
O	2.14518691754298	-1.03806357683345	-4.86313006052036
O	3.31000850581988	-2.74261912979776	-3.52631200866270
O	4.55947974621696	-1.11770924939067	-4.97958015761181
H	-0.84010241759208	0.18869451256565	-4.79569080053577
S	2.32911447619815	-2.00074853412851	0.95891011802595
O	3.75268101878644	-2.51164197586989	0.91216766827669
O	1.81059592840159	-1.91561504862086	-0.47678558752560

O	1.41216144948325	-2.84782208343457	1.78331104940977
O	2.39343241622602	-0.57072058552512	1.52676599843751
H	5.42511913035840	-1.45538098790034	-4.44397155684834
Na	0.65368988019998	0.65701796431340	2.38071737450805
Na	1.45906833679547	-1.28352915460722	-2.66299321474628
Na	1.78500679450343	0.57805669059345	-0.43728608513282
Na	-1.29183458525694	1.54645281472735	-1.54368058344792
Na	-4.19077154068341	-0.79909212473363	-0.50193502941266
Na	3.21354052745549	3.37070154274057	-0.32283115605680
Na	-2.17392269753482	2.94560216108134	1.69155402213724
Na	4.77103117109087	-0.41978970762100	1.23729628965064
Na	3.66819758588857	0.92603406657195	-4.22827134748808
Na	0.33087150162073	4.73809929420874	-1.70347410375541
Na	4.05095161680556	-2.36717255153722	-1.42556448704951
S	-1.95476487370683	0.11838979999839	1.00886122076493
O	-1.67566167362256	0.77711335452422	2.33952981355397
O	-2.87863748894645	1.04264295111456	0.18799904909622
O	-2.67591511839016	-1.20518962916102	1.16927876961167
O	-0.65332148526352	-0.07408163598462	0.26158452037878
S	4.72626603393275	0.56710764301710	-1.48956632660125
O	3.44406348156244	-0.04747081259511	-2.05558020292332
O	5.59716142064847	-0.58252745497319	-0.98699574425797
O	5.37694275252584	1.38220611693209	-2.55154416251546
O	4.33402840708510	1.39223262944402	-0.25979770050539
S	1.05552494657391	2.33025041970199	-3.11473618504004
O	1.64951543420846	2.09879724641996	-4.48895762054870
O	2.02132212650853	3.12477313546365	-2.26227843861186
O	-0.25662251600253	3.08186212061939	-3.20796497281884
O	0.76213543461977	0.98129927768546	-2.46489139911442
S	0.52667723654588	3.55418354895400	0.92141244886787
O	-0.62037427478883	3.30003918426008	-0.07901203871106
O	1.44936841398598	2.33554702805264	0.97276598765090
O	-0.08582231979339	3.77851673924156	2.26654273649391
O	1.34567292632792	4.71232802891743	0.39007751148281
N	-0.84611309537620	-3.17410546813476	0.31414212445858
H	-1.57768390887092	-2.53295910912775	0.68397875952221
H	0.01855010650153	-3.10961241942254	0.92357841736120
H	-0.59919075900753	-2.84944506215350	-0.62816744524709
H	-1.19086999271715	-4.12887071426104	0.27309071927106
N	6.73597336444125	-1.64650287212857	-3.70205504597154
H	7.07798700944416	-2.60163886823938	-3.66639886605562
H	6.65716984085268	-1.29142889634766	-2.74722012167324
H	7.45065813457237	-1.09274270214422	-4.16489198304090
N	-0.13046967120627	0.28772036111656	-5.53578583901261
H	0.52269909706280	-0.51883459307120	-5.51795854772825
H	0.47801254117707	1.11657915541747	-5.30350991788121
H	-0.57880591638677	0.37950386370730	-6.44313905328098

$Na^+(Na_2SO_4)_3(NaHSO_4)_4(NH_3)_4$

Final Gibbs free energy ... -6907.62303148 Eh

S	-1.39320881375641	-2.34052044458407	-3.38058421877332
O	-1.14547963313519	-2.80670542043794	-4.79027417444755
O	-0.38977821489857	-3.05156403088278	-2.46657305575480
O	-2.79257536240099	-2.56407745526927	-2.91646326939609
O	-1.06430891389110	-0.82664318128144	-3.31817921039840

H	-0.64200960529309	-0.33553135580995	-4.72418119637849
S	3.54416856206094	-3.07268915711258	-4.07696059064459
O	3.05142374103498	-4.25267833029191	-4.84271989810231
O	2.33166169500778	-2.18642603038193	-3.74497438958968
O	4.29424284731979	-3.46434373374863	-2.83145196647056
O	4.49504143481365	-2.18903190202136	-4.92280222723168
S	2.65736336971903	-1.17726826778580	1.17048061962940
O	4.08531626038228	-1.65927836457693	1.37208523891656
O	2.11986305006307	-1.93797075406319	-0.05741587371704
O	1.73094641718513	-1.37338301336518	2.31602414786629
O	2.75103195759558	0.32245472052655	0.86059606749067
H	5.83295194970133	-2.12914578066975	-4.25746475256080
Na	0.59504112086317	0.87005917792702	1.74680211676162
Na	0.82057291038813	-3.95721946421063	-4.34302224958814
Na	1.10738410514662	-1.19664682077351	-1.97931229883141
Na	-1.05554251115673	1.18068471826486	-2.06533272982207
Na	-3.76157051333820	-1.52438261415794	-1.23668185055571
Na	2.54980155307011	1.78054958252576	-0.87814267480643
Na	-2.58417210109452	2.63891700316261	0.73610161931682
Na	5.13952602110613	0.34342212012937	0.95530537987533
Na	3.46635868263821	-0.19010027898720	-4.36643138279304
Na	0.08500397284843	4.48630615551994	-2.62974532592692
Na	4.23831342663398	-2.33999395212260	-0.92873173647716
S	-1.86648883048494	-0.18097277616489	0.41562025517162
O	-1.77629841577276	0.64186202102274	1.67228264594296
O	-2.81720969153241	0.52434124436032	-0.57033425414616
O	-2.43134246003889	-1.56894369021179	0.66371070549449
O	-0.48780888564746	-0.28806717493146	-0.20918981484412
S	5.10685020032960	0.44848229013316	-1.93353298418918
O	3.73420734253407	-0.17197192694629	-2.05255770490518
O	6.03800706264721	-0.57157318010259	-1.29332776444050
O	5.58533151535361	0.82503669856427	-3.33286065625005
O	5.02337870137231	1.68155037083645	-1.05027038938410
S	1.32861569940316	2.07479311312255	-3.74410487779691
O	2.02101714324761	1.49029805336798	-4.95986125808436
O	2.15161498713312	3.23664651882623	-3.17276230567190
O	-0.04936774925017	2.58395418876876	-4.08397502159116
O	1.21298075314033	1.01698123229737	-2.66838813503919
S	-0.05182774501378	3.76423395740631	0.10407915813784
O	-0.99899333974813	3.17518204262528	-0.99169822382448
O	0.99415927910879	2.70972575770103	0.43476790575471
O	-0.89570171795577	4.04044007538625	1.31045759331085
O	0.60286880986624	4.97460487932271	-0.49388056458522
N	-0.28136863107387	-3.29192067745483	0.35248739723670
H	-1.06556842819608	-2.69008371460911	0.68818045185842
H	-0.22884468274151	-4.15972871345173	0.87756901296914
H	0.62131549211783	-2.76666034032546	0.41791532112456
H	-0.45337809899233	-3.45739223266109	-0.65630983400746
N	6.79496675703630	-2.09233413622021	-3.71150871160973
H	7.08662382758170	-3.04842230059210	-3.52143189201700
H	6.65190855972193	-1.59000280776604	-2.81777971235379
H	7.50794374507113	-1.61262870912604	-4.25464737279655
N	-0.33121071447184	-0.06052262033710	-5.72914662486386
H	-1.00726805044749	0.57768801512381	-6.14105904482797

H	-0.29381662911608	-0.92722302010683	-6.26346019148838
H	0.58676024607936	0.41473272024242	-5.68284097685485
N	4.82353368560810	3.45100100848851	-3.46642438751671
H	5.15548104082266	3.82945566445571	-2.58047801686753
H	5.20503040651554	2.46785581088937	-3.53826474008550
H	3.76074517536375	3.39582944334280	-3.43788467339383
H	5.13817989229532	4.03407044268724	-4.23751903781305