

**Understanding the Fast Kinetics and Mechanism of Sodium Storage in Antimony Using
ab Initio Grand Canonical Monte Carlo Simulation and Operando X-ray Scattering**

Manni Li,^{1,4,#} Tian Qiu,^{2,3,#} Samuel S. Welborn,^{1,3} Alexandre C. Foucher,¹ Jintao Fu,¹
Benjamin K. Lesel,⁵ Zeyu Wang,^{1,6} Lin Wang,¹ Eric A. Stach,^{1,3} Andrew M. Rappe,^{2,3,*} Eric
Detsi.^{1,3,*}

¹*Department of Materials Science & Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA*

²*Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA*

³*Vagelos Institute for Energy Science and Technology (VIEST), Philadelphia, Pennsylvania 19104, USA*

⁴*Automotive Engineering Research Institute, Jiangsu University, Zhenjiang 212013, China*

⁵*NanoDian, Los Angeles, California 90095, USA*

⁶*School of Materials Science & Engineering, Jiangsu University, Zhenjiang 212013, China*

Equal contribution

* *Corresponding authors: ED detsi@seas.upenn.edu, AMR rappe@sas.upenn.edu*

Detailed balance for the modified ab initio grand canonical Monte Carlo (aiGCMC)

simulation: The partition function of the μ_1, N_2, p, T ensemble is

$$Z(\mu_1, N_2, p, T) = \sum_{N_1} \frac{1}{N_1! N_2! h^{N_1 + N_2}} \int dV \int d\vec{x} d\vec{p} e^{-\beta(H - \mu_1 N_1 + pV)}$$

where h is the Plank constant, V is the volume of the system, \vec{x} and \vec{p} are the positions and momenta of all particles in the system, respectively. Define

$$z(N_1, N_2, p, T; \mu_1) = \frac{1}{N_1! N_2! h^{N_1 + N_2}} \int dV \int d\vec{x} d\vec{p} e^{-\beta(H - \mu_1 N_1 + pV)}$$

The Hamiltonian is the sum of the kinetic energy T and the potential energy U . Since the potential energy of a bulk system increases rapidly as the coordinates of atom deviates from the optimal position, here we only consider small deviations to the relaxed structure in the integral over \vec{x} , and therefore, the potential energy can be approximated as a quadratic form in V :

$$U \approx U|_{V=V_0} + \frac{\partial^2 U}{2\partial V^2} (V - V_0)^2$$

where V_0 is the volume of the optimal structure, i.e. fully relaxed structure of the given number of atoms. Define

$$B = \frac{\partial^2 U}{2\partial V^2}$$

Then

$$z(N_1, N_2, p, T; \mu_1) \approx \frac{1}{N_1! N_2! h^{N_1 + N_2}} \int d\vec{x} d\vec{p} e^{-\beta(H - \mu_1 N_1)} \Big|_{V=V_0} \int dV e^{-\beta(B(V - V_0)^2 + pV)}$$

For $\beta B V_0^2 \gg 1$,

$$\int dV e^{-\beta(B(V - V_0)^2 + pV)} = \sqrt{\frac{\pi}{\beta B}} e^{-\beta\left(pV_0 - \frac{p^2}{4B}\right)}$$

Therefore

$$z(N_1, N_2, p, T; \mu_1) = q(N_1, N_2, V = V_0, T) e^{\beta\mu_1 N_1} \sqrt{\frac{\pi}{\beta B}} e^{-\beta\left(pV_0 - \frac{p^2}{4B}\right)}$$

where $q(N_1, N_2, V, T)$ is the partition function of the canonical ensemble:

$$q(N_1, N_2, V, T) = \frac{1}{N_1! N_2! \Lambda^{N_1} \Lambda^{N_2}} \int d\vec{s} e^{-\beta U(\vec{s})}$$

The integral is over the reduced coordinates $\vec{s} = \frac{\vec{x}}{V}$. For the solid-state system under ambient

pressure, $e^{-\beta\left(pV_0 - \frac{p^2}{4B}\right)} \approx 1$. Hence,

$$z(N_1, N_2, p, T; \mu_1) \approx \frac{1}{N_1! N_2! \Lambda_1^{3N_1} \Lambda_2^{3N_2}} \int d\vec{s} e^{-\beta(U(\vec{s}) - \mu_1 N_1)} \sqrt{\frac{\pi}{\beta B}}$$

where Λ_1 and Λ_2 are the thermal de Broglie wavelength of the corresponding elements. In each iteration of the modified aiGCMC simulation, we choose to i) add one atom into the system, or ii) remove one atom from the system, or iii) switch the positions of two different atoms. Under the detailed balance condition, the acceptance probability of each choice is as follows:

i) For adding one atom:

$$P_{add} = \min\left\{1, \frac{1}{N_1 + 1} \frac{V_0^{new}}{\Lambda_1^3} \left(\frac{V_0^{new}}{V_0^{old}}\right)^{N_1} \sqrt{\frac{B^{old}}{B^{new}}} e^{-\beta(\Delta U - \mu_1)}\right\}$$

where V_0 is the volume of the relaxed system. The superscript “new” and “old” denote to which system the quantity is correspond (here “new” stands for the system with $N_1 + 1$ atoms and “old” stands for the system with N_1 atoms).

$$\Delta U = U^{new} - U^{old}$$

ii) For removing one atom:

$$P_{remove} = \min\left\{1, N_1 \frac{\Lambda_1^3}{V_0^{new}} \left(\frac{V_0^{new}}{V_0^{old}}\right)^{N_1} \sqrt{\frac{B^{new}}{B^{old}}} e^{-\beta(\Delta U + \mu_1)}\right\}$$

iii) For switching the positions of two atoms:

$$P_{switch} = \min\{1, e^{-\beta\Delta U}\}$$

In practical simulation, the square root of the ratio in B is treated as 1 to avoid frequent calculation of the bulk modulus.

SEM images of Sb with a bimodal porosity: Typical SEM images are displayed at different magnifications in **Figs. S1a-c** for the hierarchical nanoporous Sb. At low magnifications, large ligament/pore structures with size between $\sim 100\text{-}300$ nm can be observed (**Figs. S1a** and **S1b**). In turn, at high magnifications, the large ligaments are found to be composed of mesoscopic ligaments and pores with average size ~ 10 nm

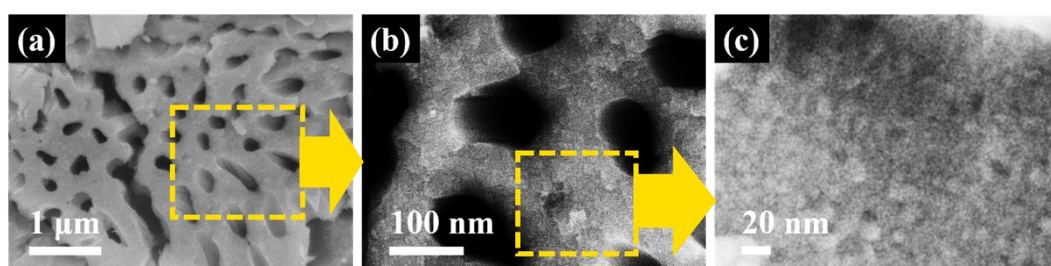


Fig. S1. SEM images of hierarchical nanoporous Sb at different magnifications. Large ligament/pore structures with size between 100-300 nm can be observed at low magnifications (a,b). At a high magnification (c), it is found that the large ligaments are in turn composed of mesoscopic ligaments and pores with average size ~ 10 nm.

(Fig. S1c),

Energy dispersive X-ray spectroscopy (EDX): As shown in **Fig. S2**, the residual Mn content was not detectable in EDX, suggesting that the Mn was almost fully removed after dealloying. The oxygen and carbon signal come from the carbon conductive tape used to hold the sample during EDX characterization, and the oxygen signal detected after dealloying may come from the dealloying process in addition to the carbon tape. As shown in **Table S1**, The atom ratio between Sb and Mn changes from ~10:90 before dealloying to ~98:2 after dealloying.

Table S1. Chemical composition of Mn-Sb parent alloy and dealloyed sample

Sample	Chemical composition (at. %)	
	Sb	Mn
Sb-Mn parent alloy	9.6	90.4
NP-Sb after dealloying	98.2	1.8

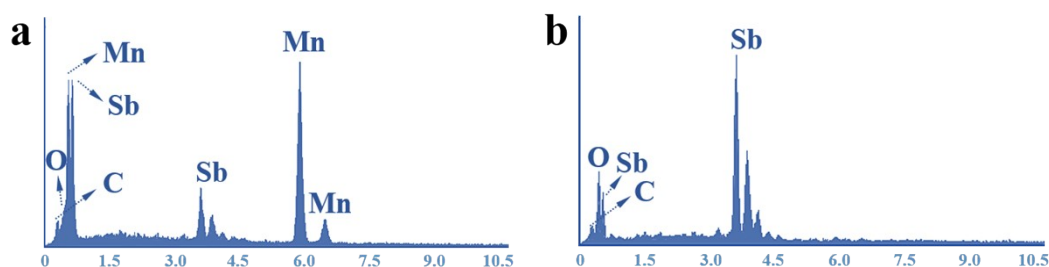


Fig. S2. EDX spectrum of $Sb_{90}Mn_{10}$ at.% before dealloying and (b) corresponding EDX spectrum of NP-Sb after dealloying.

Electrochemical impedance spectroscopy (EIS): The semicircle diameter reduced from $\sim 700 \Omega$ in the first cycle down to $\sim 300 \Omega$ in the second cycle, and was stable at $\sim 150 \Omega$ after the second cycle. The large charge transfer and reaction resistance can be attributed to the SEI formation. After the first cycle, the Sb grains were pulverized due to the volume change, leading to more area to react with sodium ions and thus fast charge-transfer.

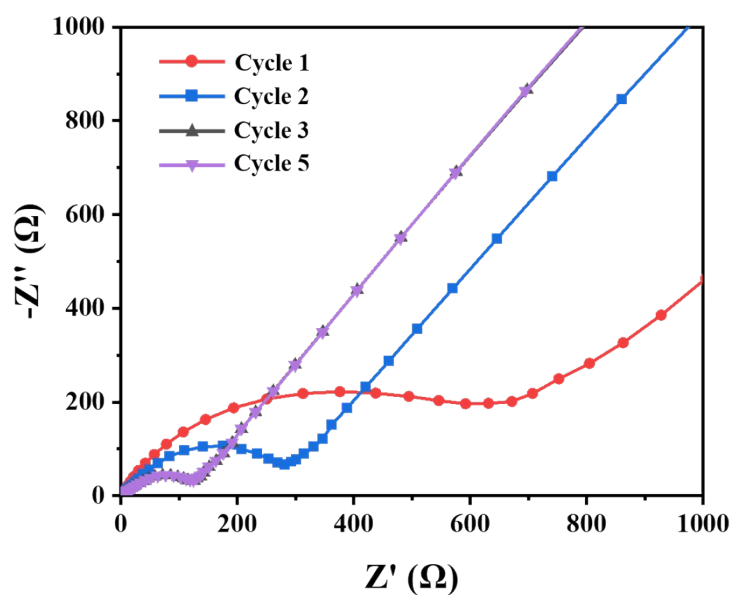


Fig. S3. Nyquist plot of NP-Sb after several representative cycles.

Coin cell configuration for the operando X-ray scattering experiment

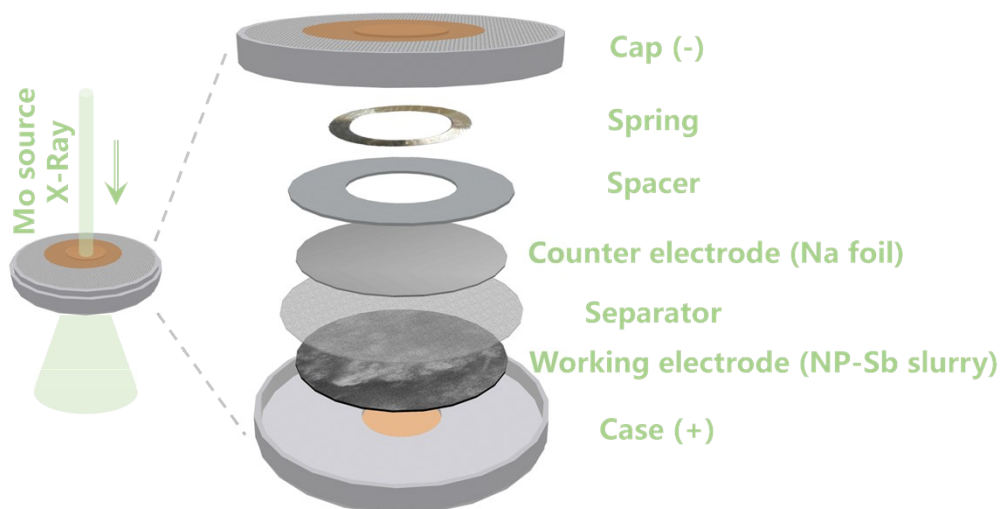


Fig. S4. Coin cell configuration used for operando WAXS measurements.

Kinetic analysis: As shown in Fig. S5, the capacitive process contributes 39.2% of the total capacity at the scan rate of 0.1 mV s^{-1} , and gradually increase to 81.8% when the scan rate grows to 5 mV s^{-1} , illustrating that the capacitive process occupies a greater proportion of the total capacity when scanning at high rates.

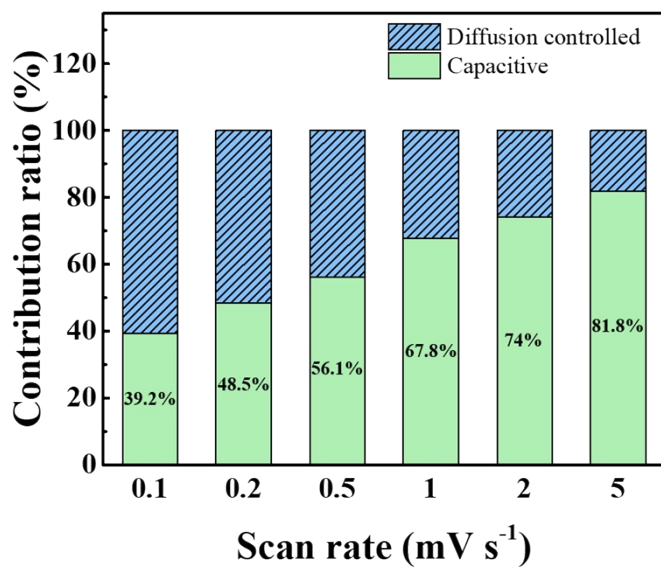


Fig. S5. The contribution ratio of the capacitive and diffusion-controlled at various scan rates.

Dynamical stability of the structures in Figure 3: The phonon dispersion calculations have been performed for all structures in Figure 3, the results are displayed as phonon density of state (DOS) show in Fig. S6

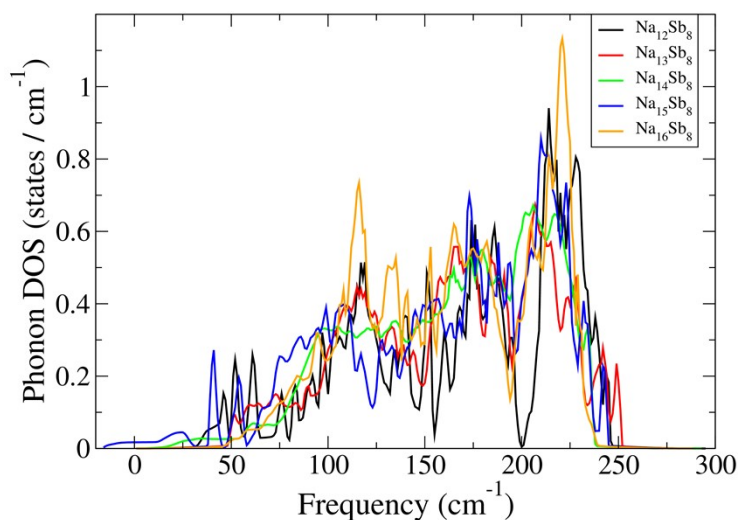


Fig. S6. The phonon DOS for structures from $\text{Na}_{12}\text{Sb}_8$ to $\text{Na}_{16}\text{Sb}_8$. $\text{Na}_{15}\text{Sb}_8$ has negative phonon frequencies but the result of structures are all dynamically stable.

Geometries of structures in .xsf format:

Na₁₂Sb₈:

PRIMVEC

10.305409821	-1.563713530	-0.599710451
-0.975221135	6.250731794	-0.090167754
0.987462025	-2.902947910	8.825090661

PRIMCOORD

20 1

Sb	3.6407303410	-2.3072216357	4.1415821641
Sb	6.5179744954	-1.8323477579	7.8712608240
Sb	8.5167332197	-1.5403090109	3.2424352386
Sb	-0.3327982145	6.5897881304	-0.2358152628
Sb	3.1528469046	0.8220935555	4.0965974353
Sb	6.9895340303	-4.8505144027	7.9145833556
Sb	9.0040246039	-4.6634323287	3.2872404303
Sb	0.1549656385	3.4646033093	-0.1907366308
Na	4.3734285602	5.7744344064	1.9140434021
Na	9.1678047313	-2.9433588253	9.2739664036
Na	6.4876300995	-3.4386854060	4.8439121442
Na	0.1216821048	1.9441354726	5.8359205276
Na	13.7242479815	0.8469830689	0.6014731045
Na	8.5870142821	0.1636984204	9.1436224922
Na	6.3154592634	-0.2566156468	5.1711486679
Na	0.5371755482	1.9780736574	2.6525326081
Na	1.0716118893	-1.1402613070	2.7701947136
Na	9.5319763240	-2.9499458870	6.0816291419
Na	3.1619480941	2.4685986641	7.1017947817
Na	3.4453253308	-0.6966615743	6.8484188185

Na₁₃Sb₈:

PRIMVEC

10.133712153	-0.012543375	-0.562836111
-0.020067045	6.458788848	-0.146241815
0.537448434	-3.025804152	8.836261650

PRIMCOORD

21 1

Sb	3.3056160188	-2.6581599966	3.7849696837
Sb	6.1887506692	0.8766439862	7.9513699713
Sb	8.3767162657	0.5003140647	3.6332270591
Sb	0.5021110071	7.1915974246	-0.2915010807
Sb	3.2954084018	0.7726193831	3.7078623256
Sb	6.1992704233	-2.6588153605	8.0295798387
Sb	8.3848873821	-2.4291072209	3.6979509493

Sb	0.5132567003	3.6774263994	-0.2115650209
Na	5.7424268623	5.5020483050	2.3084168973
Na	6.0075788700	2.3155219984	4.8651261031
Na	5.0846052049	5.5574696502	5.5498536328
Na	3.0310382604	2.4011952282	6.5207025900
Na	9.3715636655	2.3560491472	6.0053604834
Na	3.1406244454	5.4601189351	0.7245219934
Na	8.2202622325	5.4419659173	0.3971180658
Na	11.5173932064	-0.8650710187	5.2322782286
Na	8.5087042408	-0.8691753217	6.6487254958
Na	0.7174769369	-0.9444903336	2.7135298773
Na	7.2808610331	2.2262573363	1.2221231598
Na	10.7063078651	2.2754652324	2.2568386328
Na	3.4074497865	2.2258156631	0.7090647882

Na₁₄Sb₈:

PRIMVEC

10.314752329	-0.030496394	-0.563814529
-0.029781519	6.451830179	-0.156358784
0.542026008	-3.071847670	8.853287666

PRIMCOORD

22 1

Sb	3.6570611305	-0.1685244667	4.0190811256
Sb	6.3943607187	-0.1664281044	8.1687688280
Sb	8.8236250228	-0.0537478222	3.9233901979
Sb	0.8745629722	6.2407367189	-0.4971951753
Sb	3.7386510685	3.0603943901	3.9373003983
Sb	6.4087416878	-3.2847067035	8.2461325109
Sb	8.8441828146	-3.2805970250	4.0023000729
Sb	0.8929154014	3.1231647159	-0.4167145851
Na	6.2821356857	4.7502389691	4.8896131814
Na	3.8480165502	4.7098161162	6.8589673574
Na	6.3639652822	1.5189806798	5.3111356564
Na	9.0627678830	1.5029092397	6.9523981338
Na	3.8588307317	4.6145327132	1.1696764609
Na	7.4859466377	4.6483350783	1.4252274419
Na	11.4814614883	-1.6938652094	5.0956668831
Na	8.9609906784	-1.7271030979	6.9808812772
Na	0.8056120359	-1.7134654564	2.5724845451
Na	1.1502266702	1.5636215548	5.1643659571
Na	6.1971996500	1.4109461536	2.2180057869
Na	3.7871287923	1.4905126534	6.8981052228
Na	9.6190953526	1.4631055779	1.2737144330
Na	2.9741152705	1.4192351545	1.3687544126

Na₁₅Sb₈:

PRIMVEC

10.265760018	-0.053258464	-0.558019098
-0.044269507	6.532910477	-0.158212303
0.567508765	-3.075406085	8.967102307

PRIMCOORD

23 1

Sb	3.4816262338	-2.6062668149	4.1363407237
Sb	6.1968022765	0.8451461432	8.3611555580
Sb	8.4915982730	0.2963707516	3.8910048534
Sb	0.3671747752	6.9388347079	-0.4840056683
Sb	3.3678139090	0.5181870306	4.1670222725
Sb	6.0077430733	-2.5290185123	8.4648871058
Sb	8.4115199215	-2.7650964721	3.9703772637
Sb	0.4971988063	3.8442321145	-0.3176469027
Na	5.7532634738	5.6415944269	2.3640634169
Na	5.8850303870	2.3543753214	2.1616769794
Na	5.9947505952	5.4076792471	5.3964386947
Na	3.3357178963	2.4928717347	6.8773402000
Na	5.9687487487	2.1379881084	5.3353812023
Na	8.7590334502	2.1944020766	6.5919949222
Na	3.1418926899	5.3169538736	0.9337891816
Na	8.2072168911	5.3402489579	0.6851671665
Na	11.0953711353	-1.0704705555	5.3170464817
Na	8.6060136808	-1.0163618431	7.2635869073
Na	0.7137373514	-1.1382108330	2.8267566261
Na	0.8246972678	2.2342369175	4.9206389723
Na	9.2692310351	2.0633629283	1.3610947947
Na	3.5567674127	-0.7576632275	7.2822711750
Na	2.5878142488	2.0547094378	1.4897644888

Na₁₆Sb₈:

PRIMVEC

10.299445368	0.016950418	-0.610610600
0.002040696	6.774678805	-0.170202864
0.506679824	-3.198470162	9.050450911

PRIMCOORD

24 1

Sb	3.3335311052	-1.7331156053	4.1439496022
Sb	6.1616911566	0.3750275077	8.4309249499
Sb	8.4896451460	-0.0725433749	3.9029099182
Sb	0.5115531725	7.1677895888	-0.4047213580
Sb	3.3350856223	1.6547828856	4.0582107632

Sb	6.2562691839	-3.0111744658	8.5130607786
Sb	8.4885468137	-3.4594937051	3.9857624676
Sb	0.5042852913	3.7800290412	-0.3198565235
Na	5.6224937021	6.6989373614	2.4293960199
Na	5.6189280713	3.3092119950	2.5167337899
Na	6.2023444854	5.0411517597	5.4191801666
Na	3.5036184065	3.3790300779	6.7596505034
Na	6.2038253715	1.6514626089	5.5089177069
Na	8.7575440499	2.5914698684	6.9906937045
Na	3.1904543584	5.1943760027	0.6966885021
Na	8.2944161580	4.9170442407	0.9714247580
Na	10.9623603811	-1.7401879621	5.2394812127
Na	8.7199596643	-0.7892979472	7.0998173206
Na	0.8970459534	-0.1149415792	2.8297330270
Na	0.6725015890	1.6297494564	5.7546984983
Na	8.3217965182	1.5262879111	1.0694063116
Na	3.4679484069	-0.0099015668	6.8286731249
Na	11.1976077762	3.2929958967	2.1318752707
Na	3.2029395102	1.8035927382	0.7753114802

Fast Na diffusion path in Na₁₄Sb₈ under no constraint (in .axsf format):

ANIMSTEPS 17

CRYSTAL

PRIMVEC

10.3147523290 -0.0304963940 -0.5638145290

-0.0297815190 6.4518301790 -0.1563587840

0.5420260080 -3.0718476700 8.8532876660

PRIMCOORD 1

22 1

Sb	3.6570611305	-0.1685244667	4.0190811256
Sb	6.3943607187	-0.1664281044	8.1687688280
Sb	8.8236250228	-0.0537478222	3.9233901979
Sb	0.8745629722	6.2407367189	-0.4971951753
Sb	3.7386510685	3.0603943901	3.9373003983
Sb	6.4087416878	-3.2847067035	8.2461325109
Sb	8.8441828146	-3.2805970250	4.0023000729
Sb	0.8929154014	3.1231647159	-0.4167145851
Na	6.2821356857	4.7502389691	4.8896131814
Na	3.8480165502	4.7098161162	6.8589673574
Na	6.3639652822	1.5189806798	5.3111356564
Na	9.0627678830	1.5029092397	6.9523981338
Na	3.8588307317	4.6145327132	1.1696764609
Na	7.4859466377	4.6483350783	1.4252274419

Na	11.4814614883	-1.6938652094	5.0956668831
Na	8.9609906784	-1.7271030979	6.9808812772
Na	0.8056120359	-1.7134654564	2.5724845451
Na	1.1502266702	1.5636215548	5.1643659571
Na	6.1971996500	1.4109461536	2.2180057869
Na	3.7871287923	1.4905126534	6.8981052228
Na	9.6190953526	1.4631055779	1.2737144330
Na	2.9741152705	1.4192351545	1.3687544126

PRIMCOORD 2

22 1

Sb	3.6583731915	-0.1659301368	4.0173820811
Sb	6.3967394793	-0.1663036912	8.1668546444
Sb	8.8293547807	-0.0548471663	3.9231787048
Sb	0.8813600258	6.2415662280	-0.4965063673
Sb	3.7400398944	3.0568161116	3.9344348309
Sb	6.4107784594	-3.2849087164	8.2447888371
Sb	8.8505376191	-3.2796393501	4.0025305644
Sb	0.8978924611	3.1234914329	-0.4167567827
Na	6.3085071279	4.7509918884	4.8598418186
Na	3.8681547814	4.7064854066	6.8086285287
Na	6.3690595820	1.5195458220	5.2979991382
Na	9.0788515000	1.5030286114	6.9010486483
Na	3.9504442831	4.6067555138	1.2022110799
Na	7.6389828999	4.6566809828	1.3333452859
Na	11.4785402554	-1.6941658007	5.1015749785
Na	8.9909674254	-1.7285759066	7.0643755191
Na	0.9085029895	-1.7154830053	2.5816529803
Na	1.1784377801	1.5611123952	5.2039776132
Na	6.3456632054	1.4263864163	2.1861684960
Na	3.8133317846	1.4885056417	6.9169421864
Na	9.9013919292	1.4737513006	1.3933034589
Na	3.1599854354	1.3994446272	1.2725351282

PRIMCOORD 3

22 1

Sb	3.6585132335	-0.1643864954	4.0153705088
Sb	6.3994764311	-0.1647847197	8.1637414480
Sb	8.8372134682	-0.0550103611	3.9219221177
Sb	0.8865342683	6.2419753866	-0.4961775764
Sb	3.7418096208	3.0552246357	3.9315741956
Sb	6.4138768418	-3.2860136528	8.2413214206
Sb	8.9441832537	-3.2777731969	3.9959673040
Sb	0.9012836649	3.1236808192	-0.4174093747
Na	6.3482110804	4.7388906066	4.8228341669
Na	3.8868298229	4.7081307264	6.7722413310

Na	6.3765538612	1.5206069058	5.2517399469
Na	9.0720687603	1.5061789745	6.8720101209
Na	3.9953228995	4.6041907163	1.2138509868
Na	7.7377093604	4.6573851302	1.2877982893
Na	11.4921317614	-1.6885054603	5.1004781722
Na	9.0146417183	-1.7226900411	7.1222018449
Na	0.9695935229	-1.7205965398	2.5753966391
Na	1.2163919247	1.5546203366	5.2867121993
Na	6.5364985590	1.4466195315	2.1120177744
Na	3.8437276562	1.4896494156	6.9247056148
Na	10.2164968820	1.4652066850	1.5233082722
Na	3.3105029050	1.3887278362	1.2153915894

PRIMCOORD 4

22 1

Sb	3.6569465868	-0.1647134938	4.0142264457
Sb	6.4007741646	-0.1628315460	8.1588984592
Sb	8.9287971048	-0.0555291825	3.9158898808
Sb	0.8893292980	6.2416672344	-0.4946799976
Sb	3.7358861940	3.0558928510	3.9313527632
Sb	6.4141594370	-3.2890701730	8.2383109910
Sb	8.9471116700	-3.2787592972	3.9949997941
Sb	0.9037337400	3.1230719914	-0.4162628333
Na	6.3672553662	4.7548438420	4.8167630338
Na	3.8849499324	4.7050018298	6.7678366670
Na	6.3775703503	1.5226917636	5.1691570976
Na	9.0423368180	1.4995367720	6.8700306131
Na	3.9644450605	4.5961220927	1.2012321083
Na	7.7355476680	4.6614991432	1.2924014322
Na	11.5006519828	-1.6956265121	5.0967565102
Na	9.0287047697	-1.7266995807	7.1541305350
Na	0.9496583307	-1.7124682528	2.5676376559
Na	1.2334422862	1.5604464166	5.3740288012
Na	6.7806867594	1.4464166994	1.9896950700
Na	3.8721490978	1.4831524851	6.9159898649
Na	10.5185914456	1.4803572759	1.6388361014
Na	3.4608968564	1.3739771974	1.1963622555

PRIMCOORD 5

22 1

Sb	3.6535286520	-0.1653372701	4.0156913426
Sb	6.4072898431	-0.1586118461	8.1513607978
Sb	8.9334585088	-0.0557418566	3.9139228806
Sb	0.8901255306	6.1541121023	-0.4883699688
Sb	3.6432611638	3.1219012287	4.0182580260
Sb	6.4180513071	-3.2907607948	8.2327712529

Sb	8.9488388232	-3.2784685043	3.9929606944
Sb	0.9057923487	3.1182716873	-0.4142621855
Na	6.3638120331	4.7692070857	4.8241354681
Na	3.8718602174	4.7192352474	6.8151975411
Na	6.3534839751	1.5421828416	5.0540130128
Na	9.0083536824	1.4944366857	6.8525848502
Na	3.9482280502	4.5970926272	1.2027126471
Na	7.7272112398	4.6684562632	1.2939545946
Na	11.5009851003	-1.6997406184	5.1018108115
Na	9.0472155941	-1.7348341488	7.1306848888
Na	0.9226434524	-1.7204661329	2.5744666714
Na	1.2229574843	1.5511087636	5.4216800530
Na	7.0517203516	1.4448972172	1.8248227910
Na	3.9027889248	1.4862405470	6.9031170662
Na	10.7414346643	1.4680707393	1.7092125641
Na	3.6035878431	1.3863292184	1.2370125914

PRIMCOORD 6

22 1

Sb	3.6513529791	-0.1996652752	4.1009354772
Sb	6.4834380368	-0.1278817729	8.0641208142
Sb	8.9350465248	-0.0554858189	3.9119576156
Sb	0.8892836201	6.1553026700	-0.4850288987
Sb	3.6373944326	3.1235132521	4.0196143487
Sb	6.4149114437	-3.2909216738	8.2329495116
Sb	8.9485311771	-3.2788208685	3.9926471639
Sb	0.9063221677	3.1172583658	-0.4107110505
Na	6.3583000049	4.7604962430	4.8616772823
Na	3.8591368999	4.7241506301	6.8699150885
Na	6.3383382142	1.5322877102	4.9575962930
Na	8.9991568284	1.5044640140	6.8637798744
Na	3.8908810267	4.5872890387	1.1856726409
Na	7.6147199074	4.6799291108	1.3556219286
Na	11.4988792420	-1.7050445659	5.0992004030
Na	9.0608505922	-1.7374850177	7.0834692865
Na	0.8528692181	-1.7173724584	2.5655915614
Na	1.2103843748	1.5481199777	5.4619519966
Na	7.3125488589	1.4625588309	1.6488174945
Na	3.9128982191	1.4915129188	6.9012517327
Na	10.9059872921	1.4713706885	1.7641975211
Na	3.7689374175	1.3708711176	1.3015456485

PRIMCOORD 7

22 1

Sb	3.6500619936	-0.2014713873	4.1008140705
Sb	6.4840826961	-0.1276692645	8.0647007710

Sb	8.9369516701	-0.0547952695	3.9124223078
Sb	0.8896269384	6.1566685442	-0.4841265538
Sb	3.6360000503	3.1256387495	4.0199917306
Sb	6.4172779936	-3.2920782200	8.2313618187
Sb	8.9498937394	-3.2800914800	3.9926377543
Sb	0.9062660737	3.1157773271	-0.4098536731
Na	6.3548411049	4.7567210780	4.9106958092
Na	3.8491159205	4.7223907362	6.8991767469
Na	6.3435856093	1.5282627955	4.8848685750
Na	8.9912497872	1.5095682179	6.9051101899
Na	3.7918210823	4.5993346261	1.1553173378
Na	7.4197296901	4.6767841313	1.4799850876
Na	11.5128665600	-1.7062397516	5.0838567764
Na	9.0706780404	-1.7319693408	7.0246782916
Na	0.7590817940	-1.7203515284	2.5455889875
Na	1.2029400119	1.5479203943	5.4903160548
Na	7.5618530834	1.4527124490	1.4987636364
Na	3.9278273928	1.4890157500	6.8824120984
Na	11.0707718080	1.4648045373	1.8073111797
Na	3.9173032486	1.3849414575	1.3401592098

PRIMCOORD 8

22 1

Sb	3.5586709412	-0.2003782800	4.1076761737
Sb	6.4838361936	-0.1260672904	8.0640793225
Sb	8.9321098975	-0.1453434783	3.9158227787
Sb	0.8865878903	6.1584313700	-0.4838774652
Sb	3.6329902485	3.1287201009	4.0226493605
Sb	6.4984515688	-3.2909550310	8.2237602225
Sb	8.9477032799	-3.2814317630	3.9915129476
Sb	0.9002397325	3.1175987020	-0.4096872285
Na	6.3047490685	4.7564930865	4.9272079607
Na	3.8413341437	4.7382513842	6.9553993216
Na	6.3429383875	1.5175055484	4.8294746706
Na	8.9848361837	1.5184514708	6.9155928721
Na	3.7229346039	4.6213796146	1.1353259435
Na	7.3052123939	4.6670681864	1.5394927883
Na	11.5162023552	-1.7162427972	5.0895068049
Na	9.0647347194	-1.7156948960	6.9662657259
Na	0.6904249090	-1.7133391991	2.5295977454
Na	1.1642324612	1.5483054435	5.5071701384
Na	7.8164538288	1.4444709922	1.3755733147
Na	3.9308754080	1.5108796935	6.8698044523
Na	11.2400738591	1.4714545719	1.8251035012
Na	4.1435602331	1.4055326638	1.4242338739

PRIMCOORD 9

22 1

Sb	3.5588597473	-0.2017886065	4.1090242320
Sb	6.4871781330	-0.1252992114	8.0639003598
Sb	8.9306279731	-0.1456236023	3.9145375486
Sb	0.8821903545	6.1584047845	-0.4859684853
Sb	3.6355247445	3.1310145889	4.0250188822
Sb	6.5067227960	-3.2915646277	8.2271028947
Sb	8.9465765327	-3.2831199002	3.9896520781
Sb	0.8958107835	3.1174983710	-0.4117300133
Na	6.2850533169	4.7558480386	4.9465679140
Na	3.8414008839	4.7417867514	7.0214280071
Na	6.3526439408	1.5149157869	4.8184446874
Na	8.9857909716	1.5208599480	6.9308867491
Na	3.6535035683	4.6287001505	1.1141298902
Na	7.1895603780	4.6565434691	1.6126601947
Na	11.5323202674	-1.7200036170	5.0755623324
Na	9.0583642008	-1.7090421028	6.8953481925
Na	0.6063566636	-1.7156478458	2.5007844436
Na	1.1515122882	1.5465511967	5.5049409781
Na	8.0565680685	1.4360930548	1.2471689630
Na	3.9352396273	1.5163721349	6.8567535680
Na	11.4208856907	1.4686375938	1.8090545650
Na	4.4076796360	1.4127379391	1.5339396483

PRIMCOORD 10

22 1

Sb	3.5595742568	-0.2034181410	4.1101733585
Sb	6.4971661564	-0.1527583839	8.1453147422
Sb	8.8477367297	-0.1432256406	3.9155298990
Sb	0.8694178200	6.1895576374	-0.5602248696
Sb	3.6400393406	3.1319099523	4.0269135096
Sb	6.5105962873	-3.2935649441	8.2244885667
Sb	8.9458742366	-3.2846122263	3.9865349141
Sb	0.8923199347	3.1203669203	-0.4168131166
Na	6.2627636082	4.7572690387	4.9684168791
Na	3.8518337191	4.7482199225	7.0804738405
Na	6.3552763416	1.5357410305	4.8695037619
Na	8.9861785727	1.5148147791	6.9445316840
Na	3.6246965447	4.6174230194	1.1041026167
Na	7.1319590765	4.6479773057	1.6485888582
Na	11.5378779387	-1.7219618677	5.0401581926
Na	9.0469003032	-1.7091317541	6.8414356367
Na	0.5395801258	-1.6915576598	2.4591639499
Na	1.1313663721	1.5314817632	5.4661250323

Na	8.2613328583	1.4289078780	1.1547056603
Na	3.9330424834	1.5149527993	6.8512006436
Na	11.6090504513	1.4771596048	1.7430731088
Na	4.6789914778	1.3971607211	1.6743178395

PRIMCOORD 11

22 1

Sb	3.5542830148	-0.1774250542	4.0278028180
Sb	6.4974567448	-0.1565171194	8.1490852026
Sb	8.8344501671	-0.0534437416	3.9144855155
Sb	0.8634564344	6.1858399954	-0.5727155204
Sb	3.6406326298	3.1319584251	4.0288798499
Sb	6.5120732765	-3.2949821627	8.2259310541
Sb	8.8746871598	-3.2966843573	3.9819663044
Sb	0.8888103307	3.1188566843	-0.4182977715
Na	6.2345547394	4.7650862341	4.9695419911
Na	3.8542963086	4.7240378142	7.1336836608
Na	6.3418067682	1.5383679061	4.9820856198
Na	8.9967378149	1.4978220392	6.9805011617
Na	3.6189380690	4.6008678552	1.0953561512
Na	7.1143187639	4.6576956947	1.6653992813
Na	11.5401943289	-1.7186874441	5.0226329678
Na	9.0288185472	-1.7273726949	6.7942469421
Na	0.4993044521	-1.7011353569	2.4648693947
Na	1.1178860997	1.5394329870	5.4311784745
Na	8.4396212093	1.4328501746	1.0681999288
Na	3.9056589791	1.4846458218	6.8449830397
Na	11.7847765149	1.4582177278	1.6621251022
Na	4.9742200275	1.4020876187	1.8037228746

PRIMCOORD 12

22 1

Sb	3.5566381902	-0.1754407208	4.0251484733
Sb	6.4941140677	-0.1594586946	8.1516489439
Sb	8.8286480968	-0.0507635848	3.9126375107
Sb	0.7745251048	6.1844766418	-0.5750089370
Sb	3.6425102342	3.1306383197	4.0292156749
Sb	6.5088429141	-3.2926241738	8.2286739638
Sb	8.8507304792	-3.2898100370	3.9869560920
Sb	0.7961485681	3.1201500006	-0.4145392977
Na	6.2131569778	4.7694744579	4.9462637539
Na	3.8353161755	4.7122930801	7.1941068465
Na	6.3401678001	1.5419720245	5.0697397999
Na	8.9770400989	1.4974030577	6.9470415896
Na	3.6606263336	4.5975803975	1.1018430470
Na	7.1934815237	4.6595285000	1.6155851755

Na	11.5435221975	-1.7107018109	5.0304846632
Na	8.9959071756	-1.7273558300	6.7681573328
Na	0.5364550814	-1.7057393847	2.4874646926
Na	1.1079522922	1.5499634993	5.3740610115
Na	8.6152570243	1.4357440493	1.0185157005
Na	3.8533396555	1.4730470242	6.8584369039
Na	11.9817213036	1.4444110685	1.5452406880
Na	5.2462299086	1.4054440191	1.9301938184

PRIMCOORD 13

22 1

Sb	3.6472046415	-0.1758517270	4.0229436771
Sb	6.4926118756	-0.1625992836	8.1564830943
Sb	8.8246518451	-0.0504362164	3.9122940749
Sb	0.7671489811	6.1830658392	-0.5770439261
Sb	3.6433486384	3.1298318886	4.0289216689
Sb	6.4190359649	-3.2916078020	8.2351704551
Sb	8.8409765981	-3.2880580860	3.9894056799
Sb	0.7920660623	3.1207342186	-0.4155002805
Na	6.2160540442	4.7579717020	4.9396429597
Na	3.8166238282	4.7203026116	7.1776700322
Na	6.3392504286	1.5369165267	5.1606130673
Na	8.9686106870	1.5011675730	6.9475603856
Na	3.6835824771	4.5888474240	1.1147812341
Na	7.2313320705	4.6741986867	1.5746985222
Na	11.5395412649	-1.6971194300	5.0311790065
Na	8.9603771261	-1.7336633993	6.7718702998
Na	0.5547431113	-1.7210723638	2.4992178256
Na	1.1051027171	1.5555659697	5.3000868563
Na	8.7867979159	1.4487455674	1.0067318049
Na	3.8065802365	1.4726334814	6.8671205150
Na	12.2248686345	1.4161996989	1.4136016734
Na	5.5037929982	1.4226496829	2.0409678864

PRIMCOORD 14

22 1

Sb	3.6518330014	-0.1735949310	4.0228390905
Sb	6.4024656976	-0.1629033807	8.1636361934
Sb	8.8216522060	-0.0507964582	3.9152507213
Sb	0.7669786460	6.1819884020	-0.5773377864
Sb	3.6460755082	3.1290796987	4.0298194648
Sb	6.4148270840	-3.2879762458	8.2405392902
Sb	8.8382585622	-3.2858776859	3.9921035906
Sb	0.7903388310	3.1216418608	-0.4146409018
Na	6.2243705455	4.7592050686	4.9197364694
Na	3.8067923579	4.7051942400	7.1107023539

Na	6.3385731035	1.5377870410	5.2220229953
Na	8.9710560193	1.4957488587	6.9494673988
Na	3.7428088894	4.6007934629	1.1397696867
Na	7.3146125569	4.6647803661	1.5187105732
Na	11.5195958135	-1.6885171179	5.0530267334
Na	8.9283203768	-1.7310266862	6.8040002864
Na	0.6288069709	-1.7189588449	2.5270861547
Na	1.1092175846	1.5622045103	5.2390101178
Na	8.9738406642	1.4436742862	1.0393912907
Na	3.7796783893	1.4688536405	6.8824647267
Na	12.4855527513	1.4089038646	1.2568210743
Na	5.7098264491	1.4261455180	2.1256698060

PRIMCOORD 15

22 1

Sb	3.6541115817	-0.1735388680	4.0225974134
Sb	6.3985451718	-0.1653173106	8.1656904467
Sb	8.8185050769	-0.0525316310	3.9176753873
Sb	0.7712988293	6.2398674865	-0.4939530913
Sb	3.6466456896	3.1282681602	4.0299541067
Sb	6.4101752054	-3.2873460166	8.2422320480
Sb	8.8366364236	-3.2853089261	3.9942178818
Sb	0.8777332397	3.1239118378	-0.4194014309
Na	6.2345195368	4.7489640127	4.8866049984
Na	3.8176649966	4.7008175019	7.0216819376
Na	6.3365257004	1.5227623571	5.2683215319
Na	9.0130121600	1.4855087564	6.9487724335
Na	3.7705061597	4.6031718362	1.1447747408
Na	7.3816751013	4.6559635765	1.4682296581
Na	11.4950399527	-1.6985884869	5.0761414227
Na	8.9181229131	-1.7400173352	6.8415011013
Na	0.6762669961	-1.7200773743	2.5447994835
Na	1.1121115200	1.5529167074	5.1799568680
Na	9.1633510612	1.4531674613	1.0938416379
Na	3.7600447941	1.4859455601	6.8834616234
Na	12.7729014371	1.4140803770	1.1160913350
Na	5.8794966291	1.4111297446	2.1788284790

PRIMCOORD 16

22 1

Sb	3.6551834967	-0.1715651405	4.0218853080
Sb	6.3952675899	-0.1658170494	8.1682018127
Sb	8.8202221182	-0.0527010287	3.9222055435
Sb	0.7773128703	6.2418223939	-0.4931481725
Sb	3.7336998412	3.0650936425	3.9437724981
Sb	6.4063876610	-3.2857167989	8.2452981551

Sb	8.8404458716	-3.2814412307	3.9999104678
Sb	0.8865487990	3.1240686854	-0.4172971588
Na	6.2579746723	4.7515882046	4.9029013309
Na	3.8241581089	4.7146128229	6.9363198904
Na	6.3501073246	1.5209861488	5.3006129515
Na	9.0270539257	1.4860216045	6.9689674328
Na	3.7993796412	4.6044885556	1.1525578989
Na	7.4026729840	4.6547371240	1.4685333274
Na	11.4900611957	-1.6938993032	5.0869138869
Na	8.9311094317	-1.7367726990	6.9081685614
Na	0.7350839008	-1.7095742495	2.5628072110
Na	1.1322670771	1.5643110009	5.1570750513
Na	9.3747284475	1.4757510770	1.1848612442
Na	3.7592261969	1.5046815229	6.8937897152
Na	13.0320710370	1.3854685202	0.9403037158
Na	6.0434444346	1.4048574335	2.2065710558

PRIMCOORD 17

22 1

Sb	3.6570611305	-0.1685244667	4.0190811256
Sb	6.3943607187	-0.1664281044	8.1687688280
Sb	8.8236250228	-0.0537478222	3.9233901979
Sb	0.8745629722	6.2407367189	-0.4971951753
Sb	3.7386510685	3.0603943901	3.9373003983
Sb	6.4087416878	-3.2847067035	8.2461325109
Sb	8.8441828146	-3.2805970250	4.0023000729
Sb	0.8929154014	3.1231647159	-0.4167145851
Na	6.2821356857	4.7502389691	4.8896131814
Na	3.8480165502	4.7098161162	6.8589673574
Na	6.3639652822	1.5189806798	5.3111356564
Na	9.0627678830	1.5029092397	6.9523981338
Na	3.8588307317	4.6145327132	1.1696764609
Na	7.4859466377	4.6483350783	1.4252274419
Na	11.4814614883	-1.6938652094	5.0956668831
Na	8.9609906784	-1.7271030979	6.9808812772
Na	0.8056120359	-1.7134654564	2.5724845451
Na	1.1502266702	1.5636215548	5.1643659571
Na	9.6190953526	1.4631055779	1.2737144330
Na	3.7871287923	1.4905126534	6.8981052228
Na	13.2888675995	1.3887387605	0.8049398836
Na	6.1971996500	1.4109461536	2.2180057869