

## First-principles calculation on the deposition behavior of $\text{Li}_x\text{Na}_y$ ( $x+y \leq 5$ ) clusters during the hybrid storage of Li and Na atoms on graphene

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Table S1. Adsorption energies of single Li atom and Na atom on graphene calculated from different methods including GGA-PBE, TS, Grimme. (Unit: eV)

	Li atom			Na atom		
	H	B	T	H	B	T
PBE	-1.555	-1.276	-1.246	-0.916	-0.799	-0.788
PBE-TS	-1.817	-1.517	-1.497	-1.211	-1.143	-1.142
PBE-Grimme	-1.901	-1.527	-1.526	-1.267	-1.094	1.089

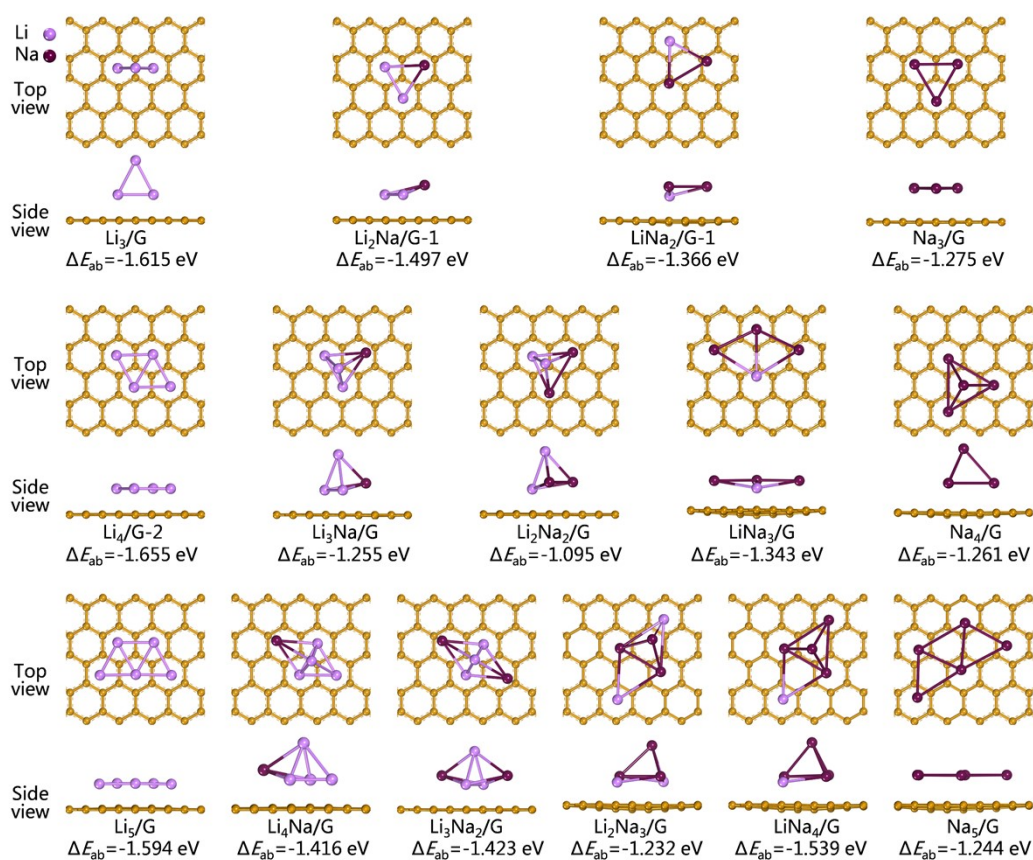


Figure S1 The metastable configurations of  $\text{Li}_x\text{Na}_y$  clusters on graphene

Table S2 Atomic coordinates and electronic states of the clusters of the relatively stable  $\text{Li}_x\text{Na}_y$  clusters on graphene

System	Li/G	Na/G	LiNa/G	Li2Na/G	Li3Na/G	Li4Na/G
Point group of cluster				C2v	C3v	C2v
Electron configuration	$(1s)^2(2s)^1$	$(1s)^2(2s)^2(2p)^6(3s)^1$	like single Li or Na atom	$(1a_1)^2(2a_1)^2(3a_1)^2(1b_2)^2(2b_2)^2(1b_1)^2(4a_1)^2(5a_1)^2(6a_1)^1$	$(1a_1)^2(2a_1)^2(2a_1)^2(1e)^2(1e)^2(2e)^2(2e)^2(3a_1)^2(4a_1)^2(5a_1)^2$	$(1a_1)^2(2a_1)^2(3a_1)^2(1b_1)^2(1b_2)^2(4a_1)^2(2b_1)^2(5a_1)^2(2b_2)^2(6a_1)^2(3b_2)^2(7a_1)^1$
number	Atom X Y Z	Atom X Y Z	Atom X Y Z	Atom X Y Z	Atom X Y Z	Atom X Y Z
1	Li1 6.3913 3.6900 11.8030	Na1 1.4190 -0.0005 9.9990	Li1 2.1305 11.0699 11.8084	Li1 6.4934 3.6306 11.9442	Li1 4.1702 2.3041 11.9342	Li1 8.6605 2.2152 11.9794
2	C1 1.4188 -0.0002 9.9986	C1 0.7090 1.2292 9.9990	C1 1.4185 0.0043 10.0264	Li2 4.1573 4.9799 11.9436	Li2 6.5639 3.6916 11.9318	Li2 6.2597 3.6105 11.9910
3	C2 0.7092 1.2288 9.9986	C2 3.5499 -1.2313 10.0006	C2 0.7085 1.2319 10.0118	C1 1.4194 -0.0005 10.0300	Li3 4.1718 5.0761 11.9338	Li3 8.6534 4.9922 11.9922
4	C3 3.5500 -1.2312 9.9994	C3 2.8388 -0.0022 10.0028	C3 3.5552 -1.2222 10.0368	C2 0.7089 1.2286 10.0284	C1 1.4135 -0.0038 10.0114	Li4 6.2531 6.3864 11.9806
5	C4 2.8384 -0.0019 10.0010	C4 5.6813 -2.4614 9.9990	C4 2.8398 0.0034 10.0294	C3 3.5507 -1.2310 10.0302	C2 0.7031 1.2268 10.0154	C1 1.4195 -0.0005 9.9948
6	C5 5.6817 -2.4614 9.9986	C5 4.9700 -1.2327 10.0028	C5 5.6858 -2.4593 10.0264	C4 2.8393 -0.0022 10.0316	C3 3.5480 -1.2360 10.0108	C2 0.7102 1.2280 9.9948
7	C6 4.9704 -1.2328 10.0010	C6 1.4175 2.4595 10.0028	C6 4.9743 -1.2290 10.0294	C5 5.6816 -2.4604 10.0266	C4 2.8327 -0.0101 10.0192	C3 3.5487 -1.2321 9.9988
8	C7 1.4175 2.4591 10.0010	C7 0.7086 3.6900 10.0006	C7 1.4187 2.4611 10.0034	C6 4.9703 -1.2317 10.0286	C5 5.6808 -2.4626 10.0072	C4 2.8386 -0.0035 9.9988
9	C8 0.7088 3.6900 9.9994	C8 3.5471 1.2274 10.0096	C8 0.7087 3.6900 9.9980	C7 1.4176 2.4583 10.0274	C6 4.9689 -1.2360 10.0160	C5 5.6805 -2.4617 9.9998
10	C9 3.5470 1.2272 10.0074	C9 2.8366 2.4582 10.0096	C9 3.5487 1.2307 10.0160	C8 0.7070 3.6889 10.0236	C7 1.4072 2.4578 10.0352	C6 4.9684 -1.2342 10.0048
11	C10 2.8363 2.4582 10.0074	C10 5.6807 -0.0044 10.0096	C10 2.8372 2.4601 10.0046	C9 3.5486 1.2264 10.0328	C8 0.7003 3.6902 10.0286	C7 1.4172 2.4585 9.9990
12	C11 5.6806 -0.0046 10.0074	C11 4.9672 1.2235 10.0130	C11 5.6827 -0.0014 10.0160	C10 2.8361 2.4545 10.0304	C9 3.5415 1.2179 10.0348	C8 0.7082 3.6878 9.9990
13	C12 4.9661 1.2215 10.0126	C12 1.4175 4.9205 10.0028	C12 4.9686 1.2259 10.0116	C11 5.6810 -0.0032 10.0280	C10 2.8255 2.4540 10.0526	C9 3.5454 1.2257 10.0134
14	C13 1.4175 4.9209 10.0010	C13 0.7090 6.1508 9.9990	C13 1.4187 4.9189 10.0034	C12 4.9684 1.2234 10.0308	C11 5.6827 -0.0106 10.0364	C10 2.8351 2.4559 10.0136
15	C14 0.7092 6.1512 9.9986	C14 3.5432 3.6900 10.0130	C14 0.7085 6.1481 10.0118	C13 1.4123 4.9204 10.0212	C12 4.9700 1.2159 10.0518	C11 5.6776 -0.0079 10.0230
16	C15 3.5409 3.6900 10.0126	C15 2.8365 4.9218 10.0096	C15 3.5452 3.6900 10.0002	C14 0.7071 6.1520 10.0176	C13 1.4072 4.9225 10.0350	C12 4.9641 1.2202 10.0364
17	C16 2.8363 4.9218 10.0074	C16 5.6777 2.4540 10.0058	C16 2.8372 4.9199 10.0046	C15 3.5439 3.6858 10.0212	C14 0.7031 6.1536 10.0150	C13 1.4163 4.9182 10.0054
18	C17 5.6767 2.4523 10.0070	C17 4.9641 3.6900 10.0058	C17 5.6784 2.4553 9.9950	C16 2.8327 4.9207 10.0130	C15 3.5385 3.6902 10.0772	C14 0.7093 6.1487 10.0000
19	C18 4.9621 3.6900 10.0070	C18 7.8121 -3.6900 9.9984	C18 4.9653 3.6900 9.9932	C17 5.6809 2.4520 10.0218	C16 2.8255 4.9264 10.0524	C15 3.5398 3.6872 10.0372
20	C19 7.8117 -3.6900 9.9986	C19 7.1012 -2.4614 9.9990	C19 7.8134 -3.6900 10.0056	C18 4.9692 3.6870 10.0198	C17 5.6837 2.4516 10.0762	C16 2.8330 4.9193 10.0240
21	C20 7.1008 -2.4614 9.9986	C20 9.9423 -4.9194 9.9998	C20 7.1039 -2.4605 10.0118	C19 7.8121 -3.6894 10.0274	C18 4.9686 3.6902 10.0814	C17 5.6707 2.4484 10.0720
22	C21 9.9422 -4.9196 10.0000	C21 9.2320 -3.6900 9.9998	C21 9.9422 -4.9196 9.9938	C20 7.1013 -2.4606 10.0262	C19 7.8108 -3.6898 10.0040	C18 4.9567 3.6851 10.0726
23	C22 9.2317 -3.6900 10.0002	C22 12.0721 -6.1495 9.9984	C22 9.2325 -3.6900 9.9948	C21 9.9422 -4.9192 10.0274	C20 7.1001 -2.4619 10.0080	C19 7.8125 -3.6900 9.9994
24	C23 12.0723 -6.1499 9.9986	C23 11.3622 -4.9199 9.9998	C23 12.0715 -6.1484 10.0056	C22 9.2320 -3.6896 10.0262	C21 9.9399 -4.9192 10.0024	C20 7.0997 -2.4626 9.9988
25	C24 11.3623 -4.9201 10.0002	C24 7.8126 -1.2327 10.0028	C24 11.3619 -4.9194 9.9948	C23 12.0718 -6.1498 10.0266	C22 9.2302 -3.6898 10.0020	C21 9.9438 -4.9185 10.0060
26	C25 7.8122 -1.2328 10.0010	C25 7.1018 -0.0044 10.0096	C25 7.8133 -1.2308 10.0034	C24 11.3618 -4.9204 10.0260	C23 12.0675 -6.1502 10.0058	C22 9.2317 -3.6909 10.0002
27	C26 7.1019 -0.0046 10.0074	C26 9.9423 -2.4606 9.9998	C26 7.1032 -0.0029 10.0046	C25 7.8122 -1.2316 10.0246	C24 11.3585 -4.9206 10.0052	C23 12.0736 -6.1491 9.9996
28	C27 9.9422 -2.4604 10.0000	C27 9.2326 -1.2313 10.0006	C27 9.9422 -2.4604 9.9938	C26 7.1021 -0.0032 10.0246	C25 7.8118 -1.2332 10.0146	C24 11.3635 -4.9205 9.9994
29	C28 9.2325 -1.2312 9.9994	C28 12.0717 -3.6900 9.9998	C28 9.2326 -1.2313 9.9980	C27 9.9420 -2.4599 10.0236	C26 7.1033 -0.0066 10.0314	C25 7.8117 -1.2366 10.0046
30	C29 12.0719 -3.6900 10.0000	C29 11.3622 -2.4601 9.9998	C29 12.0719 -3.6900 9.9938	C28 9.2323 -1.2304 10.0222	C27 9.9399 -2.4604 10.0026	C26 7.0977 -0.0116 10.0260
31	C30 11.3623 -2.4599 10.0002	C30 7.8153 1.2235 10.0130	C30 11.3619 -2.4606 9.9948	C29 12.0706 -3.6902 10.0240	C28 9.2317 -1.2311 10.0076	C27 9.9431 -2.4635 9.9974
32	C31 7.8164 1.2215 10.0126	C31 7.1048 2.4540 10.0058	C31 7.8143 1.2252 10.0002	C30 11.3617 -2.4598 10.0218	C29 12.0665 -3.6898 10.0110	C28 9.2325 -1.2373 10.0018
33	C32 7.1059 2.4523 10.0070	C32 9.9438 -0.0022 10.0028	C32 7.1043 2.4551 9.9932	C31 7.8159 1.2233 10.0226	C30 11.3585 -2.4590 10.0052	C29 12.0722 -3.6915 9.9966
34	C33 9.9441 -0.0019 10.0010	C33 9.2354 1.2274 10.0096	C33 9.9418 -0.0019 10.0034	C32 7.1059 2.4536 10.0142	C31 7.8168 1.2219 10.0366	C30 11.3628 -2.4629 9.9966

35	C34 9.2356 1.2272 10.0074	C34 12.0721 -1.2305 9.9984	C34 9.2334 1.2270 10.0046	C33 9.9431 -0.0011 10.0188	C32 7.1108 2.4522 10.0518	C31 7.8105 1.2152 10.0474
36	C35 12.0723 -1.2301 9.9986	C35 11.3635 -0.0005 9.9990	C35 12.0715 -1.2316 10.0056	C34 9.2351 1.2284 10.0188	C33 9.9417 -0.0022 10.0082	C32 7.0978 2.4465 10.0960
37	C36 11.3638 -0.0002 9.9986	C36 1.4190 7.3805 9.9990	C36 11.3614 -0.0024 10.0118	C35 12.0708 -1.2296 10.0182	C34 9.2350 1.2275 10.0172	C33 9.9473 -0.0112 10.0088
38	C37 1.4188 7.3802 9.9986	C37 0.7104 8.6105 9.9984	C37 1.4185 7.3757 10.0264	C36 11.3626 0.0007 10.0170	C35 12.0675 -1.2294 10.0058	C34 9.2388 1.2161 10.0236
39	C38 0.7102 8.6101 9.9986	C38 3.5471 6.1526 10.0096	C38 0.7055 8.6019 10.0328	C37 1.4174 7.3823 10.0174	C36 11.3607 0.0011 10.0038	C35 12.0732 -1.2337 9.9974
40	C39 3.5470 6.1528 10.0074	C39 2.8388 7.3822 10.0028	C39 3.5487 6.1493 10.0160	C38 0.7094 8.6118 10.0180	C37 1.4136 7.3842 10.0108	C36 11.3665 -0.0052 10.0020
41	C40 2.8384 7.3819 10.0010	C40 5.6777 4.9260 10.0058	C40 2.8398 7.3766 10.0294	C39 3.5465 6.1570 10.0128	C38 0.7067 8.6127 10.0032	C37 1.4181 7.3782 9.9992
42	C41 5.6767 4.9277 10.0070	C41 4.9672 6.1565 10.0130	C41 5.6784 4.9246 9.9950	C40 2.8366 7.3873 10.0208	C39 3.5415 6.1625 10.0342	C38 0.7116 8.6092 9.9992
43	C42 4.9661 6.1585 10.0126	C42 1.4204 9.8401 9.9998	C42 4.9686 6.1542 10.0116	C41 5.6832 4.9236 10.0196	C40 2.8328 7.3904 10.0186	C39 3.5398 6.1509 10.0278
44	C43 1.4202 9.8399 10.0002	C43 0.7109 11.0700 9.9998	C43 1.4157 9.8321 10.0292	C42 4.9716 6.1586 10.0206	C41 5.6837 4.9287 10.0754	C40 2.8359 7.3818 10.0058
45	C44 0.7106 11.0700 10.0000	C44 3.5499 8.6113 10.0006	C44 0.7012 11.0700 10.0306	C43 1.4202 9.8410 10.0212	C42 4.9700 6.1644 10.0510	C41 5.6686 4.9219 10.0974
46	C45 3.5500 8.6112 9.9994	C45 2.8402 9.8406 9.9998	C45 3.5552 8.6022 10.0368	C44 0.7105 11.0706 10.0232	C43 1.4178 9.8414 10.0018	C42 4.9586 6.1548 10.0498
47	C46 2.8403 9.8404 10.0000	C46 5.6807 7.3844 10.0096	C46 2.8450 9.8323 10.0306	C45 3.5504 8.6139 10.0230	C44 0.7083 11.0702 10.0016	C43 1.4204 9.8387 10.0002
48	C47 5.6806 7.3846 10.0074	C47 4.9700 8.6127 10.0028	C47 5.6827 7.3814 10.0160	C46 2.8402 9.8423 10.0236	C45 3.5480 8.6163 10.0104	C44 0.7134 11.0692 10.0056
49	C48 4.9704 8.6128 10.0010	C48 1.4204 12.2999 9.9998	C48 4.9743 8.6090 10.0294	C47 5.6840 7.3871 10.0292	C46 2.8375 9.8427 10.0028	C45 3.5457 8.6126 10.0032
50	C49 1.4202 12.3001 10.0002	C49 0.7104 13.5295 9.9984	C49 1.4157 12.3079 10.0292	C48 4.9714 8.6138 10.0262	C47 5.6827 7.3909 10.0354	C46 2.8391 9.8410 9.9980
51	C50 0.7102 13.5299 9.9986	C50 3.5506 11.0700 9.9998	C50 0.7055 13.5381 10.0328	C49 1.4204 12.3003 10.0264	C48 4.9689 8.6164 10.0154	C47 5.6735 7.3913 10.0264
52	C51 3.5508 11.0700 10.0002	C51 2.8402 12.2994 9.9998	C51 3.5598 11.0700 10.0292	C50 0.7102 13.5298 10.0278	C49 1.4178 12.2989 10.0018	C48 4.9649 8.6185 10.0108
53	C52 2.8403 12.2996 10.0000	C52 5.6813 9.8414 9.9990	C52 2.8450 12.3077 10.0306	C51 3.5512 11.0712 10.0258	C50 0.7067 13.5276 10.0034	C49 1.4214 12.2997 9.9994
54	C53 5.6817 9.8414 9.9986	C53 4.9704 11.0700 9.9984	C53 5.6858 9.8393 10.0264	C52 2.8404 12.3000 10.0278	C51 3.5496 11.0702 10.0022	C50 0.7125 13.5289 9.9994
55	C54 4.9709 11.0700 9.9986	C54 7.8184 3.6900 10.0058	C54 4.9803 11.0700 10.0328	C53 5.6821 9.8423 10.0272	C52 2.8375 12.2976 10.0030	C51 3.5494 11.0703 9.9968
56	C55 7.8205 3.6900 10.0070	C55 7.1048 4.9260 10.0058	C55 7.8169 3.6900 9.9950	C54 4.9709 11.0710 10.0262	C53 5.6808 9.8430 10.0070	C52 2.8400 12.2989 9.9966
57	C56 7.1059 4.9277 10.0070	C56 9.9460 2.4582 10.0096	C56 7.1043 4.9249 9.9932	C55 7.8197 3.6899 10.0140	C54 4.9685 11.0702 10.0034	C53 5.6797 9.8447 10.0032
58	C57 9.9462 2.4582 10.0074	C57 9.2393 3.6900 10.0130	C57 9.9424 2.4579 10.0160	C56 7.1085 4.9248 10.0214	C55 7.8233 3.6902 10.0344	C54 4.9691 11.0709 9.9980
59	C58 9.2416 3.6900 10.0126	C58 12.0735 1.2292 9.9990	C58 9.2366 3.6900 10.0116	C57 9.9454 2.4587 10.0184	C56 7.1108 4.9282 10.0512	C55 7.8126 3.6861 10.1222
60	C59 12.0733 1.2288 9.9986	C59 11.3650 2.4595 10.0028	C59 12.0695 1.2263 10.0264	C58 9.2401 3.6902 10.0220	C57 9.9454 2.4580 10.0122	C56 7.0996 4.9211 10.1228
61	C60 11.3650 2.4591 10.0010	C60 7.8153 6.1565 10.0130	C60 11.3597 2.4577 10.0294	C59 12.0724 1.2300 10.0168	C58 9.2412 3.6902 10.0198	C57 9.9537 2.4525 10.0484
62	C61 7.8164 6.1585 10.0126	C61 7.1018 7.3844 10.0096	C61 7.8143 6.1548 10.0002	C60 11.3641 2.4603 10.0184	C59 12.0701 1.2299 10.0030	C58 9.2436 3.6853 10.0970
63	C62 7.1019 7.3846 10.0074	C62 9.9460 4.9218 10.0096	C62 7.1032 7.3829 10.0046	C61 7.8163 6.1561 10.0298	C60 11.3629 2.4602 10.0042	C59 12.0763 1.2256 10.0052
64	C63 9.9462 4.9218 10.0074	C63 9.2354 6.1526 10.0096	C63 9.9424 4.9221 10.0160	C62 7.1038 7.3842 10.0314	C61 7.8168 6.1585 10.0358	C60 11.3725 2.4565 10.0272
65	C64 9.2356 6.1528 10.0074	C64 12.0739 3.6900 10.0006	C64 9.2334 6.1530 10.0046	C63 9.9454 4.9217 10.0238	C62 7.1033 7.3870 10.0306	C61 7.8144 6.1608 10.0984
66	C65 12.0737 3.6900 9.9994	C65 11.3650 4.9205 10.0028	C65 12.0634 3.6900 10.0368	C64 9.2349 6.1523 10.0270	C63 9.9454 4.9223 10.0120	C62 7.1018 7.3922 10.0506
67	C66 11.3650 4.9209 10.0010	C66 7.8126 8.6126 10.0028	C66 11.3597 4.9223 10.0294	C65 12.0733 3.6905 10.0216	C64 9.2350 6.1529 10.0170	C63 9.9555 4.9223 10.0738
68	C67 7.8122 8.6128 10.0010	C67 7.1012 9.8414 9.9990	C67 7.8133 8.6108 10.0034	C66 11.3643 4.9209 10.0242	C65 12.0718 3.6902 10.0026	C64 9.2415 6.1589 10.0744
69	C68 7.1008 9.8414 9.9986	C68 9.9438 7.3822 10.0028	C68 7.1039 9.8405 10.0118	C67 7.8132 8.6128 10.0302	C66 11.3629 4.9202 10.0042	C65 12.0793 3.6881 10.0244
70	C69 9.9441 7.3819 10.0010	C69 9.2326 8.6113 10.0006	C69 9.9418 7.3819 10.0034	C68 7.1018 9.8416 10.0290	C67 7.8118 8.6136 10.0142	C66 11.3725 4.9201 10.0382
71	C70 9.2325 8.6112 9.9994	C70 12.0735 6.1508 9.9990	C70 9.2326 8.6113 9.9980	C69 9.9435 7.3820 10.0278	C68 7.1001 9.8423 10.0078	C67 7.8145 8.6190 10.0286
72	C71 12.0733 6.1512 9.9986	C71 11.3635 7.3805 9.9990	C71 12.0695 6.1537 10.0264	C70 9.2330 8.6112 10.0292	C69 9.9417 7.3825 10.0080	C68 7.1005 9.8439 10.0062
73	C72 11.3638 7.3802 9.9986	C72 6.3913 3.6900 12.2540	C72 11.3614 7.3824 10.0118	C71 12.0732 6.1511 10.0262	C70 9.2317 8.6115 10.0076	C69 9.9482 7.3871 10.0388
74			Na1 6.3913 3.6900 12.2692	C72 11.3632 7.3804 10.0266	C71 12.0701 6.1504 10.0032	C70 9.2346 8.6153 10.0252
75				Na1 5.3302 4.3120 14.6772	C72 11.3607 7.3793 10.0038	C71 12.0771 6.1515 10.0148
76					Na1 4.9820 3.6901 14.6692	C72 11.3668 7.3817 10.0150
77						Na1 7.4584 4.2953 14.6346