

Supporting Information (SI)

The coordinates of the optimized structures of the Co_1 substituted $(111)_n$ surface of the supercell.

Singlet

1	13	0	-0.364074	6.270984	1.001860
2	13	0	-1.753138	6.179558	4.266303
3	13	0	-0.489543	2.077312	2.216555
4	8	0	-3.475381	6.255985	7.343605
5	8	0	-0.912652	6.263731	2.675479
6	8	0	0.764546	2.074877	1.054831
7	8	0	-2.173519	2.041510	4.956176
8	8	0	-3.493839	3.484917	7.352525
9	8	0	-3.485127	0.643741	7.342224
10	8	0	-0.738527	0.581694	3.049717
11	8	0	-0.762541	3.573754	3.050748
12	8	0	0.798980	4.956949	1.219079
13	8	0	0.813486	7.566104	1.219656
14	8	0	-2.198034	7.600110	5.152866
15	8	0	-2.332374	4.805476	5.147954
16	13	0	2.246079	6.255539	1.056943
17	13	0	-2.607077	2.068123	6.737545
18	13	0	-1.011823	0.631092	4.910046
19	13	0	0.727147	7.769671	3.165404
20	13	0	0.694472	4.765223	3.158753
21	13	0	-1.051052	3.483719	4.907407
22	13	0	-2.329445	4.823005	7.022192
23	13	0	2.088509	3.449631	1.043533
24	13	0	2.088042	0.696262	1.035748
25	13	0	-2.307795	7.675835	7.025258
26	8	0	3.319829	2.074534	1.115983
27	8	0	0.424384	2.104156	5.032429
28	8	0	-0.934460	6.249328	7.226793
29	8	0	1.870117	6.255113	3.033896
30	8	0	3.477917	4.918278	0.983949
31	8	0	3.489891	7.581125	0.981059
32	8	0	0.283403	7.602355	4.885152
33	8	0	0.083904	5.079125	4.834909
34	8	0	-1.027824	3.355016	6.807388
35	8	0	-1.016397	0.787038	6.817377
36	8	0	1.937750	0.691531	2.953311
37	8	0	1.913148	3.471972	2.972349
38	13	0	0.376990	2.078434	7.022456

39	13	0	1.981300	2.069855	4.085142
40	13	0	0.487348	6.313274	6.124431
41	13	0	5.009477	6.242239	1.032577
42	13	0	3.394094	6.253696	3.995703
43	13	0	4.842190	2.021510	1.917652
44	8	0	2.013768	6.247735	6.911733
45	8	0	4.938597	6.226453	3.029774
46	8	0	6.290938	2.069613	0.835427
47	8	0	3.476404	2.068211	5.042276
48	8	0	1.915650	3.398253	7.078437
49	8	0	1.907662	0.746151	7.080597
50	8	0	5.118490	0.752759	3.179036
51	8	0	5.257808	3.259650	3.208824
52	8	0	6.404279	4.969164	1.256511
53	8	0	6.397580	7.529765	1.248483
54	8	0	3.451810	7.656033	5.107364
55	8	0	3.457723	4.832184	5.094559
56	13	0	7.987056	6.252925	1.347377
57	13	0	3.173293	2.067097	7.035023
58	13	0	4.676464	0.597467	4.921604
59	13	0	6.377633	7.684223	3.158840
60	13	0	6.404193	4.836547	3.160406
61	13	0	4.690402	3.521287	4.924327
62	13	0	3.230618	4.882910	7.006795
63	13	0	7.693213	3.495963	1.050229
64	13	0	7.678693	0.645021	1.046864
65	13	0	3.234705	7.617843	7.010132
66	8	0	8.829510	2.066432	0.742085
67	8	0	6.074876	2.055101	5.327156
68	8	0	4.567582	6.246148	6.990909
69	8	0	7.538311	6.270933	3.115914
70	8	0	8.852632	4.838055	0.699365
71	8	0	8.847933	7.671771	0.704674
72	8	0	6.114560	7.738384	5.017054
73	8	0	6.125046	4.748834	5.015194
74	8	0	4.608231	3.329617	6.843358
75	8	0	4.597016	0.795418	6.842544
76	8	0	7.582473	0.701646	2.918496
77	8	0	7.674267	3.503976	2.922083
78	27	0	5.814040	2.055698	7.106371
79	13	0	7.044512	2.120611	3.758851
80	13	0	5.851228	6.244813	5.856004

triplet

1	13	0	-0.372042	6.264007	1.007553
2	13	0	-1.715275	6.240153	4.287822
3	13	0	-0.481154	2.070902	2.217335
4	8	0	-3.470294	6.258323	7.331447
5	8	0	-0.880466	6.255672	2.695055
6	8	0	0.749639	2.072014	1.030595
7	8	0	-2.155658	2.066121	4.956805
8	8	0	-3.493573	3.496338	7.330590
9	8	0	-3.492278	0.647894	7.330617
10	8	0	-0.734675	0.575916	3.055683
11	8	0	-0.742975	3.566924	3.053015
12	8	0	0.797231	4.955231	1.206983
13	8	0	0.803877	7.563063	1.211252
14	8	0	-2.241681	7.646881	5.146040
15	8	0	-2.271987	4.844521	5.144879
16	13	0	2.238825	6.255419	1.045793
17	13	0	-2.610200	2.072394	6.734402
18	13	0	-1.014234	0.639318	4.909460
19	13	0	0.729019	7.757372	3.166096
20	13	0	0.711048	4.762200	3.156649
21	13	0	-1.023554	3.499352	4.906978
22	13	0	-2.319012	4.831163	7.014555
23	13	0	2.073785	3.450310	1.020986
24	13	0	2.075101	0.693702	1.021784
25	13	0	-2.312780	7.681404	7.016371
26	8	0	3.304227	2.072842	1.094255
27	8	0	0.449104	2.081669	5.040394
28	8	0	-0.917283	6.254692	7.211884
29	8	0	1.878702	6.254977	3.023573
30	8	0	3.476179	4.922886	0.966639
31	8	0	3.480466	7.583023	0.967093
32	8	0	0.227544	7.535510	4.878787
33	8	0	0.178487	5.017175	4.862117
34	8	0	-1.021373	3.359238	6.808184
35	8	0	-1.022065	0.788327	6.811274
36	8	0	1.922477	0.690990	2.942548
37	8	0	1.913116	3.462477	2.943000
38	13	0	0.350894	2.072988	7.029476
39	13	0	1.996772	2.075994	4.061159
40	13	0	0.544900	6.266401	6.143362
41	13	0	4.984626	6.247126	1.030912
42	13	0	3.402308	6.248294	4.000415
43	13	0	4.797107	2.056895	1.955830

44	8	0	2.082449	6.247632	6.940953
45	8	0	4.935304	6.243000	3.021914
46	8	0	6.240280	2.067173	0.846731
47	8	0	3.473558	2.067826	5.035004
48	8	0	1.884251	3.349612	7.150247
49	8	0	1.875600	0.786491	7.142309
50	8	0	5.127954	0.773909	3.189616
51	8	0	5.170229	3.328616	3.197410
52	8	0	6.368749	4.984949	1.243802
53	8	0	6.363622	7.514307	1.239325
54	8	0	3.479753	7.649520	5.104149
55	8	0	3.483375	4.843568	5.102211
56	13	0	7.982199	6.250701	1.345016
57	13	0	3.212335	2.064161	6.936787
58	13	0	4.726503	0.611965	4.969330
59	13	0	6.357072	7.674254	3.159123
60	13	0	6.367413	4.832543	3.163238
61	13	0	4.735740	3.514218	4.973504
62	13	0	3.351576	4.873819	7.042125
63	13	0	7.563895	3.550579	1.017429
64	13	0	7.553001	0.582764	1.009904
65	13	0	3.349327	7.623832	7.038970
66	8	0	8.727932	2.064616	0.718534
67	8	0	6.121518	2.060868	5.269413
68	8	0	4.650812	6.249085	7.043590
69	8	0	7.519486	6.257169	3.103942
70	8	0	8.836704	4.815097	0.728720
71	8	0	8.831372	7.687743	0.725765
72	8	0	6.145288	7.738799	5.018190
73	8	0	6.151395	4.756006	5.021636
74	8	0	4.523348	3.383365	6.864672
75	8	0	4.518116	0.743114	6.862513
76	8	0	7.585318	0.677663	2.871659
77	8	0	7.615145	3.474432	2.877995
78	27	0	5.914727	2.058115	7.187695
79	13	0	7.043129	2.079946	3.740371
80	13	0	5.886233	6.248521	5.856197

quintet

1	13	0	-0.371036	6.263568	1.008661
2	13	0	-1.714109	6.239073	4.288277
3	13	0	-0.482243	2.071453	2.218438
4	8	0	-3.469074	6.258474	7.330266
5	8	0	-0.878969	6.256598	2.695947
6	8	0	0.748428	2.071944	1.031497
7	8	0	-2.156039	2.065584	4.955398
8	8	0	-3.495318	3.496073	7.329347
9	8	0	-3.493093	0.647704	7.329133
10	8	0	-0.734879	0.575703	3.055801
11	8	0	-0.742682	3.568353	3.053289
12	8	0	0.798397	4.955233	1.207120
13	8	0	0.804523	7.562999	1.210678
14	8	0	-2.239392	7.646000	5.146408
15	8	0	-2.272241	4.843761	5.144530
16	13	0	2.239420	6.255593	1.044702
17	13	0	-2.612019	2.072344	6.732394
18	13	0	-1.013511	0.639000	4.909594
19	13	0	0.729667	7.757542	3.165944
20	13	0	0.713249	4.762098	3.157560
21	13	0	-1.023756	3.499329	4.906831
22	13	0	-2.319084	4.830604	7.014407
23	13	0	2.073105	3.450089	1.019988
24	13	0	2.073729	0.693580	1.020378
25	13	0	-2.311573	7.681726	7.016683
26	8	0	3.303039	2.072467	1.092525
27	8	0	0.449560	2.081424	5.040380
28	8	0	-0.916244	6.254370	7.211655
29	8	0	1.879816	6.255065	3.022664
30	8	0	3.475695	4.922236	0.965260
31	8	0	3.480317	7.583789	0.965541
32	8	0	0.231148	7.537280	4.879732
33	8	0	0.179202	5.017919	4.862726
34	8	0	-1.022378	3.359093	6.807382
35	8	0	-1.021479	0.788170	6.811044
36	8	0	1.923442	0.690820	2.941253
37	8	0	1.914173	3.461797	2.942142
38	13	0	0.350054	2.074203	7.030084
39	13	0	1.996864	2.075259	4.060395
40	13	0	0.547158	6.267287	6.144359
41	13	0	4.984607	6.247156	1.029524
42	13	0	3.402503	6.248979	4.001283

43	13	0	4.794631	2.055355	1.955898
44	8	0	2.084755	6.248127	6.942341
45	8	0	4.933684	6.243576	3.019563
46	8	0	6.238370	2.067282	0.847147
47	8	0	3.473160	2.068471	5.035396
48	8	0	1.884265	3.351452	7.148504
49	8	0	1.875637	0.787032	7.144322
50	8	0	5.127518	0.772997	3.189564
51	8	0	5.170868	3.326454	3.197384
52	8	0	6.367321	4.984657	1.242416
53	8	0	6.363310	7.513612	1.238539
54	8	0	3.479853	7.650565	5.105389
55	8	0	3.483844	4.843874	5.102906
56	13	0	7.981357	6.250200	1.345799
57	13	0	3.212404	2.065396	6.936953
58	13	0	4.727294	0.612946	4.970778
59	13	0	6.355609	7.673701	3.159287
60	13	0	6.365146	4.832054	3.161746
61	13	0	4.735549	3.513773	4.974001
62	13	0	3.352780	4.873768	7.043443
63	13	0	7.561835	3.549723	1.016188
64	13	0	7.551763	0.582257	1.011473
65	13	0	3.352428	7.623912	7.041782
66	8	0	8.726414	2.063209	0.719104
67	8	0	6.119874	2.059787	5.268948
68	8	0	4.653091	6.249094	7.044921
69	8	0	7.517501	6.256419	3.104590
70	8	0	8.835143	4.814141	0.729747
71	8	0	8.830886	7.687597	0.727889
72	8	0	6.145098	7.739029	5.018372
73	8	0	6.149046	4.756693	5.020127
74	8	0	4.525167	3.384185	6.866093
75	8	0	4.519794	0.744493	6.864091
76	8	0	7.584256	0.677030	2.871918
77	8	0	7.614322	3.474357	2.876738
78	27	0	5.916724	2.060262	7.190217
79	13	0	7.040085	2.080073	3.738333
80	13	0	5.887824	6.248780	5.856518

septet

1	13	0	-0.551214	6.262861	0.929448
2	13	0	-1.718462	6.244588	4.280000
3	13	0	-0.567233	2.073491	2.186315
4	8	0	-3.358086	6.260520	7.339679
5	8	0	-0.723593	6.260497	2.787972
6	8	0	0.680483	2.073479	1.004782
7	8	0	-2.132749	2.067901	4.964575
8	8	0	-3.477104	3.519214	7.316835
9	8	0	-3.473537	0.626893	7.317364
10	8	0	-0.756632	0.585110	3.057008
11	8	0	-0.763544	3.563294	3.055077
12	8	0	0.793712	4.981292	1.196855
13	8	0	0.799320	7.534545	1.198415
14	8	0	-2.196863	7.644604	5.177247
15	8	0	-2.224030	4.853333	5.176270
16	13	0	2.170448	6.254775	1.134519
17	13	0	-2.628005	2.073637	6.714449
18	13	0	-0.971680	0.650289	4.907936
19	13	0	0.672691	7.718314	3.126431
20	13	0	0.663048	4.798521	3.122274
21	13	0	-0.980539	3.492038	4.906169
22	13	0	-2.193336	4.775729	7.038745
23	13	0	1.977713	3.451021	0.996699
24	13	0	1.974568	0.695059	0.996125
25	13	0	-2.186142	7.738997	7.038884
26	8	0	3.248821	2.072045	1.086548
27	8	0	0.458354	2.079265	5.053820
28	8	0	-0.866418	6.254455	7.215811
29	8	0	1.915671	6.254743	3.034114
30	8	0	3.468289	4.965000	0.907430
31	8	0	3.474594	7.536697	0.906091
32	8	0	0.281822	7.566544	4.897860
33	8	0	0.242970	4.976451	4.888446
34	8	0	-0.996809	3.344516	6.820317
35	8	0	-0.993771	0.803386	6.823041
36	8	0	1.887405	0.673419	2.919751
37	8	0	1.882182	3.475639	2.922231
38	13	0	0.370430	2.076338	7.033685
39	13	0	1.973539	2.072858	4.026178
40	13	0	0.592792	6.264679	6.118278
41	13	0	4.998640	6.245416	1.032026
42	13	0	3.399872	6.249475	4.024017
43	13	0	4.757578	2.055467	1.940897

44	8	0	2.103140	6.249633	6.974819
45	8	0	4.918195	6.241927	3.006708
46	8	0	6.227066	2.067650	0.855776
47	8	0	3.452784	2.067667	5.025922
48	8	0	1.885601	3.353122	7.159807
49	8	0	1.879071	0.788636	7.159689
50	8	0	5.104579	0.766002	3.176114
51	8	0	5.152026	3.329456	3.186064
52	8	0	6.362436	4.977570	1.242438
53	8	0	6.358241	7.519253	1.238969
54	8	0	3.495084	7.642292	5.128460
55	8	0	3.502112	4.852878	5.125030
56	13	0	7.982029	6.249370	1.336788
57	13	0	3.211235	2.066775	6.924983
58	13	0	4.714270	0.612818	4.967483
59	13	0	6.350026	7.674360	3.156378
60	13	0	6.360832	4.830048	3.158768
61	13	0	4.723964	3.513470	4.971506
62	13	0	3.366815	4.872292	7.059406
63	13	0	7.564268	3.544308	1.020521
64	13	0	7.555061	0.586570	1.018829
65	13	0	3.368536	7.625646	7.059613
66	8	0	8.731491	2.062344	0.719759
67	8	0	6.095210	2.060722	5.264776
68	8	0	4.673796	6.248838	7.070219
69	8	0	7.507332	6.256062	3.094358
70	8	0	8.841994	4.807466	0.746414
71	8	0	8.837488	7.692755	0.745756
72	8	0	6.140480	7.737379	5.009536
73	8	0	6.148425	4.756652	5.011836
74	8	0	4.515357	3.376846	6.868609
75	8	0	4.510106	0.752153	6.867412
76	8	0	7.572324	0.679736	2.879816
77	8	0	7.604493	3.471135	2.882213
78	27	0	5.905830	2.059065	7.202091
79	13	0	7.017356	2.081148	3.736069
80	13	0	5.883330	6.247633	5.856097

The coordinates of the optimized structures of the Ni_I substituted (111)_n surface of the supercell.

doublet

1	13	0	-0.369276	6.263354	1.009302
2	13	0	-1.711086	6.237566	4.289740
3	13	0	-0.483123	2.071871	2.218409
4	8	0	-3.467122	6.258414	7.330429
5	8	0	-0.876312	6.257383	2.697082
6	8	0	0.749025	2.071977	1.032887
7	8	0	-2.155718	2.064891	4.955453
8	8	0	-3.495280	3.496085	7.328644
9	8	0	-3.492550	0.647117	7.328179
10	8	0	-0.733873	0.576051	3.056464
11	8	0	-0.741761	3.568967	3.054019
12	8	0	0.800207	4.955206	1.207712
13	8	0	0.806452	7.562647	1.210982
14	8	0	-2.236161	7.644665	5.147479
15	8	0	-2.271591	4.842890	5.145260
16	13	0	2.241452	6.255665	1.045166
17	13	0	-2.612565	2.072191	6.731973
18	13	0	-1.012550	0.638707	4.910274
19	13	0	0.731282	7.757590	3.166218
20	13	0	0.715661	4.762044	3.158550
21	13	0	-1.023509	3.498904	4.907422
22	13	0	-2.317837	4.830097	7.014897
23	13	0	2.074058	3.450020	1.019670
24	13	0	2.074358	0.693455	1.019664
25	13	0	-2.309645	7.681731	7.017286
26	8	0	3.303811	2.072188	1.089958
27	8	0	0.449829	2.081702	5.042030
28	8	0	-0.914348	6.254163	7.211201
29	8	0	1.882161	6.255088	3.024066
30	8	0	3.476621	4.921449	0.963440
31	8	0	3.481805	7.584461	0.963355
32	8	0	0.235200	7.538913	4.880898
33	8	0	0.179738	5.019418	4.863360
34	8	0	-1.021676	3.358502	6.807521
35	8	0	-1.019755	0.788171	6.811556
36	8	0	1.925462	0.690597	2.940588
37	8	0	1.916384	3.461645	2.942468
38	13	0	0.351564	2.074688	7.029593
39	13	0	1.995775	2.074596	4.060462

40	13	0	0.549883	6.268558	6.145330
43	13	0	4.796086	2.054531	1.953106
44	8	0	2.085912	6.248332	6.946862
45	8	0	4.929786	6.243775	3.017407
46	8	0	6.241582	2.067247	0.844971
47	8	0	3.468567	2.068045	5.038107
48	8	0	1.890987	3.353062	7.148961
49	8	0	1.882849	0.786606	7.145937
50	8	0	5.122993	0.769399	3.184485
51	8	0	5.164956	3.329236	3.191937
52	8	0	6.367269	4.983448	1.241939
53	8	0	6.364618	7.513670	1.238379
54	8	0	3.475471	7.652839	5.110142
55	8	0	3.479184	4.842043	5.106910
56	13	0	7.982112	6.250228	1.348706
57	13	0	3.214343	2.065927	6.936777
58	13	0	4.723910	0.612137	4.965198
59	13	0	6.352636	7.672195	3.158492
60	13	0	6.360985	4.832458	3.159898
61	13	0	4.732412	3.515399	4.968266
62	13	0	3.354240	4.875770	7.047919
63	13	0	7.562963	3.549089	1.018783
64	13	0	7.553662	0.582823	1.014840
65	13	0	3.355032	7.622071	7.046961
66	8	0	8.730940	2.063242	0.719019
67	8	0	6.090441	2.061615	5.266443
68	8	0	4.654400	6.249431	7.043214
69	8	0	7.514684	6.255600	3.104801
70	8	0	8.836301	4.813879	0.733583
71	8	0	8.832499	7.687797	0.731857
72	8	0	6.141570	7.737518	5.014903
73	8	0	6.144375	4.760512	5.015254
74	8	0	4.535171	3.385473	6.862500
75	8	0	4.529414	0.743157	6.860861
76	8	0	7.581862	0.677718	2.876711
77	8	0	7.611248	3.473005	2.880863
78	28	0	5.877304	2.059349	7.159541
79	13	0	7.045479	2.079797	3.750117
80	13	0	5.896676	6.249512	5.861363

quartet

1	13	0	-0.368811	6.263744	1.010096
2	13	0	-1.708270	6.235146	4.290981
3	13	0	-0.483750	2.073006	2.218902
4	8	0	-3.466505	6.258984	7.329759
5	8	0	-0.873051	6.259373	2.698753
6	8	0	0.748004	2.072836	1.032743
7	8	0	-2.154970	2.064121	4.953597
8	8	0	-3.496983	3.496494	7.327539
9	8	0	-3.493165	0.646961	7.325799
10	8	0	-0.732181	0.576946	3.057012
11	8	0	-0.741253	3.570464	3.054539
12	8	0	0.800437	4.955347	1.207919
13	8	0	0.807220	7.563134	1.210230
14	8	0	-2.231667	7.643117	5.147935
15	8	0	-2.273190	4.841459	5.144871
16	13	0	2.241906	6.256310	1.044703
17	13	0	-2.614512	2.072838	6.729520
18	13	0	-1.010189	0.638619	4.910817
19	13	0	0.732349	7.758177	3.166090
20	13	0	0.717162	4.762681	3.159200
21	13	0	-1.023540	3.499072	4.907445
22	13	0	-2.318430	4.830185	7.014339
23	13	0	2.073940	3.450636	1.019005
24	13	0	2.073020	0.694300	1.017737
25	13	0	-2.308084	7.682201	7.017391
26	8	0	3.302826	2.072414	1.088614
27	8	0	0.450380	2.083418	5.042224
28	8	0	-0.913439	6.254465	7.209785
29	8	0	1.883371	6.255635	3.024240
30	8	0	3.476247	4.921562	0.961132
31	8	0	3.482652	7.584830	0.960487
32	8	0	0.241455	7.542902	4.882563
33	8	0	0.177255	5.023008	4.863056
34	8	0	-1.023797	3.358346	6.806588
35	8	0	-1.019105	0.789729	6.811263
36	8	0	1.926571	0.691001	2.939607
37	8	0	1.917326	3.461965	2.942956
38	13	0	0.351361	2.077730	7.029886
39	13	0	1.996553	2.074196	4.060548
40	13	0	0.551702	6.270825	6.145675
41	13	0	4.984344	6.246965	1.026685
42	13	0	3.403125	6.250431	4.008062

43	13	0	4.794627	2.051598	1.952536
44	8	0	2.086831	6.249893	6.949001
45	8	0	4.927888	6.242443	3.015930
46	8	0	6.240008	2.066955	0.844618
47	8	0	3.468785	2.067333	5.039024
48	8	0	1.890690	3.355167	7.147682
49	8	0	1.884035	0.788759	7.149753
50	8	0	5.119836	0.766615	3.184401
51	8	0	5.164080	3.326460	3.191914
52	8	0	6.365481	4.981851	1.239733
53	8	0	6.363614	7.513963	1.237842
54	8	0	3.474889	7.652926	5.112721
55	8	0	3.478732	4.842090	5.107971
56	13	0	7.982096	6.248338	1.348505
57	13	0	3.215327	2.067880	6.939090
58	13	0	4.723627	0.611573	4.966039
59	13	0	6.350900	7.670725	3.158031
60	13	0	6.358853	4.830834	3.157165
61	13	0	4.732130	3.515235	4.968378
62	13	0	3.352830	4.875115	7.048746
63	13	0	7.561662	3.547000	1.017504
64	13	0	7.554628	0.582256	1.018627
65	13	0	3.357039	7.622336	7.050027
66	8	0	8.729244	2.060938	0.721320
67	8	0	6.090347	2.061803	5.265889
68	8	0	4.655303	6.247970	7.044538
69	8	0	7.512535	6.253958	3.103265
70	8	0	8.836552	4.811322	0.734984
71	8	0	8.832925	7.686758	0.734824
72	8	0	6.140680	7.735879	5.014508
73	8	0	6.144784	4.759909	5.012982
74	8	0	4.535165	3.385971	6.862920
75	8	0	4.529103	0.744060	6.861960
76	8	0	7.579449	0.676881	2.878875
77	8	0	7.609613	3.471680	2.878963
78	28	0	5.878535	2.060135	7.157951
79	13	0	7.043459	2.080134	3.749694
80	13	0	5.896985	6.247755	5.861436

sextet

1	13	0	-0.547263	6.261996	0.928217
2	13	0	-1.711831	6.239746	4.279534
3	13	0	-0.565017	2.074900	2.187369
4	8	0	-3.358877	6.261191	7.336525
5	8	0	-0.718133	6.261642	2.787418
6	8	0	0.680821	2.073803	1.003816
7	8	0	-2.126724	2.066503	4.965841
8	8	0	-3.477799	3.519559	7.312966
9	8	0	-3.473502	0.626247	7.311377
10	8	0	-0.750172	0.587444	3.059886
11	8	0	-0.758770	3.563599	3.058705
12	8	0	0.796450	4.980396	1.196387
13	8	0	0.801950	7.534303	1.196423
14	8	0	-2.187270	7.641975	5.174893
15	8	0	-2.223115	4.850311	5.175355
16	13	0	2.173351	6.254046	1.133989
17	13	0	-2.626825	2.074013	6.713997
18	13	0	-0.964348	0.649739	4.910354
19	13	0	0.676703	7.718763	3.125734
20	13	0	0.667482	4.798790	3.122761
21	13	0	-0.975782	3.491830	4.909301
22	13	0	-2.193618	4.776496	7.037584
23	13	0	1.979406	3.451248	0.994146
24	13	0	1.974391	0.694418	0.991285
25	13	0	-2.185490	7.738136	7.035648
26	8	0	3.248378	2.071057	1.079489
27	8	0	0.462165	2.080999	5.058855
28	8	0	-0.865692	6.254426	7.214364
29	8	0	1.917723	6.254861	3.033225
30	8	0	3.468976	4.963857	0.904619
31	8	0	3.475091	7.536407	0.901309
32	8	0	0.293834	7.571877	4.900062
33	8	0	0.242487	4.982144	4.888777
34	8	0	-0.994343	3.345380	6.822908
35	8	0	-0.989364	0.802262	6.825526
36	8	0	1.891760	0.673261	2.916604
37	8	0	1.885310	3.474905	2.921603
38	13	0	0.371789	2.077649	7.037867
39	13	0	1.972526	2.071243	4.024809
40	13	0	0.596390	6.268591	6.120810
41	13	0	4.998715	6.244935	1.030669
42	13	0	3.397861	6.251168	4.029668
43	13	0	4.754864	2.053831	1.941118

44	8	0	2.102218	6.251291	6.985276
45	8	0	4.912315	6.241721	3.006867
46	8	0	6.227581	2.067539	0.858430
47	8	0	3.446389	2.067479	5.027360
48	8	0	1.890900	3.355353	7.164286
49	8	0	1.885656	0.789697	7.168579
50	8	0	5.094614	0.761477	3.171717
51	8	0	5.141963	3.331932	3.180897
52	8	0	6.362249	4.978238	1.243792
53	8	0	6.358046	7.518282	1.241504
54	8	0	3.483760	7.644336	5.135342
55	8	0	3.489472	4.852135	5.130169
56	13	0	7.984663	6.248013	1.344155
57	13	0	3.208479	2.068672	6.931371
58	13	0	4.707806	0.612849	4.960893
59	13	0	6.343861	7.673366	3.158976
60	13	0	6.354306	4.829246	3.159506
61	13	0	4.715724	3.513920	4.962890
62	13	0	3.366737	4.874589	7.064929
63	13	0	7.562036	3.545152	1.023654
64	13	0	7.554834	0.584064	1.026439
65	13	0	3.372550	7.623788	7.067922
66	8	0	8.729606	2.060577	0.727116
67	8	0	6.069384	2.060381	5.253192
68	8	0	4.672061	6.248143	7.067578
69	8	0	7.502923	6.254996	3.098512
70	8	0	8.843314	4.805509	0.751139
71	8	0	8.839470	7.692348	0.752594
72	8	0	6.130747	7.735126	5.009715
73	8	0	6.138484	4.757311	5.010436
74	8	0	4.532050	3.381442	6.861253
75	8	0	4.527135	0.749984	6.861104
76	8	0	7.568225	0.676847	2.884479
77	8	0	7.600237	3.472579	2.883489
78	28	0	5.877496	2.061883	7.149304
79	13	0	7.024559	2.081281	3.742175
80	13	0	5.891241	6.246582	5.860811