Information about surface BC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.159230	-0.876500	1.600848
2	8	0	0.188998	1.860532	1.496069
3	8	0	3.851811	-1.484886	-0.258307
4	8	0	2.592510	1.153811	-0.443504
5	8	0	-1.555275	-1.389811	-1.199236
6	8	0	-1.713298	1.143154	-0.829250
7	7	0	1.016062	-2.691237	-0.566670
8	7	0	0.481313	2.851157	-1.011303
9	6	0	0.611298	-3.116051	0.770379
10	6	0	2.312534	-3.263428	-0.947943
11	6	0	0.524147	3.775281	0.136273
12	6	0	1.690135	2.864532	-1.826617
13	6	0	0.081685	-3.067548	-1.632170
14	6	0	-0.725537	3.047374	-1.818030
15	6	0	-0.345630	-2.198205	1.529331
16	6	0	0.884295	3.092137	1.451463
17	6	0	3.542808	-2.852650	-0.149498
18	6	0	2.897907	2.398601	-1.041077
19	6	0	-1.380831	-2.776943	-1.386930
20	6	0	-1.946575	2.530878	-1.091911
21	6	0	-0.508411	-0.097850	2.593154
22	6	0	0.226403	1.205163	2.751513
23	6	0	3.388875	-0.704031	0.822697
24	6	0	3.589679	0.745168	0.476625

25	6	0	-2.722739	-0.962538	-0.637639
26	6	0	-2.790548	0.420177	-0.398973
27	6	0	-3.791113	-1.776189	-0.276023
28	6	0	-3.894652	0.967810	0.238093
29	6	0	-4.907619	-1.218594	0.356231
30	6	0	-4.953758	0.140825	0.621510
31	1	0	1.512869	-3.188504	1.382266
32	1	0	0.166682	-4.130315	0.765635
33	1	0	2.499362	-2.973393	-1.986728
34	1	0	2.268510	-4.372542	-0.929792
35	1	0	-0.465942	4.224350	0.271782
36	1	0	1.219526	4.607755	-0.046721
37	1	0	1.907110	3.864852	-2.242190
38	1	0	1.537543	2.182123	-2.669409
39	1	0	0.139457	-4.157151	-1.830439
40	1	0	0.397173	-2.556655	-2.547732
41	1	0	-0.608725	2.489293	-2.752685
42	1	0	-0.888765	4.106292	-2.075440
43	1	0	-1.356686	-2.177081	1.113691
44	1	0	-0.428389	-2.608595	2.547183
45	1	0	1.962225	2.903116	1.554426
46	1	0	0.563907	3.730732	2.286192
47	1	0	3.472523	-3.147621	0.907201
48	1	0	4.388307	-3.407154	-0.572015
49	1	0	3.761322	2.294253	-1.713062
50	1	0	3.167660	3.130693	-0.265690
51	1	0	-1.962064	-3.117011	-2.254822
52	1	0	-1.739250	-3.336890	-0.515666

53	1	0	-2.127472	3.075340	-0.153522
54	1	0	-2.836084	2.638030	-1.723501
55	1	0	-0.511652	-0.629398	3.554360
56	1	0	-1.549040	0.088208	2.291687
57	1	0	-0.279418	1.821100	3.511263
58	1	0	1.271773	1.027240	3.048961
59	1	0	3.965727	-0.937347	1.732293
60	1	0	2.327652	-0.885569	1.027142
61	1	0	3.525514	1.359581	1.387925
62	1	0	4.586524	0.880156	0.035451
63	1	0	-3.778708	-2.838329	-0.489517
64	1	0	-3.934669	2.032439	0.454405
65	1	0	-5.734393	-1.861639	0.638645
66	1	0	-5.807644	0.576299	1.128521

Information about complex Li(BC)Be

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.277012	-0.846991	1.604316
2	8	0	-0.073401	1.860892	1.385698
3	8	0	4.065509	-1.000956	-0.152197
4	8	0	2.454964	1.425136	-0.473268
5	8	0	-1.275438	-1.704123	-1.206149
6	8	0	-1.795565	0.793768	-0.945798
7	7	0	1.435232	-2.605357	-0.467456
8	7	0	0.142727	2.785304	-1.154469
9	6	0	1.059165	-3.030996	0.877685

10	6	0	2.808441	-3.003687	-0.797976
11	6	0	0.026076	3.749843	-0.045945
12	6	0	1.358618	2.937191	-1.944854
13	6	0	0.590686	-3.150242	-1.535071
14	6	0	-1.058292	2.778459	-1.993100
15	6	0	-0.036098	-2.228356	1.577919
16	6	0	0.443828	3.175440	1.303744
17	6	0	3.948010	-2.393366	0.007453
18	6	0	2.598804	2.676522	-1.116078
19	6	0	-0.903976	-3.059100	-1.332030
20	6	0	-2.213622	2.123676	-1.271006
21	6	0	-0.518519	-0.132343	2.549366
22	6	0	0.022561	1.266241	2.667973
23	6	0	3.469986	-0.251896	0.885530
24	6	0	3.475175	1.196697	0.483265
25	6	0	-2.505385	-1.424047	-0.686808
26	6	0	-2.772004	-0.056465	-0.507655
27	6	0	-3.458576	-2.365385	-0.313276
28	6	0	-3.958024	0.354510	0.083325
29	6	0	-4.658140	-1.946484	0.272228
30	6	0	-4.900745	-0.597873	0.479381
31	1	0	1.945777	-2.952189	1.510294
32	1	0	0.760972	-4.097155	0.906348
33	1	0	2.979864	-2.730545	-1.843972
34	1	0	2.919433	-4.106424	-0.734319
35	1	0	-1.020255	4.060003	0.050469
36	1	0	0.602782	4.664204	-0.249429
37	1	0	1.444371	3.941304	-2.397428

38	1	0	1.324905	2.208094	-2.761276
39	1	0	0.805345	-4.227703	-1.686344
40	1	0	0.855381	-2.635747	-2.464602
41	1	0	-0.840327	2.206727	-2.901007
42	1	0	-1.361186	3.793140	-2.297875
43	1	0	-1.029016	-2.365777	1.141266
44	1	0	-0.087141	-2.606725	2.610161
45	1	0	1.534549	3.144107	1.436449
46	1	0	0.015702	3.794319	2.104319
47	1	0	3.892169	-2.654299	1.073922
48	1	0	4.873429	-2.839254	-0.374187
49	1	0	3.485523	2.668868	-1.765392
50	1	0	2.743297	3.468657	-0.366682
51	1	0	-1.409176	-3.510810	-2.196580
52	1	0	-1.203156	-3.629876	-0.445570
53	1	0	-2.493215	2.673060	-0.360104
54	1	0	-3.092632	2.080134	-1.924502
55	1	0	-0.472441	-0.621569	3.531712
56	1	0	-1.566737	-0.106352	2.219255
57	1	0	-0.583996	1.833719	3.390824
58	1	0	1.074439	1.248810	2.993824
59	1	0	4.049916	-0.366440	1.815648
60	1	0	2.439601	-0.572945	1.075750
61	1	0	3.302055	1.830665	1.366555
62	1	0	4.454504	1.453500	0.057211
63	1	0	-3.292266	-3.422648	-0.481831
64	1	0	-4.152087	1.410458	0.254028
65	1	0	-5.393973	-2.688099	0.564421

66	1	0	-5.820025	-0.267662	0.950235
67	3	0	-3.204530	3.654708	2.568085
68	4	0	0.187260	0.941708	0.070597

Information about complex Li(BC)Mg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.077067	1.193071	1.776435
2	8	0	-1.209762	-1.180265	1.481306
3	8	0	-2.611845	1.990371	-0.221218
4	8	0	-3.359323	-0.527317	-0.622686
5	8	0	2.193633	0.989104	-1.180168
6	8	0	1.449756	-1.469878	-0.658298
7	7	0	0.219379	3.017910	-0.401839
8	7	0	-1.331221	-2.414886	-0.951977
9	6	0	0.749971	3.343997	0.923772
10	6	0	-1.019171	3.729609	-0.724405
11	6	0	-1.662041	-3.201060	0.263822
12	6	0	-2.455399	-2.338676	-1.909264
13	6	0	1.181736	3.142937	-1.501806
14	6	0	-0.151649	-2.964971	-1.663629
15	6	0	1.172930	2.115673	1.726256
16	6	0	-2.091209	-2.327935	1.434085
17	6	0	-2.227432	3.326081	0.109284
18	6	0	-3.718593	-1.708624	-1.335471
19	6	0	2.483075	2.376547	-1.316318

20	6	0	1.158142	-2.861518	-0.902703
21	6	0	0.244486	0.187022	2.786915
22	6	0	-0.996388	-0.664965	2.808007
23	6	0	-3.851511	1.581790	0.352016
24	6	0	-4.392732	0.438308	-0.485599
25	6	0	3.179588	0.157053	-0.715802
26	6	0	2.771722	-1.159638	-0.409039
27	6	0	4.513168	0.527315	-0.524408
28	6	0	3.688962	-2.065012	0.121642
29	6	0	5.434125	-0.396421	-0.011225
30	6	0	5.022320	-1.683018	0.318874
31	1	0	-0.021107	3.865850	1.498146
32	1	0	1.606512	4.038035	0.867618
33	1	0	-1.261845	3.515881	-1.770179
34	1	0	-0.897227	4.827417	-0.630941
35	1	0	-0.779111	-3.758606	0.591352
36	1	0	-2.441654	-3.951431	0.060648
37	1	0	-2.714614	-3.341649	-2.290927
38	1	0	-2.115845	-1.726470	-2.752070
39	1	0	1.461993	4.202180	-1.675391
40	1	0	0.690823	2.773258	-2.409059
41	1	0	-0.050331	-2.405420	-2.599478
42	1	0	-0.309951	-4.027452	-1.916381
43	1	0	2.048950	1.615643	1.300305
44	1	0	1.427507	2.431912	2.748410
45	1	0	-3.122223	-1.968526	1.355140
46	1	0	-1.974171	-2.906063	2.360353
47	1	0	-2.038633	3.404774	1.189332

48	1	0	-3.053064	4.010857	-0.137039
49	1	0	-4.389861	-1.460302	-2.169331
50	1	0	-4.256642	-2.392741	-0.662596
51	1	0	3.116263	2.547811	-2.198520
52	1	0	3.037356	2.734973	-0.439619
53	1	0	1.144551	-3.405776	0.050981
54	1	0	1.950977	-3.287559	-1.529153
55	1	0	0.376909	0.655887	3.772912
56	1	0	1.125295	-0.433664	2.571616
57	1	0	-0.837133	-1.501041	3.504905
58	1	0	-1.877569	-0.086015	3.120532
59	1	0	-4.576367	2.408140	0.342037
60	1	0	-3.701596	1.267722	1.395662
61	1	0	-5.272245	0.002722	0.013810
62	1	0	-4.692652	0.799491	-1.479605
63	1	0	4.847799	1.524165	-0.786601
64	1	0	3.364872	-3.058461	0.412266
65	1	0	6.467557	-0.095158	0.130305
66	1	0	5.722276	-2.397675	0.739494
67	3	0	0.984359	-4.455793	3.490556
68	12	0	-0.808063	-0.047012	-0.353906

Information about complex Li(BC)Ca

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.283604	1.530284	1.973763
2	8	0	-0.215469	-1.533221	1.403740

3	8	0	-3.529262	1.548073	-0.384602
4	8	0	-3.109540	-1.267434	-0.184348
5	8	0	1.657927	1.447341	-1.346039
6	8	0	1.630460	-1.192899	-0.663705
7	7	0	-0.783512	3.072762	-0.484598
8	7	0	-0.518060	-2.593801	-0.930628
9	6	0	-0.282895	3.627492	0.771654
10	6	0	-2.157264	3.486352	-0.780853
11	6	0	-0.525009	-3.566151	0.217609
12	6	0	-1.798217	-2.598710	-1.713046
13	6	0	0.074916	3.268638	-1.650404
14	6	0	0.591075	-2.920846	-1.890169
15	6	0	0.518647	2.652161	1.636194
16	6	0	-0.873880	-2.835595	1.499112
17	6	0	-3.218161	2.842362	0.108504
18	6	0	-3.099006	-2.465664	-0.929811
19	6	0	1.537272	2.864346	-1.507557
20	6	0	1.918929	-2.496682	-1.293671
21	6	0	0.441631	0.511930	2.640882
22	6	0	-0.341865	-0.781600	2.644089
23	6	0	-4.189326	0.728913	0.557275
24	6	0	-4.382293	-0.652809	-0.032893
25	6	0	2.775856	0.948857	-0.750899
26	6	0	2.749745	-0.400363	-0.337065
27	6	0	3.943242	1.687301	-0.504367
28	6	0	3.829645	-0.975284	0.325268
29	6	0	5.036901	1.102972	0.144731
30	6	0	4.981232	-0.221633	0.570887

31	1	0	-1.134467	3.964767	1.370145
32	1	0	0.341523	4.527996	0.608657
33	1	0	-2.388937	3.206024	-1.813248
34	1	0	-2.268699	4.588549	-0.718316
35	1	0	0.479551	-3.997427	0.337032
36	1	0	-1.210601	-4.400377	0.033729
37	1	0	-1.850231	-3.543732	-2.275809
38	1	0	-1.730314	-1.764228	-2.416445
39	1	0	0.103018	4.337533	-1.959601
40	1	0	-0.359361	2.702112	-2.480828
41	1	0	0.398771	-2.363122	-2.809634
42	1	0	0.595567	-3.994700	-2.116382
43	1	0	1.423233	2.308887	1.122343
44	1	0	0.839519	3.183453	2.549541
45	1	0	-1.944454	-2.658732	1.632350
46	1	0	-0.449712	-3.376420	2.356120
47	1	0	-2.865090	2.771517	1.146546
48	1	0	-4.125586	3.470248	0.103741
49	1	0	-3.904655	-2.467734	-1.679727
50	1	0	-3.271588	-3.334556	-0.274272
51	1	0	2.069196	3.174217	-2.417797
52	1	0	2.002116	3.382263	-0.662279
53	1	0	2.285942	-3.192479	-0.526778
54	1	0	2.680978	-2.349807	-2.062921
55	1	0	0.615073	0.792932	3.693870
56	1	0	1.425070	0.351221	2.177485
57	1	0	0.046093	-1.435673	3.432465
58	1	0	-1.405918	-0.580850	2.812827

59	1	0	-5.181080	1.140389	0.815855
60	1	0	-3.597766	0.658136	1.482995
61	1	0	-5.026909	-1.246540	0.636190
62	1	0	-4.879412	-0.569843	-1.010868
63	1	0	4.011501	2.716978	-0.834298
64	1	0	3.764039	-2.004998	0.674001
65	1	0	5.930880	1.696481	0.312202
66	1	0	5.817176	-0.677903	1.091020
67	3	0	2.717470	-4.998796	2.320562
68	20	0	-0.033351	-1.023199	-0.206415

Information about complex Na(BC)Be

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.409252	-1.212387	1.947928
2	8	0	0.459534	1.520034	1.251632
3	8	0	3.584780	-1.176917	-0.214103
4	8	0	3.013335	1.501719	-0.719074
5	8	0	-1.353790	-1.931908	-1.115665
6	8	0	-1.703995	0.687672	-1.038532
7	7	0	1.187611	-3.093207	-0.092472
8	7	0	0.472517	2.565977	-1.299322
9	6	0	0.717629	-3.493653	1.234763
10	6	0	2.613324	-3.366934	-0.296404
11	6	0	0.382930	3.486970	-0.133265
12	6	0	1.644365	2.843881	-2.162118
13	6	0	0.396654	-3.596104	-1.215839

14	6	0	-0.759064	2.620912	-2.126722
15	6	0	-0.220477	-2.489432	1.905637
16	6	0	0.932971	2.882166	1.150631
17	6	0	3.544163	-2.426575	0.461051
18	6	0	2.981597	2.728170	-1.442150
19	6	0	-1.101083	-3.336955	-1.142352
20	6	0	-1.984548	2.054011	-1.430833
21	6	0	-0.340857	-0.249542	2.683738
22	6	0	0.376840	1.073557	2.620455
23	6	0	4.241383	-0.157025	0.510925
24	6	0	4.327637	1.078526	-0.360529
25	6	0	-2.628626	-1.505294	-0.844627
26	6	0	-2.809267	-0.107390	-0.761271
27	6	0	-3.723026	-2.348894	-0.633559
28	6	0	-4.053951	0.415447	-0.417307
29	6	0	-4.978183	-1.814857	-0.314132
30	6	0	-5.140693	-0.439464	-0.194287
31	1	0	1.585719	-3.611491	1.889530
32	1	0	0.216008	-4.479500	1.218275
33	1	0	2.836395	-3.253361	-1.361714
34	1	0	2.869103	-4.409824	-0.023364
35	1	0	-0.666737	3.737973	0.055238
36	1	0	0.891101	4.439882	-0.339334
37	1	0	1.572737	3.852898	-2.601444
38	1	0	1.626540	2.110938	-2.975886
39	1	0	0.503878	-4.695673	-1.330778
40	1	0	0.784887	-3.127151	-2.125825
41	1	0	-0.568986	2.042409	-3.036421

42	1	0	-0.987397	3.657532	-2.422344
43	1	0	-1.181906	-2.404237	1.385783
44	1	0	-0.426671	-2.838887	2.930377
45	1	0	2.027103	2.876805	1.198331
46	1	0	0.530581	3.464080	1.991303
47	1	0	3.208488	-2.282468	1.498096
48	1	0	4.555219	-2.865447	0.491566
49	1	0	3.779082	2.747590	-2.198506
50	1	0	3.154429	3.570607	-0.755067
51	1	0	-1.574552	-3.781862	-2.028236
52	1	0	-1.539332	-3.815325	-0.258073
53	1	0	-2.276332	2.635722	-0.546140
54	1	0	-2.820126	2.056865	-2.139579
55	1	0	-0.429246	-0.549993	3.739711
56	1	0	-1.355947	-0.147871	2.273047
57	1	0	-0.196098	1.816092	3.192747
58	1	0	1.391318	0.988209	3.034231
59	1	0	5.266999	-0.458629	0.783341
60	1	0	3.695811	0.066165	1.441645
61	1	0	4.844764	1.875313	0.196501
62	1	0	4.901228	0.857989	-1.271963
63	1	0	-3.611290	-3.422385	-0.725313
64	1	0	-4.183170	1.484743	-0.290477
65	1	0	-5.816728	-2.485702	-0.154807
66	1	0	-6.101128	-0.014922	0.078865
67	11	0	-2.948357	4.406589	2.539758
68	4	0	0.628513	0.341556	-0.614103

Information about complex Na(BC)Mg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.586438	0.685867	1.608701
2	8	0	0.720772	-1.678784	1.158323
3	8	0	-4.289694	-0.493642	0.073642
4	8	0	-1.927759	-2.120809	-0.523393
5	8	0	0.313228	2.210525	-1.203683
6	8	0	1.737767	0.078084	-1.169682
7	7	0	-2.471415	1.992111	-0.253059
8	7	0	0.661945	-2.479371	-1.431908
9	6	0	-2.174421	2.454708	1.099641
10	6	0	-3.916099	1.865324	-0.477616
11	6	0	1.213448	-3.388301	-0.410898
12	6	0	-0.470103	-3.032171	-2.166107
13	6	0	-1.974682	2.869589	-1.317602
14	6	0	1.705484	-1.979108	-2.329996
15	6	0	-0.808689	2.083403	1.675025
16	6	0	0.720806	-3.084948	1.000270
17	6	0	-4.682502	0.831024	0.336433
18	6	0	-1.649471	-3.298843	-1.254595
19	6	0	-0.541011	3.333053	-1.202105
20	6	0	2.590368	-0.979630	-1.620791
21	6	0	0.488537	0.270867	2.450671
22	6	0	0.513314	-1.232777	2.486888
23	6	0	-3.379914	-1.020240	1.015773
24	6	0	-2.881472	-2.341940	0.501060

25	6	0	1.596457	2.383134	-0.774201
26	6	0	2.362464	1.206887	-0.718176
27	6	0	2.160896	3.591067	-0.378573
28	6	0	3.658999	1.238028	-0.225399
29	6	0	3.472467	3.620226	0.107407
30	6	0	4.211438	2.451068	0.194081
31	1	0	-2.916479	2.016389	1.770247
32	1	0	-2.289751	3.551853	1.196641
33	1	0	-4.056349	1.604397	-1.531346
34	1	0	-4.421075	2.841499	-0.321149
35	1	0	2.304453	-3.289518	-0.395044
36	1	0	1.001056	-4.439631	-0.655122
37	1	0	-0.214359	-3.969725	-2.691471
38	1	0	-0.772423	-2.300697	-2.922950
39	1	0	-2.583245	3.795128	-1.371576
40	1	0	-2.103001	2.344071	-2.269526
41	1	0	1.221020	-1.482525	-3.176980
42	1	0	2.336649	-2.789085	-2.729717
43	1	0	0.025593	2.605232	1.198470
44	1	0	-0.819849	2.397502	2.729781
45	1	0	-0.290295	-3.470787	1.192801
46	1	0	1.408830	-3.540870	1.725516
47	1	0	-4.643157	1.036342	1.415718
48	1	0	-5.734131	0.918409	0.040959
49	1	0	-2.524519	-3.588425	-1.853237
50	1	0	-1.431732	-4.126505	-0.563571
51	1	0	-0.308104	3.986513	-2.053844
52	1	0	-0.404935	3.925884	-0.290437

53	1	0	3.123880	-1.432643	-0.772332
54	1	0	3.336764	-0.575687	-2.314574
55	1	0	0.342580	0.653983	3.469685
56	1	0	1.442761	0.656346	2.064313
57	1	0	1.341458	-1.570235	3.129349
58	1	0	-0.441474	-1.627321	2.868524
59	1	0	-3.885960	-1.180829	1.981531
60	1	0	-2.529376	-0.347980	1.175770
61	1	0	-2.417491	-2.911596	1.321000
62	1	0	-3.727032	-2.922985	0.108669
63	1	0	1.603200	4.516904	-0.453918
64	1	0	4.242077	0.323669	-0.149286
65	1	0	3.902984	4.566332	0.417821
66	1	0	5.221692	2.463718	0.587838
67	12	0	-0.070594	-0.596627	0.009959
68	11	0	4.375660	-2.232658	2.027117

Information about complex Na(BC)Ca

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.341934	-1.245289	1.983272
2	8	0	0.437067	1.488323	1.296394
3	8	0	3.528582	-1.250820	-0.162620
4	8	0	3.000282	1.437799	-0.661486
5	8	0	-1.416194	-1.928006	-1.091547
6	8	0	-1.727134	0.696309	-1.007403
7	7	0	1.102122	-3.130988	-0.059473

8	7	0	0.478830	2.542293	-1.250944
9	6	0	0.619399	-3.528615	1.264031
10	6	0	2.524551	-3.425598	-0.257144
11	6	0	0.397255	3.460715	-0.082275
12	6	0	1.659117	2.805247	-2.106897
13	6	0	0.309370	-3.618173	-1.188485
14	6	0	-0.747558	2.618574	-2.084342
15	6	0	-0.306812	-2.512509	1.933535
16	6	0	0.931555	2.843455	1.202341
17	6	0	3.465642	-2.501922	0.508131
18	6	0	2.990770	2.666950	-1.380600
19	6	0	-1.184631	-3.336623	-1.121668
20	6	0	-1.984995	2.068015	-1.396532
21	6	0	-0.397260	-0.273612	2.718520
22	6	0	0.340675	1.038671	2.663281
23	6	0	4.196839	-0.243363	0.569115
24	6	0	4.306195	0.993586	-0.297751
25	6	0	-2.685794	-1.483030	-0.825500
26	6	0	-2.845697	-0.082833	-0.738373
27	6	0	-3.793884	-2.310652	-0.622768
28	6	0	-4.084064	0.457659	-0.398927
29	6	0	-5.042430	-1.758724	-0.307875
30	6	0	-5.184730	-0.381427	-0.184243
31	1	0	1.482269	-3.661724	1.922760
32	1	0	0.103018	-4.506696	1.241717
33	1	0	2.754725	-3.311929	-1.320931
34	1	0	2.763139	-4.473129	0.013685
35	1	0	-0.649440	3.726961	0.101784

36	1	0	0.920819	4.406494	-0.282590
37	1	0	1.604989	3.816666	-2.543196
38	1	0	1.634346	2.075326	-2.923194
39	1	0	0.400537	-4.718858	-1.306565
40	1	0	0.709270	-3.152176	-2.094929
41	1	0	-0.561629	2.040240	-2.995006
42	1	0	-0.958683	3.659494	-2.377636
43	1	0	-1.264188	-2.411068	1.409138
44	1	0	-0.523471	-2.862155	2.956048
45	1	0	2.025225	2.821374	1.255527
46	1	0	0.533744	3.428639	2.042921
47	1	0	3.126918	-2.356145	1.543951
48	1	0	4.469777	-2.956148	0.542263
49	1	0	3.792291	2.676770	-2.132864
50	1	0	3.172827	3.504420	-0.689838
51	1	0	-1.660265	-3.771409	-2.011408
52	1	0	-1.634552	-3.811195	-0.241213
53	1	0	-2.272443	2.651179	-0.511375
54	1	0	-2.816822	2.085838	-2.109460
55	1	0	-0.495547	-0.576145	3.773022
56	1	0	-1.408595	-0.155242	2.303068
57	1	0	-0.223869	1.787918	3.235166
58	1	0	1.351631	0.936621	3.081868
59	1	0	5.216379	-0.561349	0.845677
60	1	0	3.649982	-0.014987	1.497820
61	1	0	4.832475	1.780626	0.264540
62	1	0	4.881011	0.767375	-1.207021
63	1	0	-3.697929	-3.385406	-0.717554

64	1	0	-4.197742	1.528368	-0.269167
65	1	0	-5.891822	-2.417315	-0.155019
66	1	0	-6.140011	0.056709	0.085493
67	11	0	-2.933286	4.421906	2.577016
68	20	0	0.597687	0.313534	-0.572404

Information about complex K(BC)Be

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.655156	-0.245270	-2.439716
2	8	0	-1.910965	-0.442383	-0.725429
3	8	0	2.406578	-3.285252	-0.315528
4	8	0	0.082160	-3.217410	1.292511
5	8	0	2.303656	1.906635	0.610719
6	8	0	-0.078481	1.725731	1.698567
7	7	0	3.364478	-0.391070	-1.061951
8	7	0	-1.522683	-0.959099	2.209979
9	6	0	3.042057	0.124391	-2.395557
10	6	0	4.033067	-1.694390	-1.111426
11	6	0	-2.746427	-1.123723	1.425020
12	6	0	-1.175382	-2.118683	3.026399
13	6	0	4.121915	0.534324	-0.218166
14	6	0	-1.487406	0.262166	3.009306
15	6	0	1.657278	0.756269	-2.534195
16	6	0	-2.515688	-1.520828	-0.032418
17	6	0	3.110438	-2.853854	-1.473988
18	6	0	-0.923794	-3.417203	2.267201

19	6	0	3.555940	1.939107	-0.064879
20	6	0	-1.390350	1.570428	2.234937
21	6	0	-0.655031	0.266431	-2.646403
22	6	0	-1.683126	-0.709449	-2.100363
23	6	0	1.250323	-4.040465	-0.621553
24	6	0	0.516907	-4.405129	0.653500
25	6	0	1.556904	3.050347	0.623075
26	6	0	0.251090	2.938336	1.174401
27	6	0	1.990372	4.283496	0.131196
28	6	0	-0.589804	4.054561	1.155181
29	6	0	1.140898	5.400451	0.138542
30	6	0	-0.148395	5.282279	0.638871
31	1	0	3.090917	-0.697556	-3.116921
32	1	0	3.793351	0.863679	-2.733154
33	1	0	4.454429	-1.908272	-0.123919
34	1	0	4.884172	-1.683701	-1.823067
35	1	0	-3.309110	-0.183863	1.421456
36	1	0	-3.414981	-1.875286	1.884833
37	1	0	-1.960802	-2.341535	3.782637
38	1	0	-0.259371	-1.874719	3.573828
39	1	0	5.155041	0.678648	-0.605588
40	1	0	4.209094	0.085084	0.776955
41	1	0	-0.615918	0.212568	3.669379
42	1	0	-2.379681	0.346475	3.666426
43	1	0	1.483708	1.517502	-1.764586
44	1	0	1.605496	1.249430	-3.521680
45	1	0	-1.869216	-2.405603	-0.096396
46	1	0	-3.493181	-1.767449	-0.486175

47	1	0	2.395339	-2.548414	-2.249921
48	1	0	3.710023	-3.689898	-1.871891
49	1	0	-0.611822	-4.176942	3.002941
50	1	0	-1.843789	-3.792266	1.787542
51	1	0	4.278059	2.533672	0.513915
52	1	0	3.444544	2.423284	-1.043321
53	1	0	-2.126133	1.625085	1.422405
54	1	0	-1.598440	2.382619	2.945584
55	1	0	-0.825229	0.425665	-3.724737
56	1	0	-0.780670	1.230884	-2.133579
57	1	0	-2.627826	-0.611059	-2.662351
58	1	0	-1.309327	-1.734806	-2.241590
59	1	0	1.519592	-4.972120	-1.150237
60	1	0	0.584096	-3.454222	-1.271900
61	1	0	-0.344389	-5.039409	0.383661
62	1	0	1.169627	-4.986130	1.324362
63	1	0	2.994697	4.389430	-0.260287
64	1	0	-1.599101	3.980399	1.539957
65	1	0	1.500500	6.347694	-0.251536
66	1	0	-0.822405	6.133556	0.639664
67	19	0	-7.754569	0.426844	-2.023319
68	4	0	2.706852	-2.087714	2.640768

Information about complex K(BC)Mg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.075412	0.593061	2.064702

2	8	0	0.563706	-1.474493	1.019827
3	8	0	-3.624596	-1.327705	0.092454
4	8	0	-1.557442	-2.957952	-0.789725
5	8	0	-0.547101	2.523881	-1.016855
6	8	0	1.413114	0.768698	-1.299493
7	7	0	-3.074715	1.679651	0.299661
8	7	0	0.955165	-2.082234	-1.644023
9	6	0	-2.811029	2.205211	1.640865
10	6	0	-4.345965	0.956500	0.211722
11	6	0	1.769101	-2.773735	-0.606777
12	6	0	0.162568	-3.023699	-2.467664
13	6	0	-2.949134	2.652791	-0.785695
14	6	0	1.803229	-1.256839	-2.541576
15	6	0	-1.380931	1.983016	2.130850
16	6	0	1.108299	-2.788476	0.764675
17	6	0	-4.338869	-0.401966	0.903216
18	6	0	-0.842593	-3.835999	-1.662125
19	6	0	-1.637948	3.423949	-0.829197
20	6	0	2.449838	-0.062525	-1.860539
21	6	0	0.192978	0.281082	2.632340
22	6	0	0.468498	-1.186012	2.430038
23	6	0	-3.403686	-2.579710	0.710891
24	6	0	-2.784524	-3.513290	-0.307703
25	6	0	0.725596	3.012112	-0.869917
26	6	0	1.772297	2.069163	-0.984376
27	6	0	1.037937	4.348796	-0.605609
28	6	0	3.092308	2.469614	-0.784727
29	6	0	2.369644	4.746728	-0.428409

30	6	0	3.392471	3.809061	-0.506334
31	1	0	-3.478961	1.708228	2.350623
32	1	0	-3.041678	3.283868	1.715457
33	1	0	-4.568925	0.780783	-0.845193
34	1	0	-5.183406	1.553648	0.623688
35	1	0	2.728823	-2.259027	-0.498042
36	1	0	2.011306	-3.802676	-0.909801
37	1	0	0.822263	-3.722723	-3.007938
38	1	0	-0.383006	-2.425460	-3.205193
39	1	0	-3.748909	3.421951	-0.738220
40	1	0	-3.065351	2.111780	-1.730412
41	1	0	1.161662	-0.891957	-3.349857
42	1	0	2.605038	-1.866371	-2.988358
43	1	0	-0.647378	2.544525	1.540564
44	1	0	-1.309692	2.332375	3.173716
45	1	0	0.304896	-3.527208	0.856396
46	1	0	1.885162	-3.009025	1.510404
47	1	0	-3.876829	-0.343122	1.898834
48	1	0	-5.377483	-0.748292	1.030580
49	1	0	-1.536171	-4.320688	-2.362830
50	1	0	-0.356674	-4.625636	-1.070793
51	1	0	-1.681358	4.136538	-1.664485
52	1	0	-1.494675	4.003006	0.091240
53	1	0	3.158058	-0.357541	-1.075157
54	1	0	3.000476	0.506947	-2.618745
55	1	0	0.198196	0.493389	3.713293
56	1	0	0.988027	0.879308	2.163660
57	1	0	1.428387	-1.433994	2.902755

58	1	0	-0.326374	-1.800875	2.875015
59	1	0	-4.351128	-3.027331	1.054723
60	1	0	-2.745897	-2.467097	1.587295
61	1	0	-2.594550	-4.489058	0.163990
62	1	0	-3.470877	-3.656017	-1.153537
63	1	0	0.252206	5.091999	-0.546956
64	1	0	3.895743	1.742166	-0.818209
65	1	0	2.590852	5.789829	-0.224581
66	1	0	4.426072	4.099203	-0.348345
67	19	0	5.658746	-1.753894	2.090775
68	12	0	-0.614652	-0.648496	-0.673396

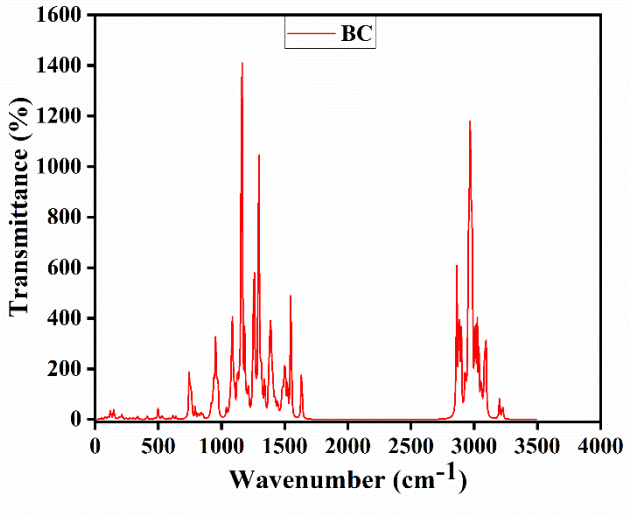
Information about complex K(BC)Ca

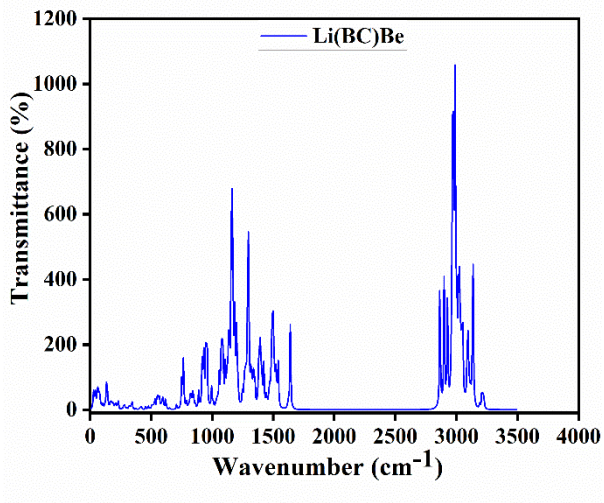
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.747809	0.593819	1.633304
2	8	0	0.950111	-1.470791	1.035252
3	8	0	-4.250243	-1.232730	0.270062
4	8	0	-1.665640	-2.370690	-0.509512
5	8	0	-0.322895	2.319725	-1.174575
6	8	0	1.475912	0.495137	-1.288352
7	7	0	-2.954049	1.558469	-0.077696
8	7	0	0.885245	-2.213627	-1.571985
9	6	0	-2.667486	2.040478	1.270469
10	6	0	-4.360199	1.165329	-0.225322
11	6	0	1.658548	-3.022953	-0.612942

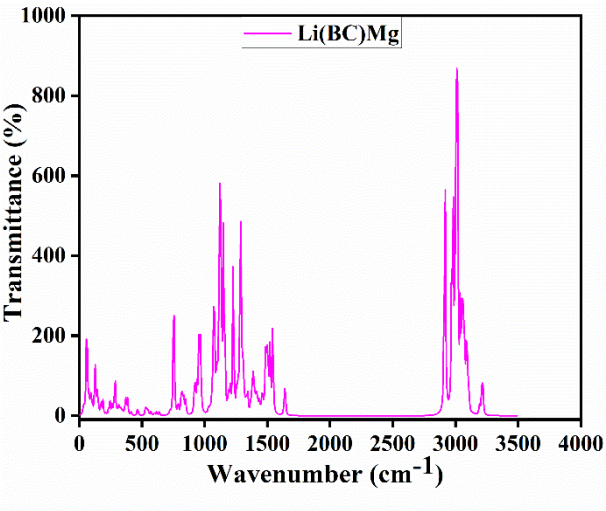
12	6	0	-0.165440	-2.955156	-2.259270
13	6	0	-2.696457	2.536185	-1.139618
14	6	0	1.759807	-1.506241	-2.510358
15	6	0	-1.223935	1.922350	1.756643
16	6	0	1.204430	-2.847920	0.832484
17	6	0	-4.867957	-0.012125	0.596634
18	6	0	-1.216184	-3.459207	-1.292447
19	6	0	-1.370916	3.260043	-1.089430
20	6	0	2.482839	-0.372451	-1.819930
21	6	0	0.435102	0.372194	2.400320
22	6	0	0.743781	-1.100019	2.386919
23	6	0	-3.202249	-1.597270	1.142665
24	6	0	-2.496845	-2.789699	0.558898
25	6	0	0.928830	2.723005	-0.811981
26	6	0	1.903936	1.712049	-0.836444
27	6	0	1.279534	4.007368	-0.409942
28	6	0	3.199102	1.977641	-0.415958
29	6	0	2.589399	4.274003	0.002858
30	6	0	3.538532	3.264247	0.010715
31	1	0	-3.271942	1.455715	1.967011
32	1	0	-2.980553	3.093701	1.408839
33	1	0	-4.512774	0.904700	-1.277412
34	1	0	-5.028940	2.024818	-0.009763
35	1	0	2.710540	-2.719860	-0.654769
36	1	0	1.632788	-4.090131	-0.878496
37	1	0	0.229295	-3.816167	-2.827833
38	1	0	-0.645098	-2.278420	-2.974267
39	1	0	-3.470037	3.330769	-1.129914

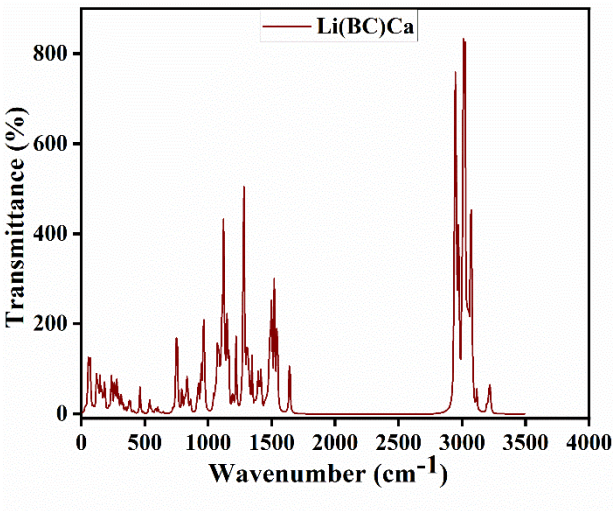
40	1	0	-2.781491	2.015930	-2.099254
41	1	0	1.140189	-1.092679	-3.312681
42	1	0	2.506282	-2.173600	-2.970379
43	1	0	-0.532944	2.602482	1.251284
44	1	0	-1.229712	2.206505	2.819899
45	1	0	0.297310	-3.422062	1.068618
46	1	0	2.008579	-3.180497	1.503276
47	1	0	-4.802316	0.174282	1.678070
48	1	0	-5.933281	-0.119149	0.363188
49	1	0	-2.056078	-3.896540	-1.850350
50	1	0	-0.805395	-4.245000	-0.641500
51	1	0	-1.316990	3.963459	-1.931458
52	1	0	-1.293356	3.848690	-0.168243
53	1	0	3.142455	-0.733989	-1.017476
54	1	0	3.096591	0.179871	-2.540945
55	1	0	0.282052	0.699344	3.437633
56	1	0	1.274750	0.939278	1.973920
57	1	0	1.658032	-1.288051	2.971080
58	1	0	-0.095005	-1.676011	2.808348
59	1	0	-3.609513	-1.870903	2.129488
60	1	0	-2.484861	-0.779710	1.276455
61	1	0	-1.885237	-3.278307	1.333034
62	1	0	-3.240596	-3.511902	0.195840
63	1	0	0.554466	4.812318	-0.424390
64	1	0	3.946945	1.188746	-0.401792
65	1	0	2.852769	5.277770	0.318938
66	1	0	4.550494	3.459588	0.347750
67	19	0	4.689932	-1.341122	1.680783

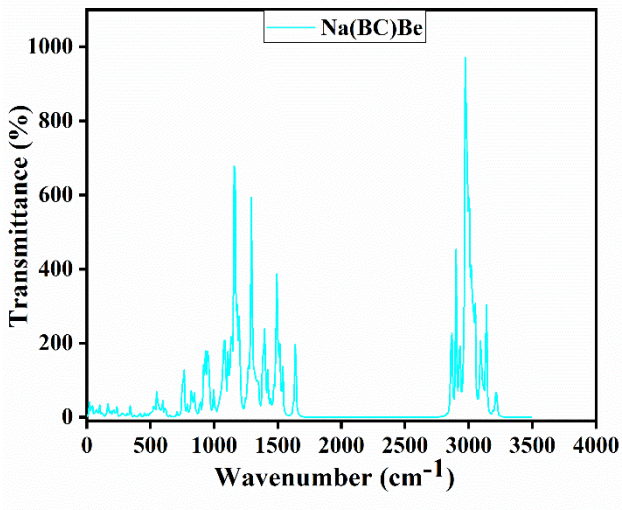
68	20	0	-0.139351	-0.608221	-0.353403

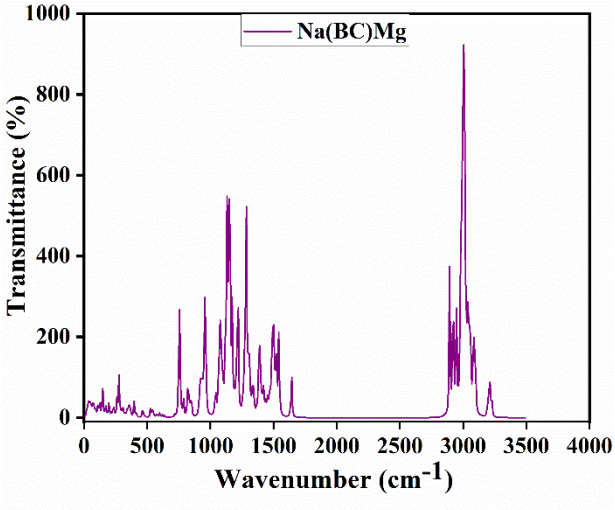

BC
Transmittance (%)
Wavenumber (cm-1)


Li(BC)Be
Transmittance (%)
Wavenumber (cm-1)


Li(BC)Mg
Transmittance (%)
Wavenumber (cm-1)


Li(BC)Ca
Transmittance (%)
Wavenumber (cm-1)


Na(BC)Be
Transmittance (%)
Wavenumber (cm-1)


Na(BC)Mg
Transmittance (%)
Wavenumber (cm-1)

IR Spectra

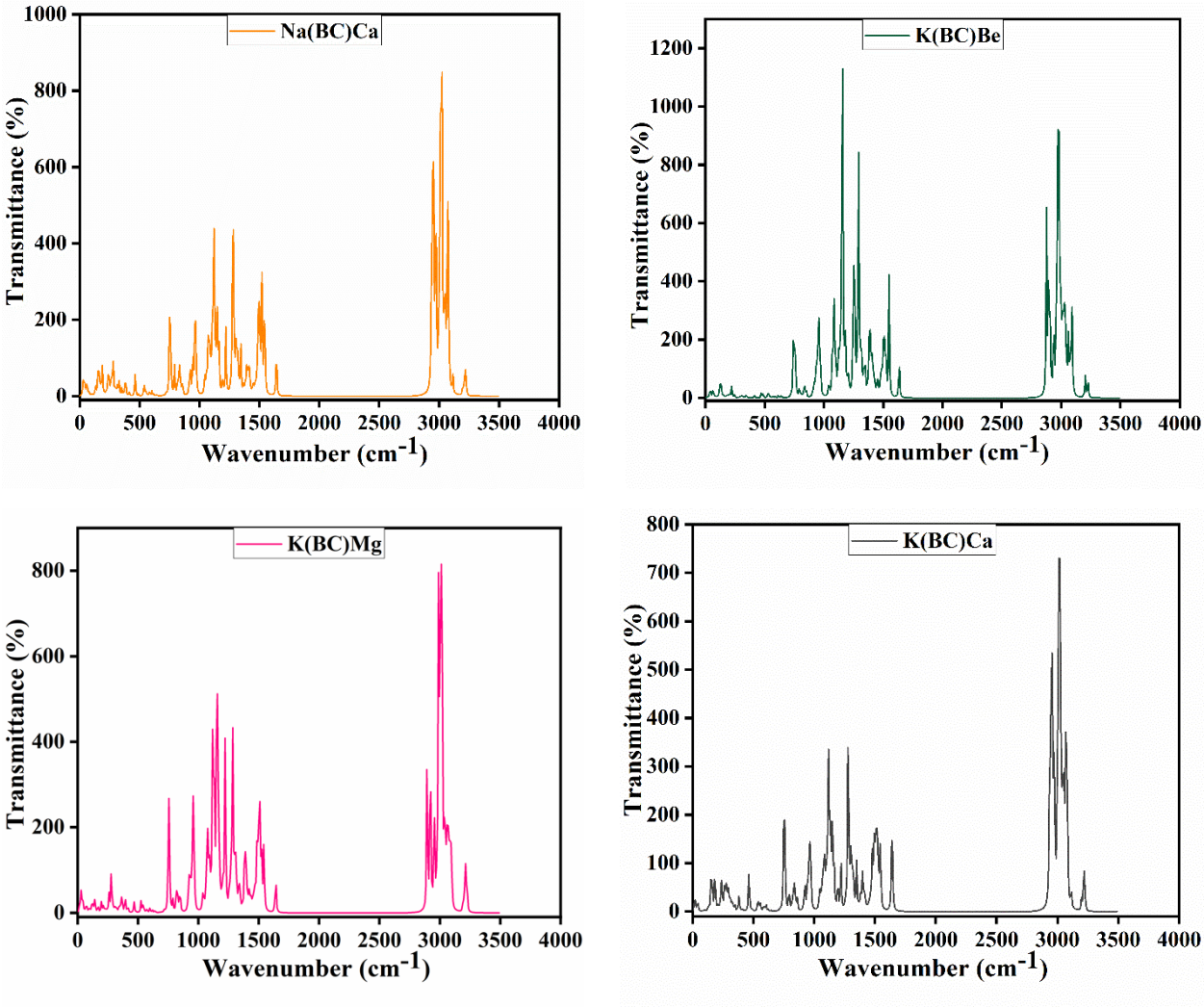


Fig. 1. IR spectra of surface BC and all the doped complexes.