

Supplementary Information

Evidence for Near-Superionic Conductivity in the Li_3BS_3 Electrolyte: Insights on the Lithium Orthothioborate Transport Mechanisms

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Contents

Supplementary Tables.....	1
Graph of MSD vs Time for 200K	2
Graph of MSD vs Time for 300K	3
Graph of MSD vs Time for 400K	4
Graph of MSD vs Time for 425K	5
Graph of MSD vs Time for 450K	6
Graph of MSD vs Time for 475K	7
Graph of MSD vs Time for 500K	8
Graph of MSD vs Time for 600K	9
Disordered Structure at High T (600K)	10
Supplementary Data File for MD.....	11
Forcefield Nonbond, Angle, and Bonding Parameters	41
Charges Implemented on Li, B, and S	42
References	43

Table 1. MSD Plot of Li⁺ Diffusion at 200K.

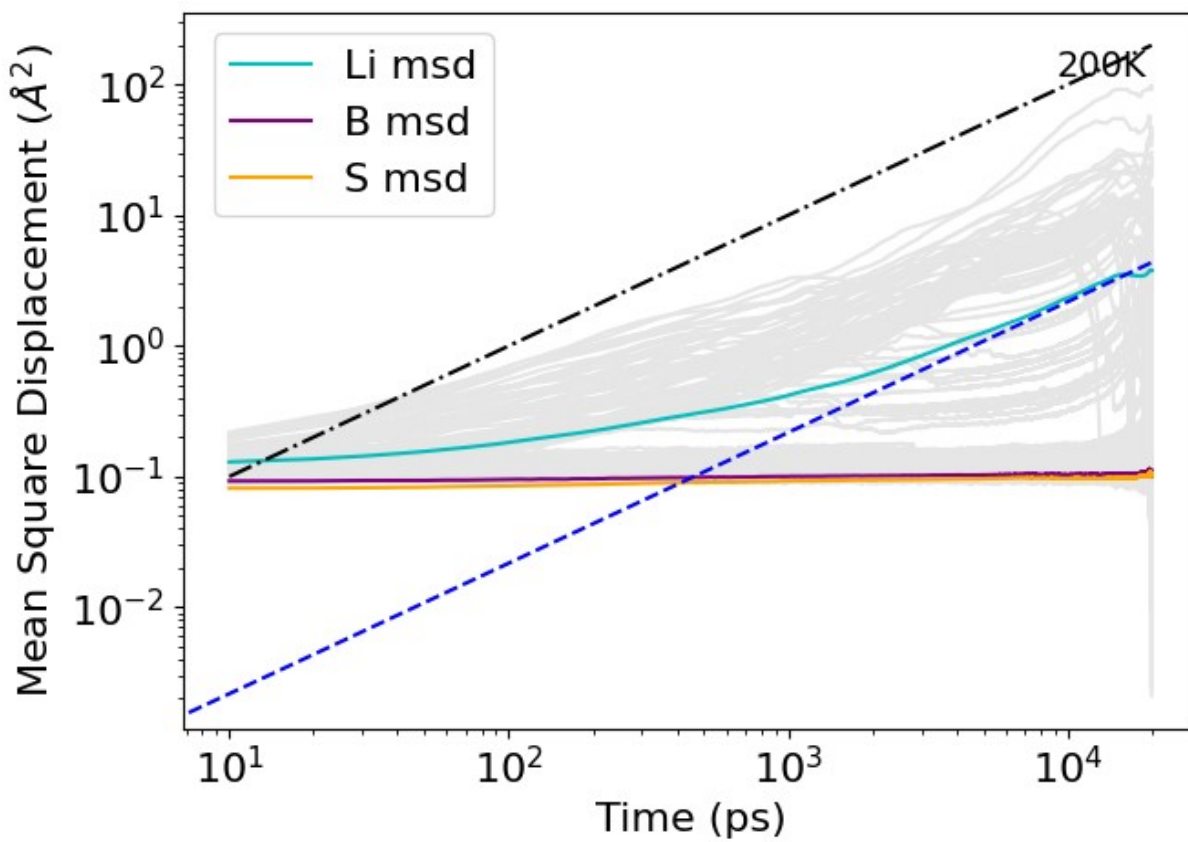


Table 2. MSD Plot of Li⁺ Diffusion at 300K.

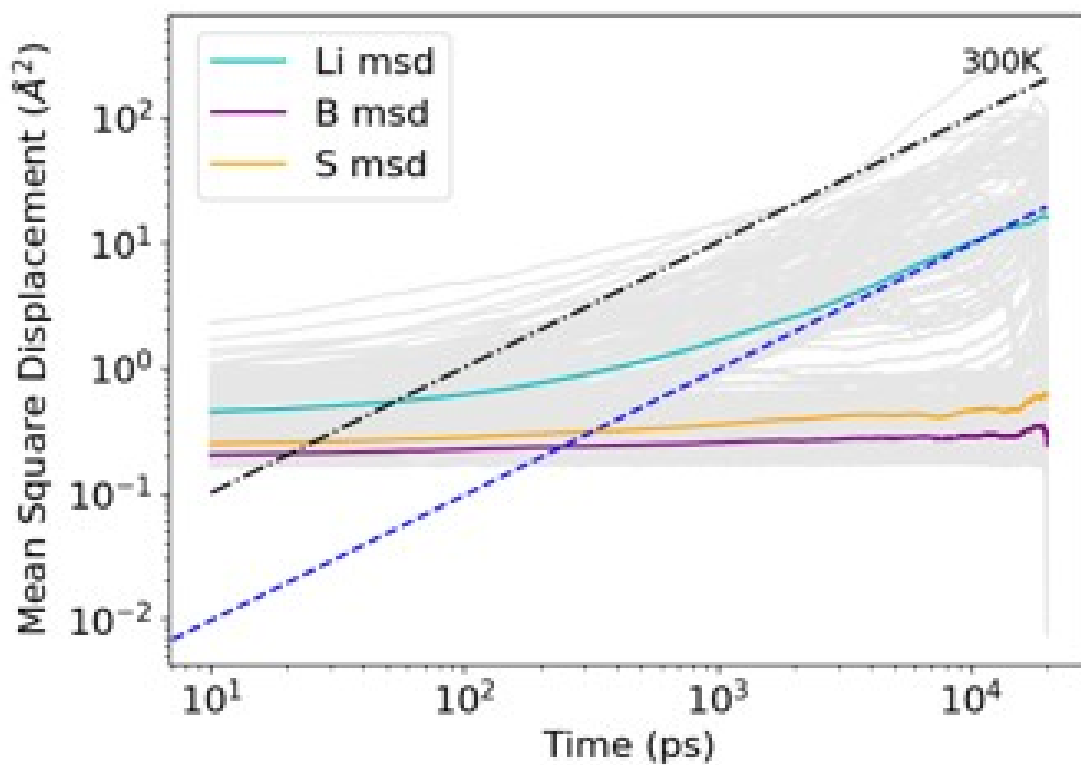


Table 3. MSD Plot of Li⁺ Diffusion at 400K.

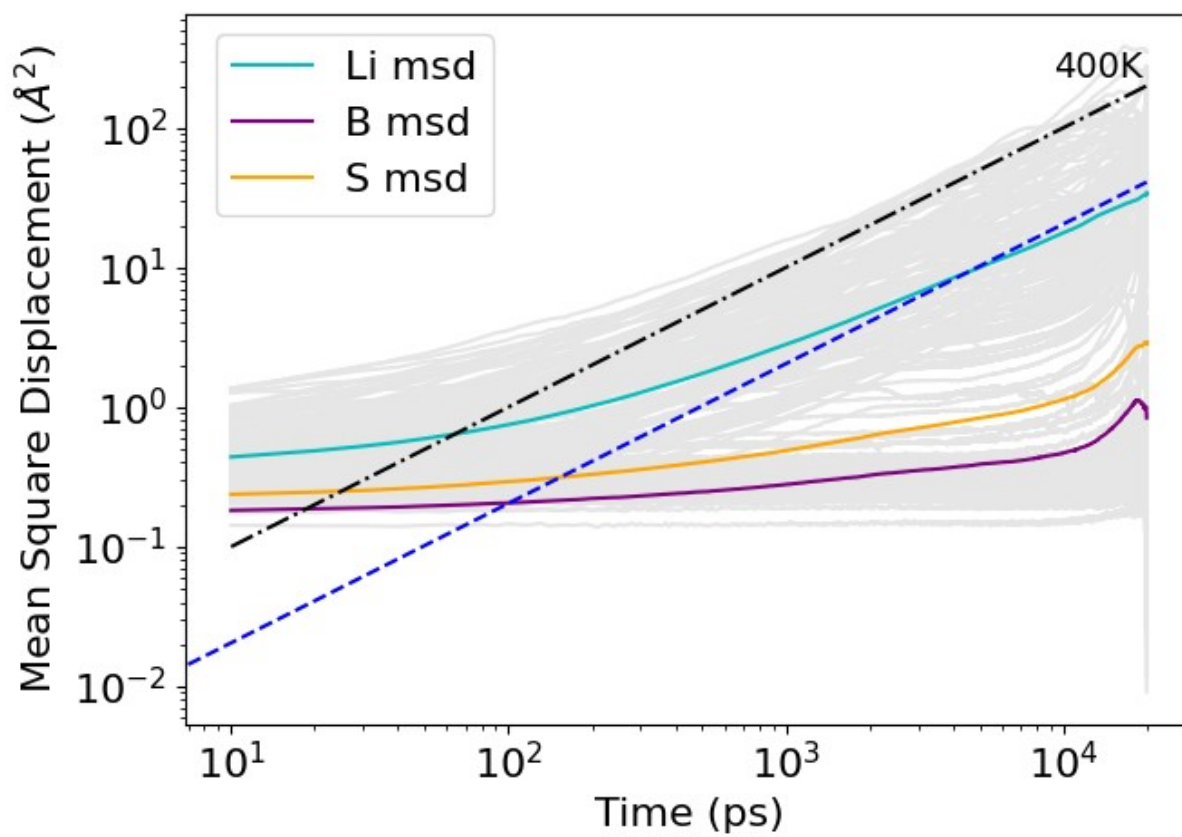


Table 4. MSD Plot of Li⁺ Diffusion at 425K

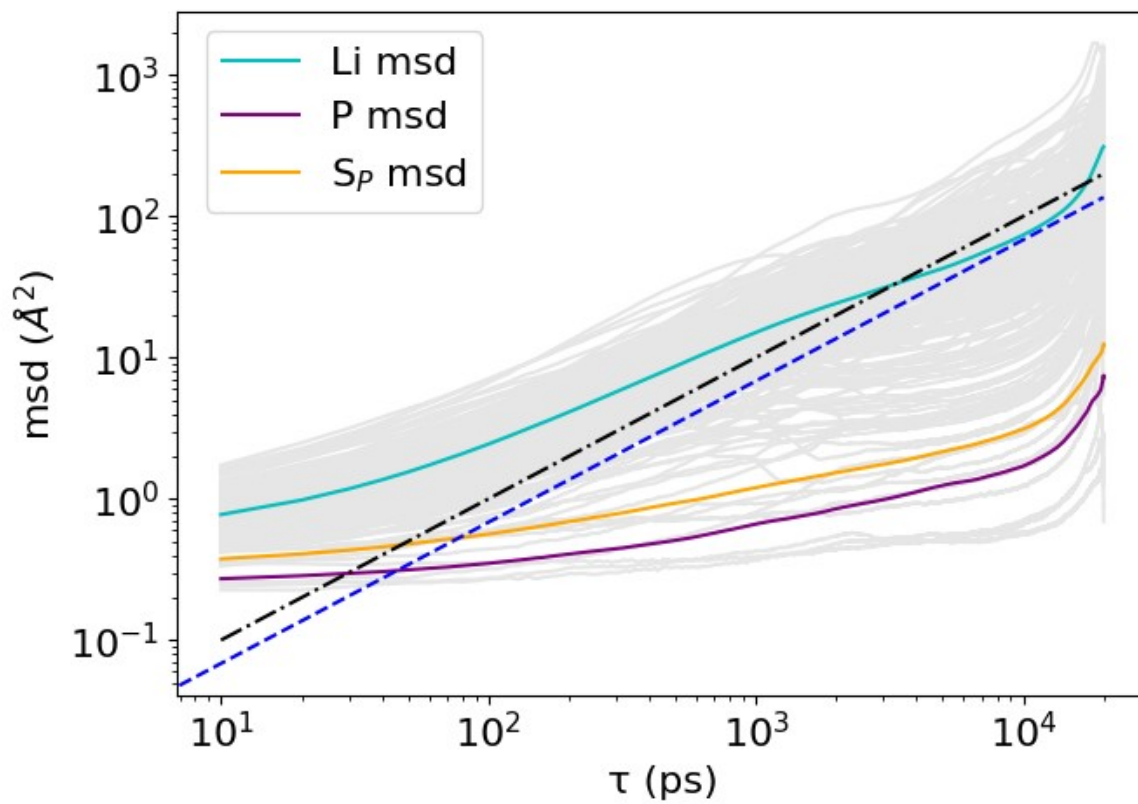


Table 5. MSD Plot of Li⁺ Diffusion at 450K

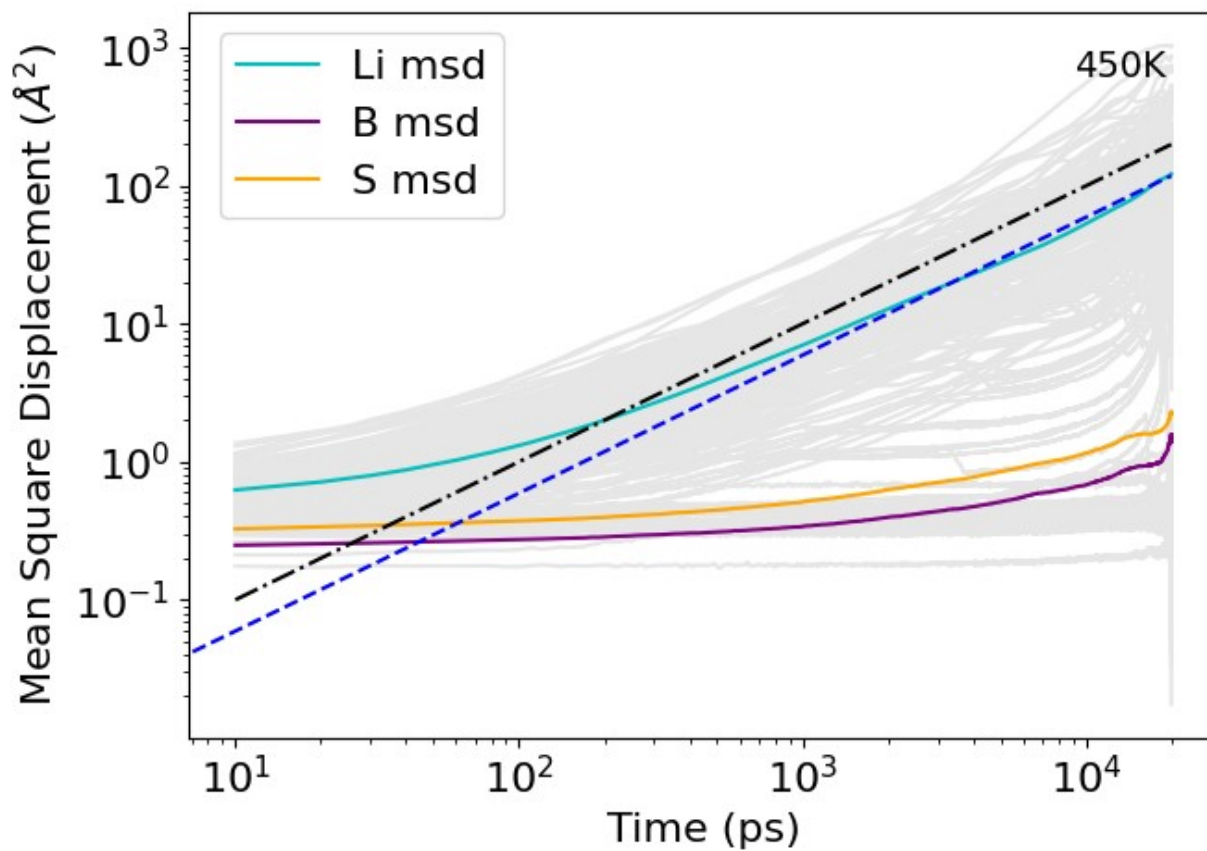


Table 6. MSD Plot of Li⁺ Diffusion at 475K

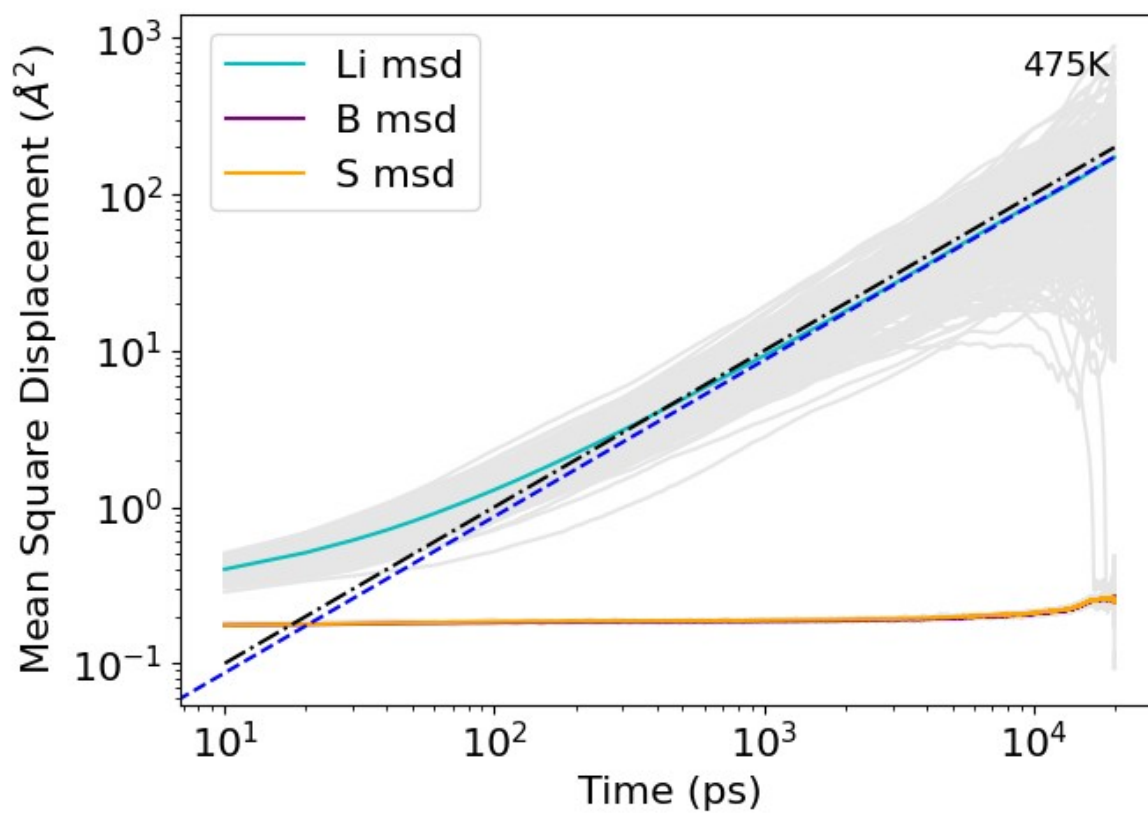


Table 7. MSD Plot of Li⁺ Diffusion at 500K.

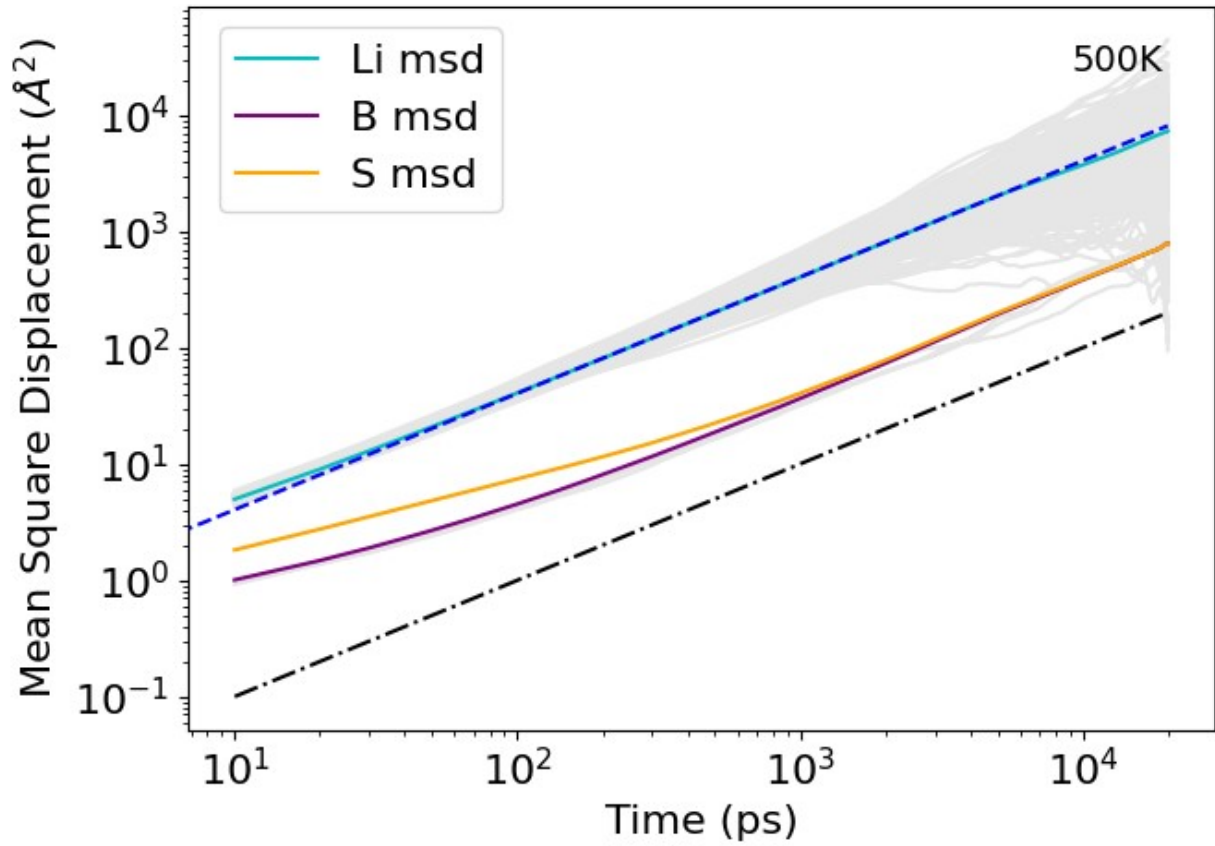


Table 8. MSD Plot of Li⁺ Diffusion at 600K.



Disordered Structure at High T (600K)

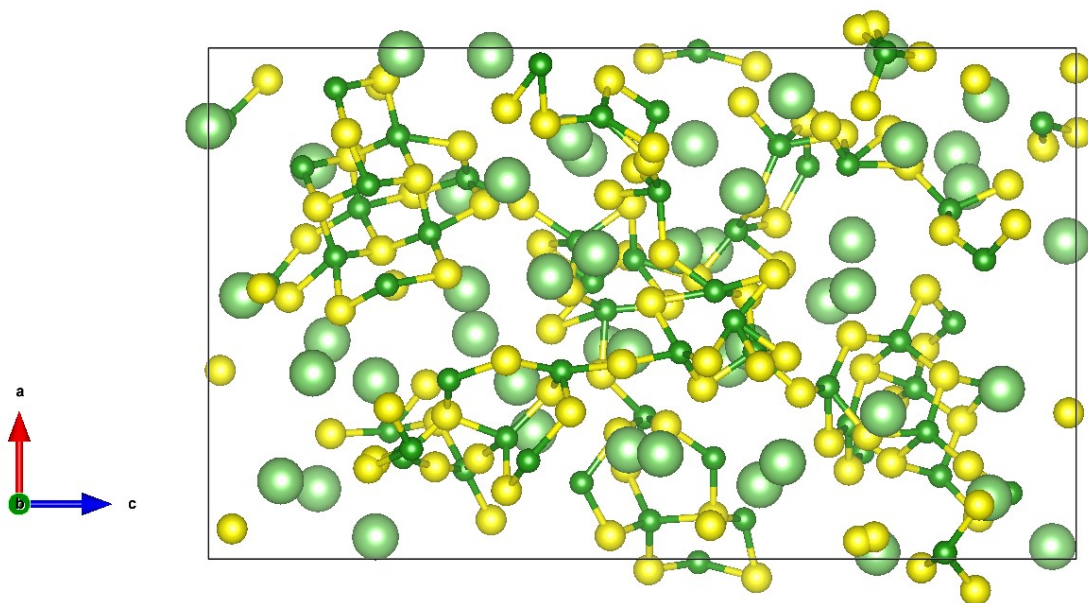


Table 9. Data File for Li3BS3 Crystal. Li charges were scaled to +.5.

Created by /net/hulk/home3/tpascal/scripts/createLammpsInput.pl on Thu May 12 13:46:48 2022

500 atoms
216 bonds
216 angles
0 dihedrals
0 impropers
3 atom types
1 bond types
1 angle types
0 dihedral types
0 improper types
0.000000 18.123460 xlo xhi
0.000000 23.878760 ylo yhi
0.000000 19.791240 zlo zhi

Masses

1 6.9410E+00 # Li
2 1.0810E+01 # B_2
3 3.2060E+01 # S_3+6

Pair Coeffs

1 0.02500000 3.20002089 # Li Li
2 0.18000001 2.29053963 # B_2 B_2
3 0.27399999 2.55088067 # S_3+6 S_3+6

Bond Coeffs

1 234.939 1.8557 # S_3+6 B_2

Angle Coeffs

1 241.304 120.00000 # S_3+6 B_2 S_3+6

Atoms

1 444 1 0.50000000 3.58406 5.37550 19.72071 0 0 0
2 444 1 0.50000000 3.58406 13.33509 9.82509 0 0 0
3 444 1 0.50000000 3.58406 13.33509 19.72071 0 0 0
4 444 1 0.50000000 3.58406 5.37550 9.82509 0 0 0

5	444	1	0.50000000	3.58406	21.29468	19.72071	0	0	0
6	444	1	0.50000000	9.62522	5.37550	9.82509	0	0	0
7	444	1	0.50000000	9.62522	13.33509	9.82509	0	0	0
8	444	1	0.50000000	9.62522	13.33509	19.72071	0	0	0
9	444	1	0.50000000	9.62522	21.29468	9.82509	0	0	0
10	444	1	0.50000000	9.62522	21.29468	19.72071	0	0	0
11	444	1	0.50000000	15.66637	5.37550	9.82509	0	0	0
12	444	1	0.50000000	0.56349	6.56387	0.07053	0	0	0
13	444	1	0.50000000	15.66637	13.33509	19.72071	0	0	0
14	444	1	0.50000000	15.66637	21.29468	9.82509	0	0	0
15	444	1	0.50000000	15.66637	21.29468	19.72071	0	0	0
16	444	1	0.50000000	0.56349	6.56387	9.96615	0	0	0
17	444	1	0.50000000	0.56349	14.52346	0.07053	0	0	0
18	444	1	0.50000000	0.56349	14.52346	9.96615	0	0	0
19	444	1	0.50000000	0.56349	22.48305	0.07053	0	0	0
20	444	1	0.50000000	0.56349	22.48305	9.96615	0	0	0
21	444	1	0.50000000	6.60464	6.56387	0.07053	0	0	0
22	444	1	0.50000000	6.60464	6.56387	9.96615	0	0	0
23	444	1	0.50000000	6.60464	14.52346	0.07053	0	0	0
24	444	1	0.50000000	6.60464	14.52346	9.96615	0	0	0
25	444	1	0.50000000	6.60464	22.48305	0.07053	0	0	0
26	444	1	0.50000000	6.60464	22.48305	9.96615	0	0	0
27	444	1	0.50000000	12.64579	6.56387	0.07053	0	0	0
28	444	1	0.50000000	12.64579	6.56387	9.96615	0	0	0
29	444	1	0.50000000	12.64579	14.52346	0.07053	0	0	0
30	444	1	0.50000000	12.64579	14.52346	9.96615	0	0	0
31	444	1	0.50000000	12.64579	22.48305	0.07053	0	0	0
32	444	1	0.50000000	12.64579	22.48305	9.96615	0	0	0
33	444	1	0.50000000	5.47767	1.39571	5.01834	0	0	0
34	444	1	0.50000000	5.47767	1.39571	14.91397	0	0	0
35	444	1	0.50000000	5.47767	9.35530	5.01834	0	0	0
36	444	1	0.50000000	5.47767	9.35530	14.91397	0	0	0
37	444	1	0.50000000	5.47767	17.31488	5.01834	0	0	0

38	444	1	0.50000000	5.47767	17.31488	14.91397	0	0	0
39	444	1	0.50000000	11.51882	1.39571	5.01834	0	0	0
40	444	1	0.50000000	11.51882	1.39571	14.91397	0	0	0
41	444	1	0.50000000	11.51882	9.35530	5.01834	0	0	0
42	444	1	0.50000000	11.51882	9.35530	14.91397	0	0	0
43	444	1	0.50000000	11.51882	17.31488	5.01834	0	0	0
44	444	1	0.50000000	11.51882	17.31488	14.91397	0	0	0
45	444	1	0.50000000	17.55997	1.39571	5.01834	0	0	0
46	444	1	0.50000000	17.55997	1.39571	14.91397	0	0	0
47	444	1	0.50000000	17.55997	9.35530	5.01834	0	0	0
48	444	1	0.50000000	17.55997	9.35530	14.91397	0	0	0
49	444	1	0.50000000	17.55997	17.31488	5.01834	0	0	0
50	444	1	0.50000000	17.55997	17.31488	14.91397	0	0	0
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52	444	1	0.50000000	2.45709	2.58408	14.77290	0	0	0
53	444	1	0.50000000	2.45709	10.54367	4.87728	0	0	0
54	444	1	0.50000000	2.45709	10.54367	14.77290	0	0	0
55	444	1	0.50000000	2.45709	18.50325	4.87728	0	0	0
56	444	1	0.50000000	2.45709	18.50325	14.77290	0	0	0
57	444	1	0.50000000	8.49824	2.58408	4.87728	0	0	0
58	444	1	0.50000000	8.49824	2.58408	14.77290	0	0	0
59	444	1	0.50000000	8.49824	10.54367	4.87728	0	0	0
60	444	1	0.50000000	8.49824	10.54367	14.77290	0	0	0
61	444	1	0.50000000	8.49824	18.50325	4.87728	0	0	0
62	444	1	0.50000000	8.49824	18.50325	14.77290	0	0	0
63	444	1	0.50000000	14.53940	2.58408	4.87728	0	0	0
64	444	1	0.50000000	14.53940	2.58408	14.77290	0	0	0
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66	444	1	0.50000000	14.53940	10.54367	14.77290	0	0	0
67	444	1	0.50000000	14.53940	18.50325	4.87728	0	0	0
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71	444	1	0.50000000	2.45709	10.54367	0.07053	0	0	0
72	444	1	0.50000000	2.45709	10.54367	9.96615	0	0	0
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75	444	1	0.50000000	8.49824	2.58408	0.07053	0	0	0
76	444	1	0.50000000	8.49824	2.58408	9.96615	0	0	0
77	444	1	0.50000000	8.49824	10.54367	0.07053	0	0	0
78	444	1	0.50000000	8.49824	10.54367	9.96615	0	0	0
79	444	1	0.50000000	8.49824	18.50325	0.07053	0	0	0
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81	444	1	0.50000000	14.53940	2.58408	0.07053	0	0	0
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85	444	1	0.50000000	14.53940	18.50325	0.07053	0	0	0
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87	444	1	0.50000000	5.47767	1.39571	9.82509	0	0	0
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89	444	1	0.50000000	5.47767	9.35530	9.82509	0	0	0
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91	444	1	0.50000000	5.47767	17.31488	9.82509	0	0	0
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95	444	1	0.50000000	11.51882	9.35530	9.82509	0	0	0
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97	444	1	0.50000000	11.51882	17.31488	9.82509	0	0	0
98	444	1	0.50000000	11.51882	17.31488	19.72071	0	0	0
99	444	1	0.50000000	17.55997	1.39571	9.82509	0	0	0
100	444	1	0.50000000	17.55997	1.39571	19.72071	0	0	0
101	444	1	0.50000000	17.55997	9.35530	9.82509	0	0	0
102	444	1	0.50000000	17.55997	9.35530	19.72071	0	0	0
103	444	1	0.50000000	17.55997	17.31488	9.82509	0	0	0

104	444	1	0.50000000	17.55997	17.31488	19.72071	0	0	0
105	444	1	0.50000000	0.56349	6.56387	4.87728	0	0	0
106	444	1	0.50000000	0.56349	6.56387	14.77290	0	0	0
107	444	1	0.50000000	0.56349	14.52346	4.87728	0	0	0
108	444	1	0.50000000	0.56349	14.52346	14.77290	0	0	0
109	444	1	0.50000000	0.56349	22.48305	4.87728	0	0	0
110	444	1	0.50000000	0.56349	22.48305	14.77290	0	0	0
111	444	1	0.50000000	6.60464	6.56387	4.87728	0	0	0
112	444	1	0.50000000	6.60464	6.56387	14.77290	0	0	0
113	444	1	0.50000000	6.60464	14.52346	4.87728	0	0	0
114	444	1	0.50000000	6.60464	14.52346	14.77290	0	0	0
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119	444	1	0.50000000	12.64579	14.52346	4.87728	0	0	0
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121	444	1	0.50000000	12.64579	22.48305	4.87728	0	0	0
122	444	1	0.50000000	12.64579	22.48305	14.77290	0	0	0
123	444	1	0.50000000	3.58406	5.37550	5.01834	0	0	0
124	444	1	0.50000000	3.58406	5.37550	14.91397	0	0	0
125	444	1	0.50000000	3.58406	13.33509	5.01834	0	0	0
126	444	1	0.50000000	3.58406	13.33509	14.91397	0	0	0
127	444	1	0.50000000	3.58406	21.29468	5.01834	0	0	0
128	444	1	0.50000000	3.58406	21.29468	14.91397	0	0	0
129	444	1	0.50000000	9.62522	5.37550	5.01834	0	0	0
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131	444	1	0.50000000	9.62522	13.33509	5.01834	0	0	0
132	444	1	0.50000000	9.62522	13.33509	14.91397	0	0	0
133	444	1	0.50000000	9.62522	21.29468	5.01834	0	0	0
134	444	1	0.50000000	9.62522	21.29468	14.91397	0	0	0
135	444	1	0.50000000	15.66637	5.37550	5.01834	0	0	0
136	444	1	0.50000000	15.66637	5.37550	14.91397	0	0	0

137	444	1	0.50000000	15.66637	13.33509	5.01834	0	0	0
138	444	1	0.50000000	15.66637	13.33509	14.91397	0	0	0
139	444	1	0.50000000	15.66637	21.29468	5.01834	0	0	0
140	444	1	0.50000000	15.66637	21.29468	14.91397	0	0	0
141	444	1	0.50000000	3.33629	7.90485	7.42172	0	0	0
142	444	1	0.50000000	3.33629	7.90485	17.31734	0	0	0
143	444	1	0.50000000	3.33629	15.86444	7.42172	0	0	0
144	444	1	0.50000000	3.33629	15.86444	17.31734	0	0	0
145	444	1	0.50000000	3.33629	23.82402	7.42172	0	0	0
146	444	1	0.50000000	3.33629	23.82402	17.31734	0	0	0
147	444	1	0.50000000	9.37745	7.90485	7.42172	0	0	0
148	444	1	0.50000000	9.37745	7.90485	17.31734	0	0	0
149	444	1	0.50000000	9.37745	15.86444	7.42172	0	0	0
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155	444	1	0.50000000	15.41860	15.86444	7.42172	0	0	0
156	444	1	0.50000000	15.41860	15.86444	17.31734	0	0	0
157	444	1	0.50000000	15.41860	23.82402	7.42172	0	0	0
158	444	1	0.50000000	15.41860	23.82402	17.31734	0	0	0
159	444	1	0.50000000	0.31572	4.03453	2.47391	0	0	0
160	444	1	0.50000000	0.31572	4.03453	12.36953	0	0	0
161	444	1	0.50000000	0.31572	11.99411	2.47391	0	0	0
162	444	1	0.50000000	0.31572	11.99411	12.36953	0	0	0
163	444	1	0.50000000	0.31572	19.95370	2.47391	0	0	0
164	444	1	0.50000000	0.31572	19.95370	12.36953	0	0	0
165	444	1	0.50000000	6.35687	4.03453	2.47391	0	0	0
166	444	1	0.50000000	6.35687	4.03453	12.36953	0	0	0
167	444	1	0.50000000	6.35687	11.99411	2.47391	0	0	0
168	444	1	0.50000000	6.35687	11.99411	12.36953	0	0	0
169	444	1	0.50000000	6.35687	19.95370	2.47391	0	0	0

170	444	1	0.50000000	6.35687	19.95370	12.36953	0	0	0
171	444	1	0.50000000	12.39802	4.03453	2.47391	0	0	0
172	444	1	0.50000000	12.39802	4.03453	12.36953	0	0	0
173	444	1	0.50000000	12.39802	11.99411	2.47391	0	0	0
174	444	1	0.50000000	12.39802	11.99411	12.36953	0	0	0
175	444	1	0.50000000	12.39802	19.95370	2.47391	0	0	0
176	444	1	0.50000000	12.39802	19.95370	12.36953	0	0	0
177	444	1	0.50000000	5.72544	3.92506	7.42172	0	0	0
178	444	1	0.50000000	5.72544	3.92506	17.31734	0	0	0
179	444	1	0.50000000	5.72544	11.88464	7.42172	0	0	0
180	444	1	0.50000000	5.72544	11.88464	17.31734	0	0	0
181	444	1	0.50000000	5.72544	19.84423	7.42172	0	0	0
182	444	1	0.50000000	5.72544	19.84423	17.31734	0	0	0
183	444	1	0.50000000	11.76659	3.92506	7.42172	0	0	0
184	444	1	0.50000000	11.76659	3.92506	17.31734	0	0	0
185	444	1	0.50000000	11.76659	11.88464	7.42172	0	0	0
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187	444	1	0.50000000	11.76659	19.84423	7.42172	0	0	0
188	444	1	0.50000000	11.76659	19.84423	17.31734	0	0	0
189	444	1	0.50000000	17.80774	3.92506	7.42172	0	0	0
190	444	1	0.50000000	17.80774	3.92506	17.31734	0	0	0
191	444	1	0.50000000	17.80774	11.88464	7.42172	0	0	0
192	444	1	0.50000000	17.80774	11.88464	17.31734	0	0	0
193	444	1	0.50000000	17.80774	19.84423	7.42172	0	0	0
194	444	1	0.50000000	17.80774	19.84423	17.31734	0	0	0
195	444	1	0.50000000	2.70486	0.05474	2.47391	0	0	0
196	444	1	0.50000000	2.70486	0.05474	12.36953	0	0	0
197	444	1	0.50000000	2.70486	8.01432	2.47391	0	0	0
198	444	1	0.50000000	2.70486	8.01432	12.36953	0	0	0
199	444	1	0.50000000	2.70486	15.97391	2.47391	0	0	0
200	444	1	0.50000000	2.70486	15.97391	12.36953	0	0	0
201	444	1	0.50000000	8.74601	0.05474	2.47391	0	0	0
202	444	1	0.50000000	8.74601	0.05474	12.36953	0	0	0

203	444	1	0.50000000	8.74601	8.01432	2.47391	0	0	0
204	444	1	0.50000000	8.74601	8.01432	12.36953	0	0	0
205	444	1	0.50000000	8.74601	15.97391	2.47391	0	0	0
206	444	1	0.50000000	8.74601	15.97391	12.36953	0	0	0
207	444	1	0.50000000	14.78717	0.05474	2.47391	0	0	0
208	444	1	0.50000000	14.78717	0.05474	12.36953	0	0	0
209	444	1	0.50000000	14.78717	8.01432	2.47391	0	0	0
210	444	1	0.50000000	14.78717	8.01432	12.36953	0	0	0
211	444	1	0.50000000	14.78717	15.97391	2.47391	0	0	0
212	444	1	0.50000000	14.78717	15.97391	12.36953	0	0	0
213	444	2	0.32142857	5.32390	7.04421	2.47391	0	0	0
214	444	2	0.32142857	5.32390	7.04421	12.36953	0	0	0
215	444	2	0.32142857	5.32390	15.00379	2.47391	0	0	0
216	444	2	0.32142857	5.32390	15.00379	12.36953	0	0	0
217	444	2	0.32142857	5.32390	22.96338	2.47391	0	0	0
218	444	2	0.32142857	5.32390	22.96338	12.36953	0	0	0
219	444	2	0.32142857	11.36505	7.04421	2.47391	0	0	0
220	444	2	0.32142857	11.36505	7.04421	12.36953	0	0	0
221	444	2	0.32142857	11.36505	15.00379	2.47391	0	0	0
222	444	2	0.32142857	11.36505	15.00379	12.36953	0	0	0
223	444	2	0.32142857	11.36505	22.96338	2.47391	0	0	0
224	444	2	0.32142857	11.36505	22.96338	12.36953	0	0	0
225	444	2	0.32142857	17.40620	7.04421	2.47391	0	0	0
226	444	2	0.32142857	17.40620	7.04421	12.36953	0	0	0
227	444	2	0.32142857	17.40620	15.00379	2.47391	0	0	0
228	444	2	0.32142857	17.40620	15.00379	12.36953	0	0	0
229	444	2	0.32142857	17.40620	22.96338	2.47391	0	0	0
230	444	2	0.32142857	17.40620	22.96338	12.36953	0	0	0
231	444	2	0.32142857	2.30332	4.89517	7.42172	0	0	0
232	444	2	0.32142857	2.30332	4.89517	17.31734	0	0	0
233	444	2	0.32142857	2.30332	12.85476	7.42172	0	0	0
234	444	2	0.32142857	2.30332	12.85476	17.31734	0	0	0
235	444	2	0.32142857	2.30332	20.81434	7.42172	0	0	0

236	444	2	0.32142857	2.30332	20.81434	17.31734	0	0	0
237	444	2	0.32142857	8.34447	4.89517	7.42172	0	0	0
238	444	2	0.32142857	8.34447	4.89517	17.31734	0	0	0
239	444	2	0.32142857	8.34447	12.85476	7.42172	0	0	0
240	444	2	0.32142857	8.34447	12.85476	17.31734	0	0	0
241	444	2	0.32142857	8.34447	20.81434	7.42172	0	0	0
242	444	2	0.32142857	8.34447	20.81434	17.31734	0	0	0
243	444	2	0.32142857	14.38563	4.89517	7.42172	0	0	0
244	444	2	0.32142857	14.38563	4.89517	17.31734	0	0	0
245	444	2	0.32142857	14.38563	12.85476	7.42172	0	0	0
246	444	2	0.32142857	14.38563	12.85476	17.31734	0	0	0
247	444	2	0.32142857	14.38563	20.81434	7.42172	0	0	0
248	444	2	0.32142857	14.38563	20.81434	17.31734	0	0	0
249	444	2	0.32142857	3.73783	3.06441	2.47391	0	0	0
250	444	2	0.32142857	3.73783	3.06441	12.36953	0	0	0
251	444	2	0.32142857	3.73783	11.02400	2.47391	0	0	0
252	444	2	0.32142857	3.73783	11.02400	12.36953	0	0	0
253	444	2	0.32142857	3.73783	18.98359	2.47391	0	0	0
254	444	2	0.32142857	3.73783	18.98359	12.36953	0	0	0
255	444	2	0.32142857	9.77898	3.06441	2.47391	0	0	0
256	444	2	0.32142857	9.77898	3.06441	12.36953	0	0	0
257	444	2	0.32142857	9.77898	11.02400	2.47391	0	0	0
258	444	2	0.32142857	9.77898	11.02400	12.36953	0	0	0
259	444	2	0.32142857	9.77898	18.98359	2.47391	0	0	0
260	444	2	0.32142857	9.77898	18.98359	12.36953	0	0	0
261	444	2	0.32142857	15.82014	3.06441	2.47391	0	0	0
262	444	2	0.32142857	15.82014	3.06441	12.36953	0	0	0
263	444	2	0.32142857	15.82014	11.02400	2.47391	0	0	0
264	444	2	0.32142857	15.82014	11.02400	12.36953	0	0	0
265	444	2	0.32142857	15.82014	18.98359	2.47391	0	0	0
266	444	2	0.32142857	15.82014	18.98359	12.36953	0	0	0
267	444	2	0.32142857	0.71725	0.91538	7.42172	0	0	0
268	444	2	0.32142857	0.71725	0.91538	17.31734	0	0	0

269	444	2	0.32142857	0.71725	8.87496	7.42172	0	0	0
270	444	2	0.32142857	0.71725	8.87496	17.31734	0	0	0
271	444	2	0.32142857	0.71725	16.83455	7.42172	0	0	0
272	444	2	0.32142857	0.71725	16.83455	17.31734	0	0	0
273	444	2	0.32142857	6.75841	0.91538	7.42172	0	0	0
274	444	2	0.32142857	6.75841	0.91538	17.31734	0	0	0
275	444	2	0.32142857	6.75841	8.87496	7.42172	0	0	0
276	444	2	0.32142857	6.75841	8.87496	17.31734	0	0	0
277	444	2	0.32142857	6.75841	16.83455	7.42172	0	0	0
278	444	2	0.32142857	6.75841	16.83455	17.31734	0	0	0
279	444	2	0.32142857	12.79956	0.91538	7.42172	0	0	0
280	444	2	0.32142857	12.79956	0.91538	17.31734	0	0	0
281	444	2	0.32142857	12.79956	8.87496	7.42172	0	0	0
282	444	2	0.32142857	12.79956	8.87496	17.31734	0	0	0
283	444	2	0.32142857	12.79956	16.83455	7.42172	0	0	0
284	444	2	0.32142857	12.79956	16.83455	17.31734	0	0	0
285	444	3	-0.60714286	4.45319	7.39179	0.90526	0	0	0
286	444	3	-0.60714286	4.45319	7.39179	10.80088	0	0	0
287	444	3	-0.60714286	4.45319	15.35138	0.90526	0	0	0
288	444	3	-0.60714286	4.45319	15.35138	10.80088	0	0	0
289	444	3	-0.60714286	4.45319	23.31097	0.90526	0	0	0
290	444	3	-0.60714286	4.45319	23.31097	10.80088	0	0	0
291	444	3	-0.60714286	10.49434	7.39179	0.90526	0	0	0
292	444	3	-0.60714286	10.49434	7.39179	10.80088	0	0	0
293	444	3	-0.60714286	10.49434	15.35138	0.90526	0	0	0
294	444	3	-0.60714286	10.49434	15.35138	10.80088	0	0	0
295	444	3	-0.60714286	10.49434	23.31097	0.90526	0	0	0
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297	444	3	-0.60714286	16.53549	7.39179	0.90526	0	0	0
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303	444	3	-0.60714286	1.43261	4.54758	8.99036	0	0	0
304	444	3	-0.60714286	1.43261	4.54758	18.88598	0	0	0
305	444	3	-0.60714286	1.43261	12.50717	8.99036	0	0	0
306	444	3	-0.60714286	1.43261	12.50717	18.88598	0	0	0
307	444	3	-0.60714286	1.43261	20.46676	8.99036	0	0	0
308	444	3	-0.60714286	1.43261	20.46676	18.88598	0	0	0
309	444	3	-0.60714286	7.47376	4.54758	8.99036	0	0	0
310	444	3	-0.60714286	7.47376	4.54758	18.88598	0	0	0
311	444	3	-0.60714286	7.47376	12.50717	8.99036	0	0	0
312	444	3	-0.60714286	7.47376	12.50717	18.88598	0	0	0
313	444	3	-0.60714286	7.47376	20.46676	8.99036	0	0	0
314	444	3	-0.60714286	7.47376	20.46676	18.88598	0	0	0
315	444	3	-0.60714286	13.51492	4.54758	8.99036	0	0	0
316	444	3	-0.60714286	13.51492	4.54758	18.88598	0	0	0
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321	444	3	-0.60714286	4.60854	3.41200	4.04255	0	0	0
322	444	3	-0.60714286	4.60854	3.41200	13.93817	0	0	0
323	444	3	-0.60714286	4.60854	11.37159	4.04255	0	0	0
324	444	3	-0.60714286	4.60854	11.37159	13.93817	0	0	0
325	444	3	-0.60714286	4.60854	19.33117	4.04255	0	0	0
326	444	3	-0.60714286	4.60854	19.33117	13.93817	0	0	0
327	444	3	-0.60714286	10.64970	3.41200	4.04255	0	0	0
328	444	3	-0.60714286	10.64970	3.41200	13.93817	0	0	0
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330	444	3	-0.60714286	10.64970	11.37159	13.93817	0	0	0
331	444	3	-0.60714286	10.64970	19.33117	4.04255	0	0	0
332	444	3	-0.60714286	10.64970	19.33117	13.93817	0	0	0
333	444	3	-0.60714286	16.69085	3.41200	4.04255	0	0	0
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335	444	3	-0.60714286	16.69085	11.37159	4.04255	0	0	0
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337	444	3	-0.60714286	16.69085	19.33117	4.04255	0	0	0
338	444	3	-0.60714286	16.69085	19.33117	13.93817	0	0	0
339	444	3	-0.60714286	1.58797	0.56779	5.85307	0	0	0
340	444	3	-0.60714286	1.58797	0.56779	15.74869	0	0	0
341	444	3	-0.60714286	1.58797	8.52738	5.85307	0	0	0
342	444	3	-0.60714286	1.58797	8.52738	15.74869	0	0	0
343	444	3	-0.60714286	1.58797	16.48696	5.85307	0	0	0
344	444	3	-0.60714286	1.58797	16.48696	15.74869	0	0	0
345	444	3	-0.60714286	7.62912	0.56779	5.85307	0	0	0
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347	444	3	-0.60714286	7.62912	8.52738	5.85307	0	0	0
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353	444	3	-0.60714286	13.67027	8.52738	5.85307	0	0	0
354	444	3	-0.60714286	13.67027	8.52738	15.74869	0	0	0
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356	444	3	-0.60714286	13.67027	16.48696	15.74869	0	0	0
357	444	3	-0.60714286	1.58797	0.56779	8.99036	0	0	0
358	444	3	-0.60714286	1.58797	0.56779	18.88598	0	0	0
359	444	3	-0.60714286	1.58797	8.52738	8.99036	0	0	0
360	444	3	-0.60714286	1.58797	8.52738	18.88598	0	0	0
361	444	3	-0.60714286	1.58797	16.48696	8.99036	0	0	0
362	444	3	-0.60714286	1.58797	16.48696	18.88598	0	0	0
363	444	3	-0.60714286	7.62912	0.56779	8.99036	0	0	0
364	444	3	-0.60714286	7.62912	0.56779	18.88598	0	0	0
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367	444	3	-0.60714286	7.62912	16.48696	8.99036	0	0	0

368	444	3	-0.60714286	7.62912	16.48696	18.88598	0	0	0
369	444	3	-0.60714286	13.67027	0.56779	8.99036	0	0	0
370	444	3	-0.60714286	13.67027	0.56779	18.88598	0	0	0
371	444	3	-0.60714286	13.67027	8.52738	8.99036	0	0	0
372	444	3	-0.60714286	13.67027	8.52738	18.88598	0	0	0
373	444	3	-0.60714286	13.67027	16.48696	8.99036	0	0	0
374	444	3	-0.60714286	13.67027	16.48696	18.88598	0	0	0
375	444	3	-0.60714286	4.60854	3.41200	0.90526	0	0	0
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377	444	3	-0.60714286	4.60854	11.37159	0.90526	0	0	0
378	444	3	-0.60714286	4.60854	11.37159	10.80088	0	0	0
379	444	3	-0.60714286	4.60854	19.33117	0.90526	0	0	0
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389	444	3	-0.60714286	16.69085	11.37159	0.90526	0	0	0
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393	444	3	-0.60714286	1.43261	4.54758	5.85307	0	0	0
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395	444	3	-0.60714286	1.43261	12.50717	5.85307	0	0	0
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397	444	3	-0.60714286	1.43261	20.46676	5.85307	0	0	0
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401	444	3	-0.60714286	7.47376	12.50717	5.85307	0	0	0
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405	444	3	-0.60714286	13.51492	4.54758	5.85307	0	0	0
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411	444	3	-0.60714286	4.45319	7.39179	4.04255	0	0	0
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414	444	3	-0.60714286	4.45319	15.35138	13.93817	0	0	0
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429	444	3	-0.60714286	5.06558	1.61201	7.42172	0	0	0
430	444	3	-0.60714286	5.06558	1.61201	17.31734	0	0	0
431	444	3	-0.60714286	5.06558	9.57160	7.42172	0	0	0
432	444	3	-0.60714286	5.06558	9.57160	17.31734	0	0	0
433	444	3	-0.60714286	5.06558	17.53119	7.42172	0	0	0

434	444	3	-0.60714286	5.06558	17.53119	17.31734	0	0	0
435	444	3	-0.60714286	11.10673	1.61201	7.42172	0	0	0
436	444	3	-0.60714286	11.10673	1.61201	17.31734	0	0	0
437	444	3	-0.60714286	11.10673	9.57160	7.42172	0	0	0
438	444	3	-0.60714286	11.10673	9.57160	17.31734	0	0	0
439	444	3	-0.60714286	11.10673	17.53119	7.42172	0	0	0
440	444	3	-0.60714286	11.10673	17.53119	17.31734	0	0	0
441	444	3	-0.60714286	17.14789	1.61201	7.42172	0	0	0
442	444	3	-0.60714286	17.14789	1.61201	17.31734	0	0	0
443	444	3	-0.60714286	17.14789	9.57160	7.42172	0	0	0
444	444	3	-0.60714286	17.14789	9.57160	17.31734	0	0	0
445	444	3	-0.60714286	17.14789	17.53119	7.42172	0	0	0
446	444	3	-0.60714286	17.14789	17.53119	17.31734	0	0	0
447	444	3	-0.60714286	2.04500	2.36778	2.47391	0	0	0
448	444	3	-0.60714286	2.04500	2.36778	12.36953	0	0	0
449	444	3	-0.60714286	2.04500	10.32736	2.47391	0	0	0
450	444	3	-0.60714286	2.04500	10.32736	12.36953	0	0	0
451	444	3	-0.60714286	2.04500	18.28695	2.47391	0	0	0
452	444	3	-0.60714286	2.04500	18.28695	12.36953	0	0	0
453	444	3	-0.60714286	8.08616	2.36778	2.47391	0	0	0
454	444	3	-0.60714286	8.08616	2.36778	12.36953	0	0	0
455	444	3	-0.60714286	8.08616	10.32736	2.47391	0	0	0
456	444	3	-0.60714286	8.08616	10.32736	12.36953	0	0	0
457	444	3	-0.60714286	8.08616	18.28695	2.47391	0	0	0
458	444	3	-0.60714286	8.08616	18.28695	12.36953	0	0	0
459	444	3	-0.60714286	14.12731	2.36778	2.47391	0	0	0
460	444	3	-0.60714286	14.12731	2.36778	12.36953	0	0	0
461	444	3	-0.60714286	14.12731	10.32736	2.47391	0	0	0
462	444	3	-0.60714286	14.12731	10.32736	12.36953	0	0	0
463	444	3	-0.60714286	14.12731	18.28695	2.47391	0	0	0
464	444	3	-0.60714286	14.12731	18.28695	12.36953	0	0	0
465	444	3	-0.60714286	3.99615	5.59181	7.42172	0	0	0
466	444	3	-0.60714286	3.99615	5.59181	17.31734	0	0	0

467	444	3	-0.60714286	3.99615	13.55139	7.42172	0	0	0
468	444	3	-0.60714286	3.99615	13.55139	17.31734	0	0	0
469	444	3	-0.60714286	3.99615	21.51098	7.42172	0	0	0
470	444	3	-0.60714286	3.99615	21.51098	17.31734	0	0	0
471	444	3	-0.60714286	10.03730	5.59181	7.42172	0	0	0
472	444	3	-0.60714286	10.03730	5.59181	17.31734	0	0	0
473	444	3	-0.60714286	10.03730	13.55139	7.42172	0	0	0
474	444	3	-0.60714286	10.03730	13.55139	17.31734	0	0	0
475	444	3	-0.60714286	10.03730	21.51098	7.42172	0	0	0
476	444	3	-0.60714286	10.03730	21.51098	17.31734	0	0	0
477	444	3	-0.60714286	16.07846	5.59181	7.42172	0	0	0
478	444	3	-0.60714286	16.07846	5.59181	17.31734	0	0	0
479	444	3	-0.60714286	16.07846	13.55139	7.42172	0	0	0
480	444	3	-0.60714286	16.07846	13.55139	17.31734	0	0	0
481	444	3	-0.60714286	16.07846	21.51098	7.42172	0	0	0
482	444	3	-0.60714286	16.07846	21.51098	17.31734	0	0	0
483	444	3	-0.60714286	0.97557	6.34757	2.47391	0	0	0
484	444	3	-0.60714286	0.97557	6.34757	12.36953	0	0	0
485	444	3	-0.60714286	0.97557	14.30716	2.47391	0	0	0
486	444	3	-0.60714286	0.97557	14.30716	12.36953	0	0	0
487	444	3	-0.60714286	0.97557	22.26674	2.47391	0	0	0
488	444	3	-0.60714286	0.97557	22.26674	12.36953	0	0	0
489	444	3	-0.60714286	7.01673	6.34757	2.47391	0	0	0
490	444	3	-0.60714286	7.01673	6.34757	12.36953	0	0	0
491	444	3	-0.60714286	7.01673	14.30716	2.47391	0	0	0
492	444	3	-0.60714286	7.01673	14.30716	12.36953	0	0	0
493	444	3	-0.60714286	7.01673	22.26674	2.47391	0	0	0
494	444	3	-0.60714286	7.01673	22.26674	12.36953	0	0	0
495	444	3	-0.60714286	13.05788	6.34757	2.47391	0	0	0
496	444	3	-0.60714286	13.05788	6.34757	12.36953	0	0	0
497	444	3	-0.60714286	13.05788	14.30716	2.47391	0	0	0
498	444	3	-0.60714286	13.05788	14.30716	12.36953	0	0	0
499	444	3	-0.60714286	13.05788	22.26674	2.47391	0	0	0

500 444 3 -0.60714286 13.05788 22.26674 12.36953 0 0 0

Bonds

1	1	213	285
2	1	213	411
3	1	213	489
4	1	214	286
5	1	214	412
6	1	214	490
7	1	215	287
8	1	215	413
9	1	215	491
10	1	216	288
11	1	216	414
12	1	216	492
13	1	217	289
14	1	217	415
15	1	217	493
16	1	218	290
17	1	218	416
18	1	218	494
19	1	219	291
20	1	219	417
21	1	219	495
22	1	220	292
23	1	220	418
24	1	220	496
25	1	221	293
26	1	221	419
27	1	221	497
28	1	222	294
29	1	222	420
30	1	222	498

31	1	223	295
32	1	223	421
33	1	223	499
34	1	224	296
35	1	224	422
36	1	224	500
37	1	225	297
38	1	225	423
39	1	225	483
40	1	226	298
41	1	226	424
42	1	226	484
43	1	227	299
44	1	227	425
45	1	227	485
46	1	228	300
47	1	228	426
48	1	228	486
49	1	229	301
50	1	229	427
51	1	229	487
52	1	230	302
53	1	230	428
54	1	230	488
55	1	231	303
56	1	231	393
57	1	231	465
58	1	232	304
59	1	232	394
60	1	232	466
61	1	233	305
62	1	233	395
63	1	233	467

64	1	234	306
65	1	234	396
66	1	234	468
67	1	235	307
68	1	235	397
69	1	235	469
70	1	236	308
71	1	236	398
72	1	236	470
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75	1	237	471
76	1	238	310
77	1	238	400
78	1	238	472
79	1	239	311
80	1	239	401
81	1	239	473
82	1	240	312
83	1	240	402
84	1	240	474
85	1	241	313
86	1	241	403
87	1	241	475
88	1	242	314
89	1	242	404
90	1	242	476
91	1	243	315
92	1	243	405
93	1	243	477
94	1	244	316
95	1	244	406
96	1	244	478

97	1	245	317
98	1	245	407
99	1	245	479
100	1	246	318
101	1	246	408
102	1	246	480
103	1	247	319
104	1	247	409
105	1	247	481
106	1	248	320
107	1	248	410
108	1	248	482
109	1	249	321
110	1	249	375
111	1	249	447
112	1	250	322
113	1	250	376
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117	1	251	449
118	1	252	324
119	1	252	378
120	1	252	450
121	1	253	325
122	1	253	379
123	1	253	451
124	1	254	326
125	1	254	380
126	1	254	452
127	1	255	327
128	1	255	381
129	1	255	453

130	1	256	328
131	1	256	382
132	1	256	454
133	1	257	329
134	1	257	383
135	1	257	455
136	1	258	330
137	1	258	384
138	1	258	456
139	1	259	331
140	1	259	385
141	1	259	457
142	1	260	332
143	1	260	386
144	1	260	458
145	1	261	333
146	1	261	387
147	1	261	459
148	1	262	334
149	1	262	388
150	1	262	460
151	1	263	335
152	1	263	389
153	1	263	461
154	1	264	336
155	1	264	390
156	1	264	462
157	1	265	337
158	1	265	391
159	1	265	463
160	1	266	338
161	1	266	392
162	1	266	464

163	1	267	339
164	1	267	357
165	1	267	441
166	1	268	340
167	1	268	358
168	1	268	442
169	1	269	341
170	1	269	359
171	1	269	443
172	1	270	342
173	1	270	360
174	1	270	444
175	1	271	343
176	1	271	361
177	1	271	445
178	1	272	344
179	1	272	362
180	1	272	446
181	1	273	345
182	1	273	363
183	1	273	429
184	1	274	346
185	1	274	364
186	1	274	430
187	1	275	347
188	1	275	365
189	1	275	431
190	1	276	348
191	1	276	366
192	1	276	432
193	1	277	349
194	1	277	367
195	1	277	433

196	1	278	350
197	1	278	368
198	1	278	434
199	1	279	351
200	1	279	369
201	1	279	435
202	1	280	352
203	1	280	370
204	1	280	436
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206	1	281	371
207	1	281	437
208	1	282	354
209	1	282	372
210	1	282	438
211	1	283	355
212	1	283	373
213	1	283	439
214	1	284	356
215	1	284	374
216	1	284	440

Angles

1	1	357	267	339
2	1	358	268	340
3	1	359	269	341
4	1	360	270	342
5	1	361	271	343
6	1	362	272	344
7	1	363	273	345
8	1	364	274	346
9	1	365	275	347
10	1	366	276	348
11	1	367	277	349

12	1	368	278	350
13	1	369	279	351
14	1	370	280	352
15	1	371	281	353
16	1	372	282	354
17	1	373	283	355
18	1	374	284	356
19	1	375	249	321
20	1	376	250	322
21	1	377	251	323
22	1	378	252	324
23	1	379	253	325
24	1	380	254	326
25	1	381	255	327
26	1	382	256	328
27	1	383	257	329
28	1	384	258	330
29	1	385	259	331
30	1	386	260	332
31	1	387	261	333
32	1	388	262	334
33	1	389	263	335
34	1	390	264	336
35	1	391	265	337
36	1	392	266	338
37	1	393	231	303
38	1	394	232	304
39	1	395	233	305
40	1	396	234	306
41	1	397	235	307
42	1	398	236	308
43	1	399	237	309
44	1	400	238	310

45	1	401	239	311
46	1	402	240	312
47	1	403	241	313
48	1	404	242	314
49	1	405	243	315
50	1	406	244	316
51	1	407	245	317
52	1	408	246	318
53	1	409	247	319
54	1	410	248	320
55	1	411	213	285
56	1	412	214	286
57	1	413	215	287
58	1	414	216	288
59	1	415	217	289
60	1	416	218	290
61	1	417	219	291
62	1	418	220	292
63	1	419	221	293
64	1	420	222	294
65	1	421	223	295
66	1	422	224	296
67	1	423	225	297
68	1	424	226	298
69	1	425	227	299
70	1	426	228	300
71	1	427	229	301
72	1	428	230	302
73	1	429	273	345
74	1	429	273	363
75	1	430	274	346
76	1	430	274	364
77	1	431	275	347

78	1	431	275	365
79	1	432	276	348
80	1	432	276	366
81	1	433	277	349
82	1	433	277	367
83	1	434	278	350
84	1	434	278	368
85	1	435	279	351
86	1	435	279	369
87	1	436	280	352
88	1	436	280	370
89	1	437	281	353
90	1	437	281	371
91	1	438	282	354
92	1	438	282	372
93	1	439	283	355
94	1	439	283	373
95	1	440	284	356
96	1	440	284	374
97	1	441	267	339
98	1	441	267	357
99	1	442	268	340
100	1	442	268	358
101	1	443	269	341
102	1	443	269	359
103	1	444	270	342
104	1	444	270	360
105	1	445	271	343
106	1	445	271	361
107	1	446	272	344
108	1	446	272	362
109	1	447	249	321
110	1	447	249	375

111	1	448	250	322
112	1	448	250	376
113	1	449	251	323
114	1	449	251	377
115	1	450	252	324
116	1	450	252	378
117	1	451	253	325
118	1	451	253	379
119	1	452	254	326
120	1	452	254	380
121	1	453	255	327
122	1	453	255	381
123	1	454	256	328
124	1	454	256	382
125	1	455	257	329
126	1	455	257	383
127	1	456	258	330
128	1	456	258	384
129	1	457	259	331
130	1	457	259	385
131	1	458	260	332
132	1	458	260	386
133	1	459	261	333
134	1	459	261	387
135	1	460	262	334
136	1	460	262	388
137	1	461	263	335
138	1	461	263	389
139	1	462	264	336
140	1	462	264	390
141	1	463	265	337
142	1	463	265	391
143	1	464	266	338

144	1	464	266	392
145	1	465	231	303
146	1	465	231	393
147	1	466	232	304
148	1	466	232	394
149	1	467	233	305
150	1	467	233	395
151	1	468	234	306
152	1	468	234	396
153	1	469	235	307
154	1	469	235	397
155	1	470	236	308
156	1	470	236	398
157	1	471	237	309
158	1	471	237	399
159	1	472	238	310
160	1	472	238	400
161	1	473	239	311
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166	1	475	241	403
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169	1	477	243	315
170	1	477	243	405
171	1	478	244	316
172	1	478	244	406
173	1	479	245	317
174	1	479	245	407
175	1	480	246	318
176	1	480	246	408

177	1	481	247	319
178	1	481	247	409
179	1	482	248	320
180	1	482	248	410
181	1	483	225	297
182	1	483	225	423
183	1	484	226	298
184	1	484	226	424
185	1	485	227	299
186	1	485	227	425
187	1	486	228	300
188	1	486	228	426
189	1	487	229	301
190	1	487	229	427
191	1	488	230	302
192	1	488	230	428
193	1	489	213	285
194	1	489	213	411
195	1	490	214	286
196	1	490	214	412
197	1	491	215	287
198	1	491	215	413
199	1	492	216	288
200	1	492	216	414
201	1	493	217	289
202	1	493	217	415
203	1	494	218	290
204	1	494	218	416
205	1	495	219	291
206	1	495	219	417
207	1	496	220	292
208	1	496	220	418
209	1	497	221	293

210	1	497	221	419
211	1	498	222	294
212	1	498	222	420
213	1	499	223	295
214	1	499	223	421
215	1	500	224	296
216	1	500	224	422

Table 10. Forcefield Parameters Used

Pair Coeffs

1	0.02500000	3.20002089	# Li Li
2	0.18000001	2.29053963	# B_2 B_2
3	0.27399999	2.55088067	# S_3+6 S_3+6

Bond Coeffs

1	234.939	1.8557	# S_3+6 B_2
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Angle Coeffs

1	241.304	120.00000	# S_3+6 B_2 S_3+6
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