SUPPLEMENTAL MATERIAL: **Best Fit Force Constants**

Diagonal terms

Stretch

1	Fe	NP1	1.17
2	Fe	NP2	1.12
3	Fe	NP3	1.17
4	Fe	NP4	1.12
5	AC1	NP1	5.4
6	AC2	NP1	5.4
7	AC3	NP2	5.4
8	AC4	NP2	5.4
9	AC5	NP3	5.4
10	AC6	NP3	5.4
11	AC7	NP4	5.4
12	AC8	NP4	5.4
13	AC1	BC1	4.4
14	AC1	MC4	4.3
15	AC2	BC2	4.4
16	AC2	MC1	4.3
17	AC3	BC3	4.7
18	AC3	MC1	4.7
19	AC4	BC4	4.7
20	AC4	MC2	4.7
21	AC5	BC5	4.4
22	AC5	MC2	4.3
23	AC6	BC6	4.4
24	AC6	MC3	4.3
25	AC7	BC7	4.1
26	AC7	MC3	4.1
27	AC8	BC8	4.1
28	AC8	MC4	4.1
29	BC1	BC2	4.1
30	BC1	xC1	7.8
31	BC2	xC2	7.8
32	BC3	BC4	4.1
33	BC3	xC3	9.4
34	BC4	xC4	9.4
35	BC5	BC6	4.1
36	BC5	xC5	7.8
37	BC6	xC6	7.8
38	BC7	BC8	4.1
39	BC7	xC7	9.4
40	BC8	xC8	9.4

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41    xC1   yC1   4.1
42    xC2   yC2   4.1
43    xC3   yC3   4.1
44    xC4   yC4   4.1
45    xC5   yC5   5.1
46    xC6   yC6   5.1
47    xC7   yC7   5.1
48    xC8   yC8   5.1

      Bend
49    AC1   NP1   Fe    0.17
50    AC2   NP1   Fe    0.17
51    AC3   NP2   Fe    0.04
52    AC4   NP2   Fe    0.04
53    AC5   NP3   Fe    0.17
54    AC6   NP3   Fe    0.17
55    AC7   NP4   Fe    0.04
56    AC8   NP4   Fe    0.04
57    NP1   Fe    NP2   0.12
58    NP1   Fe    NP3   0.06
59    NP1   Fe    NP4   0.12
60    BC1   AC1   NP1   0.04
61    MC4   AC1   NP1   0.28
62    BC2   AC2   NP1   0.04
63    MC1   AC2   NP1   0.28
64    NP2   Fe    NP3   0.12
65    NP2   Fe    NP4   0.06
66    BC3   AC3   NP2   0.04
67    MC1   AC3   NP2   0.34
68    BC4   AC4   NP2   0.04
69    MC2   AC4   NP2   0.34
70    NP3   Fe    NP4   0.12
71    BC5   AC5   NP3   0.04
72    MC2   AC5   NP3   0.28
73    BC6   AC6   NP3   0.04
74    MC3   AC6   NP3   0.28
75    BC7   AC7   NP4   0.04
76    MC3   AC7   NP4   0.34
77    BC8   AC8   NP4   0.04
78    MC4   AC8   NP4   0.34
79    AC1   NP1   AC2   0.99
80    AC1   BC1   BC2   0.43
81    AC1   BC1   xC1   0.17
82    AC1   MC4   AC8   0.06
83    AC2   BC2   BC1   0.43
84    AC2   BC2   xC2   0.17
85    AC2   MC1   AC3   0.06
86    AC3   NP2   AC4   0.99
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87   AC3  BC3  BC4  0.43
88   AC3  BC3  xC3  0.17
89   AC4  BC4  BC3  0.43
90   AC4  BC4  xC4  0.17
91   AC4  MC2  AC5  0.06
92   AC5  NP3  AC6  0.99
93   AC5  BC5  BC6  0.43
94   AC5  BC5  xC5  0.17
95   AC6  BC6  BC5  0.43
96   AC6  BC6  xC6  0.17
97   AC6  MC3  AC7  0.06
98   AC7  NP4  AC8  0.99
99   AC7  BC7  BC8  0.43
100  AC7  BC7  xC7  0.17
101  AC8  BC8  BC7  0.43
102  AC8  BC8  xC8  0.17
103  BC1  AC1  MC4  0.17
104  BC1  BC2  xC2  0.05
105  BC1  xC1  yC1  0.11
106  BC2  AC2  MC1  0.17
107  BC2  BC1  xC1  0.05
108  BC2  xC2  yC2  0.11
109  BC3  AC3  MC1  0.17
110  BC3  BC4  xC4  0.05
111  BC3  xC3  yC3  0.11
112  BC4  AC4  MC2  0.17
113  BC4  BC3  xC3  0.05
114  BC4  xC4  yC4  0.11
115  BC5  AC5  MC2  0.17
116  BC5  BC6  xC6  0.05
117  BC5  xC5  yC5  0.11
118  BC6  AC6  MC3  0.17
119  BC6  BC5  xC5  0.05
120  BC6  xC6  yC6  0.11
121  BC7  AC7  MC3  0.17
122  BC7  BC8  xC8  0.05
123  BC7  xC7  yC7  0.11
124  BC8  AC8  MC4  0.17
125  BC8  BC7  xC7  0.05
126  BC8  xC8  yC8  0.11

     Torsion
127  BC1  AC1  NP1  Fe   0.012
128  Fe   NP1  AC1  MC4  0.006
129  BC2  AC2  NP1  Fe   0.012
130  Fe   NP1  AC2  MC1  0.006
131  BC3  AC3  NP2  Fe   0.012
132  Fe   NP2  AC3  MC1  0.006
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133  BC4  AC4  NP2  Fe   0.012
134  Fe   NP2  AC4  MC2  0.006
135  BC5  AC5  NP3  Fe   0.012
136  Fe   NP3  AC5  MC2  0.006
137  BC6  AC6  NP3  Fe   0.012
138  Fe   NP3  AC6  MC3  0.006
139  BC7  AC7  NP4  Fe   0.012
140  Fe   NP4  AC7  MC3  0.006
141  BC8  AC8  NP4  Fe   0.012
142  Fe   NP4  AC8  MC4  0.006
143  AC3  NP2  Fe   NP1  0.01
144  AC4  NP2  Fe   NP1  0.01
145  AC5  NP3  Fe   NP1  0.02
146  AC6  NP3  Fe   NP1  0.02
147  AC7  NP4  Fe   NP1  0.01
148  AC8  NP4  Fe   NP1  0.01
149  BC2  BC1  AC1  NP1  0.015
150  NP1  AC1  BC1  xC1  0.015
151  AC8  MC4  AC1  NP1  0.03
152  BC1  BC2  AC2  NP1  0.015
153  NP1  AC2  BC2  xC2  0.015
154  AC3  MC1  AC2  NP1  0.03
155  AC1  NP1  Fe   NP2  0.01
156  AC2  NP1  Fe   NP2  0.01
157  AC5  NP3  Fe   NP2  0.01
158  AC6  NP3  Fe   NP2  0.01
159  AC7  NP4  Fe   NP2  0.02
160  AC8  NP4  Fe   NP2  0.02
161  BC4  BC3  AC3  NP2  0.015
162  NP2  AC3  BC3  xC3  0.015
163  AC2  MC1  AC3  NP2  0.03
164  BC3  BC4  AC4  NP2  0.015
165  NP2  AC4  BC4  xC4  0.015
166  AC5  MC2  AC4  NP2  0.03
167  AC1  NP1  Fe   NP3  0.02
168  AC2  NP1  Fe   NP3  0.02
169  AC3  NP2  Fe   NP3  0.01
170  AC4  NP2  Fe   NP3  0.01
171  AC7  NP4  Fe   NP3  0.01
172  AC8  NP4  Fe   NP3  0.01
173  BC6  BC5  AC5  NP3  0.015
174  NP3  AC5  BC5  xC5  0.015
175  AC4  MC2  AC5  NP3  0.03
176  BC5  BC6  AC6  NP3  0.015
177  NP3  AC6  BC6  xC6  0.015
178  AC7  MC3  AC6  NP3  0.03
179  AC1  NP1  Fe   NP4  0.01
180  AC2  NP1  Fe   NP4  0.01
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181  AC3  NP2  Fe   NP4  0.02
182  AC4  NP2  Fe   NP4  0.02
183  AC5  NP3  Fe   NP4  0.01
184  AC6  NP3  Fe   NP4  0.01
185  BC8  BC7  AC7  NP4  0.015
186  NP4  AC7  BC7  xC7  0.015
187  AC6  MC3  AC7  NP4  0.03
188  BC7  BC8  AC8  NP4  0.015
189  NP4  AC8  BC8  xC8  0.015
190  AC1  MC4  AC8  NP4  0.03
191  AC1  NP1  AC2  BC2  0.02
192  AC1  NP1  AC2  MC1  0.002
193  AC2  BC2  BC1  AC1  0.016
194  AC1  BC1  BC2  xC2  0.003
195  AC1  BC1  xC1  yC1  0.002
196  AC1  MC4  AC8  BC8  0.015
197  AC2  NP1  AC1  BC1  0.02
198  AC2  NP1  AC1  MC4  0.002
199  AC2  BC2  BC1  xC1  0.003
200  AC2  BC2  xC2  yC2  0.002
201  AC2  MC1  AC3  BC3  0.015
202  AC3  NP2  AC4  BC4  0.02
203  AC3  NP2  AC4  MC2  0.002
204  AC4  BC4  BC3  AC3  0.016
205  AC3  BC3  BC4  xC4  0.003
206  AC3  BC3  xC3  yC3  0.002
207  AC3  MC1  AC2  BC2  0.015
208  AC4  NP2  AC3  BC3  0.02
209  AC4  NP2  AC3  MC1  0.002
210  AC4  BC4  BC3  xC3  0.003
211  AC4  BC4  xC4  yC4  0.002
212  AC4  MC2  AC5  BC5  0.015
213  AC5  NP3  AC6  BC6  0.02
214  AC5  NP3  AC6  MC3  0.002
215  AC6  BC6  BC5  AC5  0.016
216  AC5  BC5  BC6  xC6  0.003
217  AC5  BC5  xC5  yC5  0.002
218  AC5  MC2  AC4  BC4  0.015
219  AC6  NP3  AC5  BC5  0.02
220  AC6  NP3  AC5  MC2  0.002
221  AC6  BC6  BC5  xC5  0.003
222  AC6  BC6  xC6  yC6  0.002
223  AC6  MC3  AC7  BC7  0.015
224  AC7  NP4  AC8  BC8  0.02
225  AC7  NP4  AC8  MC4  0.002
226  AC8  BC8  BC7  AC7  0.016
227  AC7  BC7  BC8  xC8  0.003
228  AC7  BC7  xC7  yC7  0.002
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229  AC7  MC3  AC6  BC6  0.015
230  AC8  NP4  AC7  BC7  0.02
231  AC8  NP4  AC7  MC3  0.002
232  AC8  BC8  BC7  xC7  0.003
233  AC8  BC8  xC8  yC8  0.002
234  AC8  MC4  AC1  BC1  0.015
235  BC1  BC2  AC2  MC1  0.003
236  BC1  BC2  xC2  yC2  0.021
237  BC2  BC1  AC1  MC4  0.003
238  BC2  BC1  xC1  yC1  0.021
239  BC3  BC4  AC4  MC2  0.003
240  BC3  BC4  xC4  yC4  0.021
241  BC4  BC3  AC3  MC1  0.003
242  BC4  BC3  xC3  yC3  0.021
243  BC5  BC6  AC6  MC3  0.003
244  BC5  BC6  xC6  yC6  0.021
245  BC6  BC5  AC5  MC2  0.003
246  BC6  BC5  xC5  yC5  0.021
247  BC7  BC8  AC8  MC4  0.003
248  BC7  BC8  xC8  yC8  0.021
249  BC8  BC7  AC7  MC3  0.003
250  BC8  BC7  xC7  yC7  0.021
251  MC1  AC2  BC2  xC2  0.003
252  MC1  AC3  BC3  xC3  0.003
253  MC2  AC4  BC4  xC4  0.003
254  MC2  AC5  BC5  xC5  0.003
255  MC3  AC6  BC6  xC6  0.003
256  MC3  AC7  BC7  xC7  0.003
257  MC4  AC1  BC1  xC1  0.003
258  MC4  AC8  BC8  xC8  0.003
259  xC2  BC2  BC1  xC1  0.072
260  xC4  BC4  BC3  xC3  0.072
261  xC6  BC6  BC5  xC5  0.072
262  xC8  BC8  BC7  xC7  0.072

     Out-of-plane
263-323   All       1.19


     Off-diagonal terms

{Explanation: The first column represents the set of the
force constants (1 means first force constant from the
table, 2 - second and so on), the second column gives the
off-diagonal term value.

For example:
"1,2,3,4"     0.1
```

means that there is off-diagonal coupling between the force constants:

1 and 2
1 and 3
1 and 4
2 and 3
2 and 4
3 and 4
and for all of them the off-diagonal coupling constant equals 0.1.}

"1,3,79,92" 0.04
"2,4,86,98" 0.05
5-48 -2.6
"67,69,76,78" 0.06
"80,83,87,89,93,95,99,101" 0.03
"81,94" -0.05
"84,96" -0.05
"88,100" -0.04
"90,102" -0.04
"82,85,91,97" 0.02
"127,129,131,133,135,137,139,141" -0.03
"267,268" 0.2
"272,273" -0.6