

A multi-scale approach to spin crossover in Fe(II) compounds

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Table S1. Vibrational frequencies^a (cm⁻¹) from OPBE/TZP and IntraFF force field parameters

Freq.	IntraFF	OPBE/TZP singlet	<i>diff.</i>	IntraFF	OPBE/TZP quintet	<i>diff.</i>
7	86.5	57.3	29.1	78.6	37.2	41.4
8	111.3	64.1	47.2	107.8	54.0	53.9
9	111.3	64.1	47.2	107.8	54.0	53.9
10	131.5	76.5	54.9	128.6	55.6	73.0
11	131.5	76.5	54.9	128.6	55.6	73.0
12	137.9	78.7	59.2	133.6	58.4	75.1
13	137.9	78.7	59.2	133.6	58.4	75.1
14	171.4	121.5	50.0	164.0	75.4	88.6
15	179.1	144.1	35.1	177.1	91.2	85.9
16	197.2	158.0	39.2	194.7	104.7	89.9
17	198.6	163.7	34.9	194.7	104.7	89.9
18	198.6	176.9	21.7	195.7	110.7	85.0
19	202.0	176.9	25.1	198.4	133.2	65.2
20	202.0	182.5	19.5	198.4	133.2	65.2
21	236.5	182.5	54.0	224.7	133.4	91.3
22	236.5	203.4	33.1	224.7	133.4	91.3
23	270.5	203.4	67.1	257.2	155.4	101.8
24	283.1	211.1	72.0	275.5	162.0	113.5
25	295.9	242.0	53.9	282.3	168.0	114.3
26	307.1	256.0	51.1	301.1	191.1	110.0
27	310.6	317.0	-6.3	307.7	191.1	116.5
28	318.6	317.0	1.7	316.1	197.1	119.0
29	318.7	328.9	-10.2	316.1	242.1	74.0
30	326.5	328.9	-2.4	323.7	276.0	47.7
31	326.5	334.2	-7.8	323.7	276.0	47.7
32	386.9	340.7	46.2	376.1	280.6	95.5
33	425.9	340.7	85.2	399.9	280.6	119.3
34	426.0	347.3	78.7	399.9	321.2	78.8
35	478.5	347.3	131.2	473.9	321.2	152.7
36	487.6	354.9	132.7	479.3	325.7	153.6
37	487.6	411.0	76.5	479.3	325.8	153.5
38	487.8	411.0	76.8	482.7	325.8	156.9
39	488.0	430.9	57.1	482.8	327.9	154.8
40	506.3	613.3	-107.0	501.8	617.1	-115.3
41	506.3	617.2	-110.9	501.9	620.1	-118.3
42	515.4	619.4	-104.0	505.0	620.9	-115.9
43	525.4	619.4	-94.0	506.0	620.9	-114.9
44	545.9	622.4	-76.5	532.8	628.9	-96.1
45	545.9	622.4	-76.4	532.9	628.9	-96.0
46	637.6	655.3	-17.7	648.1	663.6	-15.5
47	637.7	668.3	-30.6	648.4	664.9	-16.5
48	643.0	669.6	-26.6	664.0	674.9	-10.9
49	643.0	669.6	-26.6	664.2	674.9	-10.7
50	661.1	679.3	-18.2	685.5	679.1	6.4
51	670.7	679.3	-8.6	695.1	679.1	16.0
52	692.4	721.1	-28.7	700.1	731.1	-31.0
53	701.5	721.1	-19.6	700.3	731.1	-30.8
54	701.6	722.9	-21.3	714.4	733.1	-18.7
55	718.6	722.9	-4.4	715.2	733.1	-17.9
56	728.3	728.8	-0.6	720.7	742.0	-21.2
57	742.8	732.9	9.9	720.9	745.1	-24.2
58	742.8	733.9	8.8	726.0	746.6	-20.6
59	748.3	733.9	14.4	732.0	746.6	-14.6
60	752.2	736.5	15.7	764.4	748.3	16.0
61	752.3	736.5	15.8	764.4	748.3	16.0
62	754.3	800.2	-45.8	770.3	783.4	-13.1
63	754.4	801.1	-46.7	770.3	785.4	-15.1
64	782.9	807.8	-24.9	803.9	827.4	-23.5
65	782.9	811.6	-28.7	804.0	830.0	-26.0
66	787.6	811.6	-24.0	804.1	830.6	-26.5
67	787.6	811.8	-24.2	804.6	830.6	-25.9
Freq.	IntraFF	OPBE/TZP	<i>diff.</i>	IntraFF	OPBE/TZP	<i>diff.</i>

	singlet			quintet		
68	800.4	811.9	-11.6	804.8	831.8	-27.0
69	814.6	811.9	2.7	816.9	831.8	-15.0
70	848.3	857.4	-9.1	836.2	869.6	-33.4
71	848.3	858.5	-10.2	836.2	871.0	-34.8
72	850.8	858.7	-7.9	841.7	871.0	-29.3
73	850.8	858.7	-7.9	841.7	873.1	-31.3
74	854.6	858.9	-4.3	870.4	873.5	-3.1
75	859.0	858.9	0.1	875.8	873.5	2.3
76	884.8	912.5	-27.7	895.6	910.9	-15.3
77	884.9	912.5	-27.6	898.5	910.9	-12.4
78	888.8	912.7	-24.0	898.6	911.8	-13.2
79	888.8	912.7	-23.9	901.7	911.8	-10.1
80	896.4	919.0	-22.6	905.2	915.8	-10.6
81	899.6	919.3	-19.8	905.2	916.6	-11.4
82	903.4	977.5	-74.2	926.8	976.6	-49.7
83	920.4	977.5	-57.1	932.6	977.7	-45.2
84	920.5	978.8	-58.3	932.8	979.6	-46.8
85	933.6	978.8	-45.1	936.4	979.6	-43.2
86	951.1	980.3	-29.2	937.4	980.3	-42.9
87	951.1	986.7	-35.5	937.6	980.3	-42.7
88	992.5	1042.5	-50.0	985.5	1052.8	-67.3
89	992.5	1042.5	-50.0	985.7	1052.8	-67.2
90	994.2	1042.5	-48.3	997.7	1055.7	-58.0
91	994.6	1042.5	-47.9	997.7	1055.7	-58.0
92	1000.6	1063.8	-63.2	1003.3	1065.1	-61.8
93	1000.6	1065.4	-64.8	1003.3	1066.8	-63.5
94	1010.1	1065.4	-55.3	1010.2	1071.3	-61.1
95	1017.2	1067.4	-50.2	1014.9	1071.3	-56.4
96	1017.8	1067.4	-49.6	1017.8	1072.1	-54.3
97	1017.8	1071.2	-53.4	1017.8	1072.1	-54.3
98	1021.1	1093.3	-72.2	1021.6	1092.2	-70.6
99	1021.1	1101.0	-79.8	1021.6	1094.2	-72.6
100	1092.8	1124.5	-31.7	1090.8	1128.7	-37.9
101	1092.8	1124.5	-31.7	1090.8	1128.7	-37.9
102	1093.6	1125.3	-31.8	1092.3	1128.9	-36.6
103	1093.6	1125.3	-31.8	1092.3	1128.9	-36.6
104	1130.6	1189.7	-59.1	1127.7	1187.0	-59.3
105	1134.8	1189.7	-54.9	1131.2	1187.0	-55.8
106	1175.2	1193.3	-18.1	1173.9	1189.3	-15.5
107	1175.2	1193.3	-18.1	1173.9	1189.3	-15.5
108	1185.5	1197.6	-12.1	1181.4	1194.4	-13.0
109	1185.5	1198.1	-12.5	1181.4	1195.5	-14.1
110	1242.3	1237.3	5.0	1238.3	1243.3	-5.0
111	1243.5	1237.3	6.2	1238.5	1245.4	-7.0
112	1280.5	1237.8	42.8	1288.7	1245.5	43.3
113	1280.5	1237.8	42.8	1288.7	1246.4	42.4
114	1286.8	1242.6	44.2	1294.0	1246.7	47.3
115	1286.8	1246.6	40.2	1294.0	1246.7	47.3
116	1330.7	1333.3	-2.6	1328.1	1332.1	-4.0
117	1330.7	1333.3	-2.6	1328.1	1332.6	-4.5
118	1332.1	1338.2	-6.1	1329.8	1332.6	-2.8
119	1332.1	1338.2	-6.1	1329.8	1333.0	-3.2
120	1382.2	1338.2	43.9	1377.7	1333.9	43.9
121	1382.4	1338.8	43.6	1378.8	1333.9	44.9
122	1439.8	1433.4	6.4	1429.2	1419.0	10.2
123	1439.8	1433.4	6.4	1429.2	1419.0	10.2
124	1441.7	1435.9	5.8	1430.7	1419.4	11.3
125	1441.7	1435.9	5.8	1430.7	1419.4	11.3
126	1447.2	1444.6	2.6	1443.9	1439.5	4.5
127	1450.3	1444.6	5.8	1444.1	1440.2	3.8
128	1459.2	1445.2	14.0	1456.7	1442.3	14.4
129	1459.2	1445.2	14.0	1457.4	1442.3	15.1
130	1463.5	1445.5	18.0	1458.0	1442.4	15.6
Freq.	IntraFF	OPBE/TZP singlet	diff.	IntraFF	OPBE/TZP quintet	diff.

131	1463.5	1445.6	17.9	1458.0	1442.4	15.6
132	1466.6	1455.8	10.8	1459.4	1445.4	14.0
133	1467.6	1456.8	10.8	1459.4	1445.8	13.7
134	1535.5	1514.8	20.7	1543.4	1523.7	19.6
135	1535.5	1514.8	20.8	1543.4	1523.7	19.7
136	1537.6	1516.5	21.1	1543.5	1524.0	19.4
137	1537.6	1516.5	21.1	1543.5	1524.0	19.4
138	1537.9	1524.7	13.3	1543.7	1529.9	13.8
139	1537.9	1525.1	12.8	1543.7	1530.5	13.2
140	2552.8	2552.4	0.4	2535.8	2535.4	0.4
141	2552.8	2553.2	-0.4	2535.8	2536.1	-0.3
142	3210.4	3210.3	0.1	3205.2	3205.0	0.1
143	3210.4	3210.3	0.1	3205.2	3205.0	0.1
144	3210.4	3210.4	0.0	3205.2	3205.1	0.1
145	3210.4	3210.4	0.0	3205.2	3205.2	-0.1
146	3210.4	3210.5	-0.1	3205.2	3205.2	0.0
147	3210.4	3210.6	-0.2	3205.2	3205.5	-0.3
148	3229.7	3229.7	0.1	3218.8	3218.5	0.2
149	3229.7	3229.7	0.1	3218.8	3218.5	0.2
150	3229.7	3229.7	0.1	3218.8	3218.7	0.1
151	3229.7	3229.7	0.1	3218.8	3218.8	-0.1
152	3229.8	3229.8	0.0	3218.8	3218.8	0.0
153	3229.8	3230.2	-0.4	3218.8	3219.4	-0.6
154	3244.9	3244.4	0.5	3233.8	3233.7	0.1
155	3244.9	3244.6	0.3	3233.8	3233.7	0.1
156	3244.9	3244.6	0.3	3233.8	3233.7	0.1
157	3244.9	3245.2	-0.3	3233.8	3233.9	0.0
158	3244.9	3245.2	-0.2	3233.8	3233.9	0.0
159	3244.9	3245.6	-0.7	3233.8	3234.0	-0.2

a) indicated in **boldface** are those frequencies where the quintet value is higher than the singlet value

Table S2. Macroscopic density (kg/l) of dichloromethane and box-radius (a.u.) at different temperatures

Temperature (K)	Macroscopic density (kg/l)	Box-radius (Bohr)
200	1.4759	29.4824
210	1.4618	29.5735
220	1.4472	29.6689
230	1.4321	29.7687
240	1.4166	29.8731
250	1.4005	29.9823
260	1.3841	30.0965
270	1.3671	30.2158
280	1.3497	30.3405
290	1.3318	30.4709
300	1.3135	30.6071
310	1.2947	30.7495
320	1.2754	30.8984
330	1.2557	31.0540
340	1.2355	31.2169
350	1.2148	31.3872
360	1.1936	31.5655
370	1.1720	31.7523
380	1.1500	31.9479
390	1.1274	32.1529
400	1.1044	32.3681
410	1.0810	32.5939
420	1.0570	32.8311
430	1.0326	33.0805
440	1.0077	33.3431
450	0.9824	33.6197

Macroscopic densities from CRC Handbook:

Temperature (°C)	Density (kg/l)
0	1.362
10	1.344
20	1.326
30	1.307
40	1.289
50	1.269
60	1.250
70	1.229
80	1.208
90	1.187
100	1.165

Force field parameters for iron-compound in low and high state

Singlet

bond	i1	i2	k	R	
BOND	Fe1	N2	146.9601	1.959737	
BOND	Fe1	N4	146.9601	1.959737	
BOND	Fe1	N6	146.9601	1.959737	
BOND	Fe1	N18	146.9601	1.959737	
BOND	Fe1	N20	146.9601	1.959737	
BOND	N19	Fe1	146.9601	1.959737	
BOND	N2	N3	155.5122	1.346781	
BOND	N4	N5	155.5122	1.346781	
BOND	N6	N7	155.5122	1.346781	
BOND	N18	N23	155.5122	1.346781	
BOND	N19	N25	155.5122	1.346781	
BOND	N20	N22	155.5122	1.346781	
BOND	N2	C10	260.5812	1.339798	
BOND	N4	C13	260.5812	1.339798	
BOND	N6	C16	260.5812	1.339798	
BOND	N18	C24	260.5812	1.339798	
BOND	N19	C26	260.5812	1.339798	
BOND	N20	C27	260.5812	1.339798	
BOND	N3	C8	264.5643	1.348575	
BOND	N5	C11	264.5643	1.348575	
BOND	N7	C14	264.5643	1.348575	
BOND	N22	C28	264.5643	1.348575	
BOND	N23	C29	264.5643	1.348575	
BOND	N25	C31	264.5643	1.348575	
BOND	N3	B17	160.3521	1.534820	
BOND	N5	B17	160.3521	1.534820	
BOND	N7	B21	160.3521	1.534820	
BOND	B17	N22	160.3521	1.534820	
BOND	B21	N23	160.3521	1.534820	
BOND	B21	N25	160.3521	1.534820	
BOND	C8	C9	353.5446	1.385210	
BOND	C11	C12	353.5446	1.385210	
BOND	C14	C15	353.5446	1.385210	
BOND	C28	C33	353.5446	1.385210	
BOND	C29	C30	353.5446	1.385210	
BOND	C31	C32	353.5446	1.385210	
BOND	C8	H49	406.9132	1.083067	
BOND	C11	H48	406.9132	1.083067	
BOND	C14	H52	406.9132	1.083067	
BOND	C28	H50	406.9132	1.083067	
BOND	C29	H53	406.9132	1.083067	
BOND	C31	H51	406.9132	1.083067	
BOND	C9	C10	218.5871	1.399173	
BOND	C12	C13	218.5871	1.399173	
BOND	C15	C16	218.5871	1.399173	
BOND	C24	C30	218.5871	1.399173	
BOND	C26	C32	218.5871	1.399173	
BOND	C27	C33	218.5871	1.399173	
BOND	C9	H39	402.3165	1.083567	
BOND	C12	H41	402.3165	1.083567	
BOND	C15	H40	402.3165	1.083567	
BOND	C30	H37	402.3165	1.083567	
BOND	C32	H36	402.3165	1.083567	
BOND	C33	H38	402.3165	1.083567	
BOND	C10	H43	411.5010	1.081516	
BOND	C13	H47	411.5010	1.081516	
BOND	C16	H42	411.5010	1.081516	
BOND	C24	H45	411.5010	1.081516	
BOND	C26	H46	411.5010	1.081516	
BOND	C27	H44	411.5010	1.081516	
BOND	B17	H35	249.9358	1.202551	
BOND	B21	H34	249.9358	1.202551	
angle	i1	i2	i3	k	theta
ANGLE	N18	Fe1	N6	203.8032	88.675256
ANGLE	N19	Fe1	N18	203.8032	88.675256
ANGLE	N19	Fe1	N6	203.8032	88.675256
ANGLE	N20	Fe1	N2	203.8032	88.675256
ANGLE	N20	Fe1	N4	203.8032	88.675256
ANGLE	N4	Fe1	N2	203.8032	88.675256
ANGLE	N18	Fe1	N4	208.4059	91.324744
ANGLE	N19	Fe1	N2	208.4059	91.324744
ANGLE	N19	Fe1	N20	208.4059	91.324744
ANGLE	N20	Fe1	N18	208.4059	91.324744
ANGLE	N6	Fe1	N2	208.4059	91.324744

Supplementary Material (ESI) for PCCP
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ANGLE	N6	Fe1	N4	208.4059	91.324744
ANGLE	C10	C9	C8	174.1487	104.640706
ANGLE	C13	C12	C11	174.1487	104.640706
ANGLE	C16	C15	C14	174.1487	104.640706
ANGLE	C28	C33	C27	174.1487	104.640706
ANGLE	C29	C30	C24	174.1487	104.640706
ANGLE	C31	C32	C26	174.1487	104.640706
ANGLE	C10	N2	N3	117.2426	106.892006
ANGLE	C13	N4	N5	117.2426	106.892006
ANGLE	C16	N6	N7	117.2426	106.892006
ANGLE	C24	N18	N23	117.2426	106.892006
ANGLE	C26	N19	N25	117.2426	106.892006
ANGLE	C27	N20	N22	117.2426	106.892006
ANGLE	C12	C11	N5	144.1767	108.059935
ANGLE	C15	C14	N7	144.1767	108.059935
ANGLE	C30	C29	N23	144.1767	108.059935
ANGLE	C32	C31	N25	144.1767	108.059935
ANGLE	C33	C28	N22	144.1767	108.059935
ANGLE	C9	C8	N3	144.1767	108.059935
ANGLE	H34	B21	N23	42.6076	111.452821
ANGLE	H34	B21	N25	42.6076	111.452821
ANGLE	H34	B21	N7	42.6076	111.452821
ANGLE	H35	B17	N22	42.6076	111.452821
ANGLE	H35	B17	N3	42.6076	111.452821
ANGLE	H35	B17	N5	42.6076	111.452821
ANGLE	N22	B17	N3	109.7677	107.418981
ANGLE	N22	B17	N5	109.7677	107.418981
ANGLE	N23	B21	N7	109.7677	107.418981
ANGLE	N25	B21	N23	109.7677	107.418981
ANGLE	N25	B21	N7	109.7677	107.418981
ANGLE	N5	B17	N3	109.7677	107.418981
ANGLE	C11	N5	N4	75.9716	110.285087
ANGLE	C14	N7	N6	75.9716	110.285087
ANGLE	C28	N22	N20	75.9716	110.285087
ANGLE	C29	N23	N18	75.9716	110.285087
ANGLE	C31	N25	N19	75.9716	110.285087
ANGLE	C8	N3	N2	75.9716	110.285087
ANGLE	C12	C13	N4	99.4151	110.122266
ANGLE	C15	C16	N6	99.4151	110.122266
ANGLE	C30	C24	N18	99.4151	110.122266
ANGLE	C32	C26	N19	99.4151	110.122266
ANGLE	C33	C27	N20	99.4151	110.122266
ANGLE	C9	C10	N2	99.4151	110.122266
ANGLE	N22	N20	Fe1	126.0035	119.671539
ANGLE	N23	N18	Fe1	126.0035	119.671539
ANGLE	N25	N19	Fe1	126.0035	119.671539
ANGLE	N3	N2	Fe1	126.0035	119.671539
ANGLE	N5	N4	Fe1	126.0035	119.671539
ANGLE	N7	N6	Fe1	126.0035	119.671539
ANGLE	H42	C16	N6	23.5399	120.087054
ANGLE	H43	C10	N2	23.5399	120.087054
ANGLE	H44	C27	N20	23.5399	120.087054
ANGLE	H45	C24	N18	23.5399	120.087054
ANGLE	H46	C26	N19	23.5399	120.087054
ANGLE	H47	C13	N4	23.5399	120.087054
ANGLE	H48	C11	N5	35.1998	120.555715
ANGLE	H49	C8	N3	35.1998	120.555715
ANGLE	H50	C28	N22	35.1998	120.555715
ANGLE	H51	C31	N25	35.1998	120.555715
ANGLE	H52	C14	N7	35.1998	120.555715
ANGLE	H53	C29	N23	35.1998	120.555715
ANGLE	B17	N3	N2	92.1472	117.977134
ANGLE	B17	N5	N4	92.1472	117.977134
ANGLE	N20	N22	B17	92.1472	117.977134
ANGLE	B21	N23	N18	92.1472	117.977134
ANGLE	B21	N25	N19	92.1472	117.977134
ANGLE	B21	N7	N6	92.1472	117.977134
ANGLE	H36	C32	C31	33.4945	127.587229
ANGLE	H37	C30	C29	33.4945	127.587229
ANGLE	H38	C33	C28	33.4945	127.587229
ANGLE	H39	C9	C8	33.4945	127.587229
ANGLE	H40	C15	C14	33.4945	127.587229
ANGLE	H41	C12	C11	33.4945	127.587229
ANGLE	H36	C32	C26	33.8889	127.772066
ANGLE	H37	C30	C24	33.8889	127.772066
ANGLE	H38	C33	C27	33.8889	127.772066
ANGLE	H39	C9	C10	33.8889	127.772066
ANGLE	H40	C15	C16	33.8889	127.772066
ANGLE	H41	C12	C13	33.8889	127.772066
ANGLE	B17	N3	C8	99.0962	131.737778

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ANGLE	B17	N5	C11			99.0962		131.737778	
ANGLE	B21	N7	C14			99.0962		131.737778	
ANGLE	C28	N22	B17			99.0962		131.737778	
ANGLE	C29	N23	B21			99.0962		131.737778	
ANGLE	C31	N25	B21			99.0962		131.737778	
ANGLE	H42	C16	C15			37.2325		129.790680	
ANGLE	H43	C10	C9			37.2325		129.790680	
ANGLE	H44	C27	C33			37.2325		129.790680	
ANGLE	H45	C24	C30			37.2325		129.790680	
ANGLE	H46	C26	C32			37.2325		129.790680	
ANGLE	H47	C13	C12			37.2325		129.790680	
ANGLE	H48	C11	C12			32.5688		131.384349	
ANGLE	H49	C8	C9			32.5688		131.384349	
ANGLE	H50	C28	C33			32.5688		131.384349	
ANGLE	H51	C31	C32			32.5688		131.384349	
ANGLE	H52	C14	C15			32.5688		131.384349	
ANGLE	H53	C29	C30			32.5688		131.384349	
ANGLE	C10	N2	Fe1			124.3723		133.436455	
ANGLE	C13	N4	Fe1			124.3723		133.436455	
ANGLE	C16	N6	Fe1			124.3723		133.436455	
ANGLE	C24	N18	Fe1			124.3723		133.436455	
ANGLE	C26	N19	Fe1			124.3723		133.436455	
ANGLE	C27	N20	Fe1			124.3723		133.436455	
dihedral	i1	i2	i3	i4			k	divf	phi
DIHEDRAL	C10	C9	C8	N3	1	12.0427	1.0	360.000000	
DIHEDRAL	C13	C12	C11	N5	1	12.0427	1.0	360.000000	
DIHEDRAL	C16	C15	C14	N7	1	12.0427	1.0	360.000000	
DIHEDRAL	C26	C32	C31	N25	1	12.0427	1.0	360.000000	
DIHEDRAL	C24	C30	C29	N23	1	12.0427	1.0	360.000000	
DIHEDRAL	C27	C33	C28	N22	1	12.0427	1.0	360.000000	
DIHEDRAL	C11	C12	C13	N4	1	12.0738	1.0	0.000000	
DIHEDRAL	C8	C9	C10	N2	1	12.0738	1.0	0.000000	
DIHEDRAL	C14	C15	C16	N6	1	12.0738	1.0	0.000000	
DIHEDRAL	C28	C33	C27	N20	1	12.0738	1.0	0.000000	
DIHEDRAL	C29	C30	C24	N18	1	12.0738	1.0	0.000000	
DIHEDRAL	C31	C32	C26	N19	1	12.0738	1.0	0.000000	
DIHEDRAL	C8	N3	N2	C10	1	13.2685	1.0	360.000000	
DIHEDRAL	C11	N5	N4	C13	1	13.2685	1.0	360.000000	
DIHEDRAL	C14	N7	N6	C16	1	13.2685	1.0	360.000000	
DIHEDRAL	C28	N22	N20	C27	1	13.2685	1.0	360.000000	
DIHEDRAL	C29	N23	N18	C24	1	13.2685	1.0	360.000000	
DIHEDRAL	C31	N25	N19	C26	1	13.2685	1.0	360.000000	
DIHEDRAL	C9	C8	N3	N2	1	11.7401	1.0	0.000000	
DIHEDRAL	C12	C11	N5	N4	1	11.7401	1.0	0.000000	
DIHEDRAL	C15	C14	N7	N6	1	11.7401	1.0	0.000000	
DIHEDRAL	C30	C29	N23	N18	1	11.7401	1.0	0.000000	
DIHEDRAL	C32	C31	N25	N19	1	11.7401	1.0	0.000000	
DIHEDRAL	C33	C28	N22	N20	1	11.7401	1.0	0.000000	
DIHEDRAL	C9	C10	N2	N3	1	13.1558	1.0	0.000000	
DIHEDRAL	C12	C13	N4	N5	1	13.1558	1.0	0.000000	
DIHEDRAL	C15	C16	N6	N7	1	13.1558	1.0	0.000000	
DIHEDRAL	C30	C24	N18	N23	1	13.1558	1.0	0.000000	
DIHEDRAL	C32	C26	N19	N25	1	13.1558	1.0	0.000000	
DIHEDRAL	C33	C27	N20	N22	1	13.1558	1.0	0.000000	
DIHEDRAL	B17	N3	N2	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	B17	N22	N20	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	B17	N5	N4	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	B21	N23	N18	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	B21	N25	N19	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	B21	N7	N6	Fe1	1	11.0914	1.0	0.000000	
DIHEDRAL	C28	N22	B17	H35	1	3.4239	1.0	0.000000	
DIHEDRAL	C29	N23	B21	H34	1	3.4239	1.0	0.000000	
DIHEDRAL	C31	N25	B21	H34	1	3.4239	1.0	0.000000	
DIHEDRAL	H34	B21	N7	C14	1	3.4239	1.0	0.000000	
DIHEDRAL	H35	B17	N3	C8	1	3.4239	1.0	0.000000	
DIHEDRAL	H35	B17	N5	C11	1	3.4239	1.0	0.000000	
DIHEDRAL	H36	C32	C26	H46	1	1.8548	1.0	360.000000	
DIHEDRAL	H37	C30	C24	H45	1	1.8548	1.0	360.000000	
DIHEDRAL	H38	C33	C27	H44	1	1.8548	1.0	360.000000	
DIHEDRAL	H42	C16	C15	H40	1	1.8548	1.0	360.000000	
DIHEDRAL	H43	C10	C9	H39	1	1.8548	1.0	360.000000	
DIHEDRAL	H47	C13	C12	H41	1	1.8548	1.0	360.000000	
DIHEDRAL	H36	C32	C31	H51	1	1.6613	1.0	0.000000	
DIHEDRAL	H37	C30	C29	H53	1	1.6613	1.0	0.000000	
DIHEDRAL	H38	C33	C28	H50	1	1.6613	1.0	0.000000	
DIHEDRAL	H39	C9	C8	H49	1	1.6613	1.0	0.000000	
DIHEDRAL	H40	C15	C14	H52	1	1.6613	1.0	0.000000	
DIHEDRAL	H41	C12	C11	H48	1	1.6613	1.0	0.000000	
DIHEDRAL	H42	C16	N6	Fe1	1	3.2473	1.0	0.000000	
DIHEDRAL	H43	C10	N2	Fe1	1	3.2473	1.0	0.000000	

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DIHEDRAL	H44	C27	N20	Fe1	1	3.2473	1.0	0.000000
DIHEDRAL	H45	C24	N18	Fe1	1	3.2473	1.0	0.000000
DIHEDRAL	H46	C26	N19	Fe1	1	3.2473	1.0	0.000000
DIHEDRAL	H47	C13	N4	Fe1	1	3.2473	1.0	0.000000
DIHEDRAL	H48	C11	N5	B17	1	2.8966	1.0	0.000000
DIHEDRAL	H49	C8	N3	B17	1	2.8966	1.0	0.000000
DIHEDRAL	H50	C28	N22	B17	1	2.8966	1.0	0.000000
DIHEDRAL	H51	C31	N25	B21	1	2.8966	1.0	0.000000
DIHEDRAL	H52	C14	N7	B21	1	2.8966	1.0	0.000000
DIHEDRAL	H53	C29	N23	B21	1	2.8966	1.0	0.000000
DIHEDRAL	C13	N4	Fe1	N6	1	4.6634	1.0	44.352598
DIHEDRAL	C16	N6	Fe1	N4	1	4.6634	1.0	44.352598
DIHEDRAL	N19	Fe1	N2	C10	1	4.6634	1.0	44.352598
DIHEDRAL	C24	N18	Fe1	N20	1	4.6634	1.0	44.352598
DIHEDRAL	C26	N19	Fe1	N2	1	4.6634	1.0	44.352598
DIHEDRAL	C27	N20	Fe1	N18	1	4.6634	1.0	44.352598
DIHEDRAL	N19	Fe1	N6	N7	1	8.0036	1.0	44.352598
DIHEDRAL	N22	N20	Fe1	N2	1	8.0036	1.0	44.352598
DIHEDRAL	N23	N18	Fe1	N6	1	8.0036	1.0	44.352598
DIHEDRAL	N25	N19	Fe1	N18	1	8.0036	1.0	44.352598
DIHEDRAL	N3	N2	Fe1	N4	1	8.0036	1.0	44.352598
DIHEDRAL	N5	N4	Fe1	N20	1	8.0036	1.0	44.352598
DIHEDRAL	N19	N25	B21	N7	1	12.5208	1.0	57.646905
DIHEDRAL	N20	N22	B17	N5	1	12.5208	1.0	57.646905
DIHEDRAL	N22	B17	N3	N2	1	12.5208	1.0	57.646905
DIHEDRAL	N23	B21	N7	N6	1	12.5208	1.0	57.646905
DIHEDRAL	N25	B21	N23	N18	1	12.5208	1.0	57.646905
DIHEDRAL	N4	N5	B17	N3	1	12.5208	1.0	57.646905
DIHEDRAL	N22	B17	N5	C11	1	9.8988	1.0	122.353095
DIHEDRAL	N25	B21	N7	C14	1	9.8988	1.0	122.353095
DIHEDRAL	C28	N22	B17	N3	1	9.8988	1.0	122.353095
DIHEDRAL	C29	N23	B21	N7	1	9.8988	1.0	122.353095
DIHEDRAL	C31	N25	B21	N23	1	9.8988	1.0	122.353095
DIHEDRAL	N5	B17	N3	C8	1	9.8988	1.0	122.353095
DIHEDRAL	C10	N2	Fe1	N20	1	5.0085	1.0	135.647402
DIHEDRAL	C13	N4	Fe1	N2	1	5.0085	1.0	135.647402
DIHEDRAL	C16	N6	Fe1	N18	1	5.0085	1.0	135.647402
DIHEDRAL	N19	Fe1	N18	C24	1	5.0085	1.0	135.647402
DIHEDRAL	C26	N19	Fe1	N6	1	5.0085	1.0	135.647402
DIHEDRAL	C27	N20	Fe1	N4	1	5.0085	1.0	135.647402
DIHEDRAL	N22	N20	Fe1	N19	1	8.4273	1.0	135.647402
DIHEDRAL	N23	N18	Fe1	N4	1	8.4273	1.0	135.647402
DIHEDRAL	N25	N19	Fe1	N20	1	8.4273	1.0	135.647402
DIHEDRAL	N3	N2	Fe1	N6	1	8.4273	1.0	135.647402
DIHEDRAL	N5	N4	Fe1	N18	1	8.4273	1.0	135.647402
DIHEDRAL	N7	N6	Fe1	N2	1	8.4273	1.0	135.647402
DIHEDRAL	C10	C9	C8	H49	1	3.1773	1.0	180.000000
DIHEDRAL	H51	C31	C32	C26	1	3.1773	1.0	180.000000
DIHEDRAL	C13	C12	C11	H48	1	3.1773	1.0	180.000000
DIHEDRAL	C16	C15	C14	H52	1	3.1773	1.0	180.000000
DIHEDRAL	H50	C28	C33	C27	1	3.1773	1.0	180.000000
DIHEDRAL	H53	C29	C30	C24	1	3.1773	1.0	180.000000
DIHEDRAL	C11	N5	N4	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C14	N7	N6	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C28	N22	N20	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C29	N23	N18	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C31	N25	N19	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C8	N3	N2	Fe1	1	15.1425	1.0	180.000000
DIHEDRAL	C12	C11	N5	B17	1	13.6363	1.0	180.000000
DIHEDRAL	C9	C8	N3	B17	1	13.6363	1.0	180.000000
DIHEDRAL	C15	C14	N7	B21	1	13.6363	1.0	180.000000
DIHEDRAL	C30	C29	N23	B21	1	13.6363	1.0	180.000000
DIHEDRAL	C32	C31	N25	B21	1	13.6363	1.0	180.000000
DIHEDRAL	C33	C28	N22	B17	1	13.6363	1.0	180.000000
DIHEDRAL	C12	C13	N4	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	C15	C16	N6	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	C30	C24	N18	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	C32	C26	N19	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	C33	C27	N20	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	C9	C10	N2	Fe1	1	11.9261	1.0	180.000000
DIHEDRAL	B17	N3	N2	C10	1	17.8712	1.0	180.000000
DIHEDRAL	B17	N5	N4	C13	1	17.8712	1.0	180.000000
DIHEDRAL	B21	N23	N18	C24	1	17.8712	1.0	180.000000
DIHEDRAL	B21	N25	N19	C26	1	17.8712	1.0	180.000000
DIHEDRAL	B21	N7	N6	C16	1	17.8712	1.0	180.000000
DIHEDRAL	C27	N20	N22	B17	1	17.8712	1.0	180.000000
DIHEDRAL	N20	N22	B17	H35	1	5.8716	1.0	180.000000
DIHEDRAL	H34	B21	N23	N18	1	5.8716	1.0	180.000000
DIHEDRAL	H34	B21	N25	N19	1	5.8716	1.0	180.000000
DIHEDRAL	H34	B21	N7	N6	1	5.8716	1.0	180.000000

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DIHEDRAL	H35	B17	N3	N2	1	5.8716	1.0	180.000000
DIHEDRAL	H35	B17	N5	N4	1	5.8716	1.0	180.000000
DIHEDRAL	C28	C33	C27	H44	1	3.7068	1.0	180.000000
DIHEDRAL	C29	C30	C24	H45	1	3.7068	1.0	180.000000
DIHEDRAL	C31	C32	C26	H46	1	3.7068	1.0	180.000000
DIHEDRAL	H42	C16	C15	C14	1	3.7068	1.0	180.000000
DIHEDRAL	H43	C10	C9	C8	1	3.7068	1.0	180.000000
DIHEDRAL	H47	C13	C12	C11	1	3.7068	1.0	180.000000
DIHEDRAL	H36	C32	C26	N19	1	3.4020	1.0	180.000000
DIHEDRAL	H37	C30	C24	N18	1	3.4020	1.0	180.000000
DIHEDRAL	H38	C33	C27	N20	1	3.4020	1.0	180.000000
DIHEDRAL	H39	C9	C10	N2	1	3.4020	1.0	180.000000
DIHEDRAL	H40	C15	C16	N6	1	3.4020	1.0	180.000000
DIHEDRAL	H41	C12	C13	N4	1	3.4020	1.0	180.000000
DIHEDRAL	H36	C32	C31	N25	1	3.4365	1.0	180.000000
DIHEDRAL	H37	C30	C29	N23	1	3.4365	1.0	180.000000
DIHEDRAL	H38	C33	C28	N22	1	3.4365	1.0	180.000000
DIHEDRAL	H39	C9	C8	N3	1	3.4365	1.0	180.000000
DIHEDRAL	H40	C15	C14	N7	1	3.4365	1.0	180.000000
DIHEDRAL	H41	C12	C11	N5	1	3.4365	1.0	180.000000
DIHEDRAL	H42	C16	N6	N7	1	4.3084	1.0	180.000000
DIHEDRAL	H45	C24	N18	N23	1	4.3084	1.0	180.000000
DIHEDRAL	H48	C11	N5	N4	1	4.3084	1.0	180.000000
DIHEDRAL	H49	C8	N3	N2	1	4.3084	1.0	180.000000
DIHEDRAL	H50	C28	N22	N20	1	4.3084	1.0	180.000000
DIHEDRAL	H51	C31	N25	N19	1	4.3084	1.0	180.000000
DIHEDRAL	H43	C10	N2	N3	1	4.5102	1.0	180.000000
DIHEDRAL	H44	C27	N20	N22	1	4.5102	1.0	180.000000
DIHEDRAL	H46	C26	N19	N25	1	4.5102	1.0	180.000000
DIHEDRAL	H47	C13	N4	N5	1	4.5102	1.0	180.000000
DIHEDRAL	H52	C14	N7	N6	1	4.5102	1.0	180.000000
DIHEDRAL	H53	C29	N23	N18	1	4.5102	1.0	180.000000
DIHEDRAL	C10	N2	Fe1	N4	1	5.0085	1.0	224.352598
DIHEDRAL	C13	N4	Fe1	N20	1	5.0085	1.0	224.352598
DIHEDRAL	N19	Fe1	N6	C16	1	5.0085	1.0	224.352598
DIHEDRAL	C24	N18	Fe1	N6	1	5.0085	1.0	224.352598
DIHEDRAL	C26	N19	Fe1	N18	1	5.0085	1.0	224.352598
DIHEDRAL	C27	N20	Fe1	N2	1	5.0085	1.0	224.352598
DIHEDRAL	N19	Fe1	N2	N3	1	8.4276	1.0	224.352598
DIHEDRAL	N22	N20	Fe1	N18	1	8.4276	1.0	224.352598
DIHEDRAL	N23	N18	Fe1	N20	1	8.4276	1.0	224.352598
DIHEDRAL	N25	N19	Fe1	N2	1	8.4276	1.0	224.352598
DIHEDRAL	N5	N4	Fe1	N6	1	8.4276	1.0	224.352598
DIHEDRAL	N7	N6	Fe1	N4	1	8.4276	1.0	224.352598
DIHEDRAL	C11	N5	B17	N3	1	9.8954	1.0	237.646905
DIHEDRAL	N22	B17	N3	C8	1	9.8954	1.0	237.646905
DIHEDRAL	N23	B21	N7	C14	1	9.8954	1.0	237.646905
DIHEDRAL	C28	N22	B17	N5	1	9.8954	1.0	237.646905
DIHEDRAL	C29	N23	B21	N25	1	9.8954	1.0	237.646905
DIHEDRAL	C31	N25	B21	N7	1	9.8954	1.0	237.646905
DIHEDRAL	N18	N23	B21	N7	1	12.5207	1.0	302.353095
DIHEDRAL	N20	N22	B17	N3	1	12.5207	1.0	302.353095
DIHEDRAL	N22	B17	N5	N4	1	12.5207	1.0	302.353095
DIHEDRAL	N23	B21	N25	N19	1	12.5207	1.0	302.353095
DIHEDRAL	N25	B21	N7	N6	1	12.5207	1.0	302.353095
DIHEDRAL	N5	B17	N3	N2	1	12.5207	1.0	302.353095
DIHEDRAL	C10	N2	Fe1	N6	1	4.6632	1.0	315.647402
DIHEDRAL	C13	N4	Fe1	N18	1	4.6632	1.0	315.647402
DIHEDRAL	C16	N6	Fe1	N2	1	4.6632	1.0	315.647402
DIHEDRAL	C24	N18	Fe1	N4	1	4.6632	1.0	315.647402
DIHEDRAL	C26	N19	Fe1	N20	1	4.6632	1.0	315.647402
DIHEDRAL	C27	N20	Fe1	N19	1	4.6632	1.0	315.647402
DIHEDRAL	N19	Fe1	N18	N23	1	8.0041	1.0	315.647402
DIHEDRAL	N22	N20	Fe1	N4	1	8.0041	1.0	315.647402
DIHEDRAL	N25	N19	Fe1	N6	1	8.0041	1.0	315.647402
DIHEDRAL	N5	N4	Fe1	N2	1	8.0041	1.0	315.647402
DIHEDRAL	N7	N6	Fe1	N18	1	8.0041	1.0	315.647402
DIHEDRAL	N3	N2	Fe1	N20	1	8.0041	1.0	315.647402
improper	i1	i2	i3	i4				k divf phi
IMPROPER	C10	Fe1	N2	N3	1	7.5297	2.0	180.000000
IMPROPER	C13	Fe1	N4	N5	1	7.5297	2.0	180.000000
IMPROPER	C16	Fe1	N6	N7	1	7.5297	2.0	180.000000
IMPROPER	C24	Fe1	N18	N23	1	7.5297	2.0	180.000000
IMPROPER	C26	Fe1	N19	N25	1	7.5297	2.0	180.000000
IMPROPER	C27	Fe1	N20	N22	1	7.5297	2.0	180.000000
IMPROPER	B17	N2	N3	C8	1	10.2565	2.0	180.000000
IMPROPER	B17	N4	N5	C11	1	10.2565	2.0	180.000000
IMPROPER	B17	N20	N22	C28	1	10.2565	2.0	180.000000
IMPROPER	B21	N6	N7	C14	1	10.2565	2.0	180.000000
IMPROPER	B21	N18	N23	C29	1	10.2565	2.0	180.000000

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IMPROPER	B21	N19	N25	C31	1	10.2565	2.0	180.000000
IMPROPER	H49	C9	C8	N3	1	2.8950	2.0	180.000000
IMPROPER	H48	C12	C11	N5	1	2.8950	2.0	180.000000
IMPROPER	H52	C15	C14	N7	1	2.8950	2.0	180.000000
IMPROPER	H50	C33	C28	N22	1	2.8950	2.0	180.000000
IMPROPER	H53	C30	C29	N23	1	2.8950	2.0	180.000000
IMPROPER	H51	C32	C31	N25	1	2.8950	2.0	180.000000
IMPROPER	H39	C10	C9	C8	1	3.3400	2.0	180.000000
IMPROPER	H41	C13	C12	C11	1	3.3400	2.0	180.000000
IMPROPER	H40	C16	C15	C14	1	3.3400	2.0	180.000000
IMPROPER	H37	C24	C30	C29	1	3.3400	2.0	180.000000
IMPROPER	H36	C26	C32	C31	1	3.3400	2.0	180.000000
IMPROPER	H38	C27	C33	C28	1	3.3400	2.0	180.000000
IMPROPER	H43	N2	C10	C9	1	4.8267	2.0	180.000000
IMPROPER	H47	N4	C13	C12	1	4.8267	2.0	180.000000
IMPROPER	H42	N6	C16	C15	1	4.8267	2.0	180.000000
IMPROPER	H45	N18	C24	C30	1	4.8267	2.0	180.000000
IMPROPER	H46	N19	C26	C32	1	4.8267	2.0	180.000000
IMPROPER	H44	N20	C27	C33	1	4.8267	2.0	180.000000

Quintet

bond	i1	i2	k	R
BOND	Fe1	N2	120.0055	2.209972
BOND	Fe1	N4	120.0055	2.209972
BOND	Fe1	N6	120.0055	2.209972
BOND	Fe1	N18	120.0055	2.209972
BOND	Fe1	N20	120.0055	2.209972
BOND	N19	Fe1	120.0055	2.209972
BOND	N2	N3	155.4822	1.346206
BOND	N4	N5	155.4822	1.346206
BOND	N6	N7	155.4822	1.346206
BOND	N18	N23	155.4822	1.346206
BOND	N19	N25	155.4822	1.346206
BOND	N20	N22	155.4822	1.346206
BOND	N2	C10	249.8327	1.337455
BOND	N4	C13	249.8327	1.337455
BOND	N6	C16	249.8327	1.337455
BOND	N18	C24	249.8327	1.337455
BOND	N19	C26	249.8327	1.337455
BOND	N20	C27	249.8327	1.337455
BOND	N3	C8	239.5794	1.347595
BOND	N5	C11	239.5794	1.347595
BOND	N7	C14	239.5794	1.347595
BOND	N22	C28	239.5794	1.347595
BOND	N23	C29	239.5794	1.347595
BOND	N25	C31	239.5794	1.347595
BOND	N3	B17	149.4677	1.541661
BOND	N5	B17	149.4677	1.541661
BOND	N7	B21	149.4677	1.541661
BOND	B17	N22	149.4677	1.541661
BOND	B21	N23	149.4677	1.541661
BOND	B21	N25	149.4677	1.541661
BOND	C8	C9	367.8865	1.386359
BOND	C11	C12	367.8865	1.386359
BOND	C14	C15	367.8865	1.386359
BOND	C28	C33	367.8865	1.386359
BOND	C29	C30	367.8865	1.386359
BOND	C31	C32	367.8865	1.386359
BOND	C8	H49	404.2351	1.083381
BOND	C11	H48	404.2351	1.083381
BOND	C14	H52	404.2351	1.083381
BOND	C28	H50	404.2351	1.083381
BOND	C29	H53	404.2351	1.083381
BOND	C31	H51	404.2351	1.083381
BOND	C9	C10	234.1878	1.398562
BOND	C12	C13	234.1878	1.398562
BOND	C15	C16	234.1878	1.398562
BOND	C24	C30	234.1878	1.398562
BOND	C26	C32	234.1878	1.398562
BOND	C27	C33	234.1878	1.398562
BOND	C9	H39	408.0013	1.083711
BOND	C12	H41	408.0013	1.083711
BOND	C15	H40	408.0013	1.083711
BOND	C30	H37	408.0013	1.083711
BOND	C32	H36	408.0013	1.083711
BOND	C33	H38	408.0013	1.083711
BOND	C10	H43	401.5456	1.083641

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BOND	C13	H47		401.5456	1.083641
BOND	C16	H42		401.5456	1.083641
BOND	C24	H45		401.5456	1.083641
BOND	C26	H46		401.5456	1.083641
BOND	C27	H44		401.5456	1.083641
BOND	B17	H35		246.7146	1.204167
BOND	B21	H34		246.7146	1.204167
angle	i1	i2	i3	k	theta
ANGLE	N18	Fe1	N6	196.2044	85.085129
ANGLE	N19	Fe1	N18	196.2044	85.085129
ANGLE	N19	Fe1	N6	196.2044	85.085129
ANGLE	N20	Fe1	N2	196.2044	85.085129
ANGLE	N20	Fe1	N4	196.2044	85.085129
ANGLE	N4	Fe1	N2	196.2044	85.085129
ANGLE	N18	Fe1	N4	178.9674	94.914871
ANGLE	N19	Fe1	N2	178.9674	94.914871
ANGLE	N19	Fe1	N20	178.9674	94.914871
ANGLE	N20	Fe1	N18	178.9674	94.914871
ANGLE	N6	Fe1	N2	178.9674	94.914871
ANGLE	N6	Fe1	N4	178.9674	94.914871
ANGLE	C10	C9	C8	164.0692	104.181489
ANGLE	C13	C12	C11	164.0692	104.181489
ANGLE	C16	C15	C14	164.0692	104.181489
ANGLE	C28	C33	C27	164.0692	104.181489
ANGLE	C29	C30	C24	164.0692	104.181489
ANGLE	C31	C32	C26	164.0692	104.181489
ANGLE	C10	N2	N3	120.6098	106.631946
ANGLE	C13	N4	N5	120.6098	106.631946
ANGLE	C16	N6	N7	120.6098	106.631946
ANGLE	C24	N18	N23	120.6098	106.631946
ANGLE	C26	N19	N25	120.6098	106.631946
ANGLE	C27	N20	N22	120.6098	106.631946
ANGLE	C12	C11	N5	140.5382	108.240442
ANGLE	C15	C14	N7	140.5382	108.240442
ANGLE	C30	C29	N23	140.5382	108.240442
ANGLE	C32	C31	N25	140.5382	108.240442
ANGLE	C33	C28	N22	140.5382	108.240442
ANGLE	C9	C8	N3	140.5382	108.240442
ANGLE	H34	B21	N23	43.3253	109.234141
ANGLE	H34	B21	N25	43.3253	109.234141
ANGLE	H34	B21	N7	43.3253	109.234141
ANGLE	H35	B17	N22	43.3253	109.234141
ANGLE	H35	B17	N3	43.3253	109.234141
ANGLE	H35	B17	N5	43.3253	109.234141
ANGLE	N22	B17	N3	107.9889	109.707256
ANGLE	N22	B17	N5	107.9889	109.707256
ANGLE	N23	B21	N7	107.9889	109.707256
ANGLE	N25	B21	N23	107.9889	109.707256
ANGLE	N25	B21	N7	107.9889	109.707256
ANGLE	N5	B17	N3	107.9889	109.707256
ANGLE	C11	N5	N4	83.5808	110.329746
ANGLE	C14	N7	N6	83.5808	110.329746
ANGLE	C28	N22	N20	83.5808	110.329746
ANGLE	C29	N23	N18	83.5808	110.329746
ANGLE	C31	N25	N19	83.5808	110.329746
ANGLE	C8	N3	N2	83.5808	110.329746
ANGLE	C12	C13	N4	95.6402	110.616377
ANGLE	C15	C16	N6	95.6402	110.616377
ANGLE	C30	C24	N18	95.6402	110.616377
ANGLE	C32	C26	N19	95.6402	110.616377
ANGLE	C33	C27	N20	95.6402	110.616377
ANGLE	C9	C10	N2	95.6402	110.616377
ANGLE	N22	N20	Fe1	136.3735	117.110707
ANGLE	N23	N18	Fe1	136.3735	117.110707
ANGLE	N25	N19	Fe1	136.3735	117.110707
ANGLE	N3	N2	Fe1	136.3735	117.110707
ANGLE	N5	N4	Fe1	136.3735	117.110707
ANGLE	N7	N6	Fe1	136.3735	117.110707
ANGLE	H42	C16	N6	25.3521	119.823702
ANGLE	H43	C10	N2	25.3521	119.823702
ANGLE	H44	C27	N20	25.3521	119.823702
ANGLE	H45	C24	N18	25.3521	119.823702
ANGLE	H46	C26	N19	25.3521	119.823702
ANGLE	H47	C13	N4	25.3521	119.823702
ANGLE	H48	C11	N5	35.4524	120.693228
ANGLE	H49	C8	N3	35.4524	120.693228
ANGLE	H50	C28	N22	35.4524	120.693228
ANGLE	H51	C31	N25	35.4524	120.693228
ANGLE	H52	C14	N7	35.4524	120.693228
ANGLE	H53	C29	N23	35.4524	120.693228

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ANGLE	B17	N3	N2			91.8493		120.795366
ANGLE	B17	N5	N4			91.8493		120.795366
ANGLE	N20	N22	B17			91.8493		120.795366
ANGLE	B21	N23	N18			91.8493		120.795366
ANGLE	B21	N25	N19			91.8493		120.795366
ANGLE	B21	N7	N6			91.8493		120.795366
ANGLE	H36	C32	C31			33.9263		127.544449
ANGLE	H37	C30	C29			33.9263		127.544449
ANGLE	H38	C33	C28			33.9263		127.544449
ANGLE	H39	C9	C8			33.9263		127.544449
ANGLE	H40	C15	C14			33.9263		127.544449
ANGLE	H41	C12	C11			33.9263		127.544449
ANGLE	H36	C32	C26			33.4787		128.274062
ANGLE	H37	C30	C24			33.4787		128.274062
ANGLE	H38	C33	C27			33.4787		128.274062
ANGLE	H39	C9	C10			33.4787		128.274062
ANGLE	H40	C15	C16			33.4787		128.274062
ANGLE	H41	C12	C13			33.4787		128.274062
ANGLE	B17	N3	C8			103.6144		128.874889
ANGLE	B17	N5	C11			103.6144		128.874889
ANGLE	B21	N7	C14			103.6144		128.874889
ANGLE	C28	N22	B17			103.6144		128.874889
ANGLE	C29	N23	B21			103.6144		128.874889
ANGLE	C31	N25	B21			103.6144		128.874889
ANGLE	H42	C16	C15			36.5874		129.559920
ANGLE	H43	C10	C9			36.5874		129.559920
ANGLE	H44	C27	C33			36.5874		129.559920
ANGLE	H45	C24	C30			36.5874		129.559920
ANGLE	H46	C26	C32			36.5874		129.559920
ANGLE	H47	C13	C12			36.5874		129.559920
ANGLE	H48	C11	C12			32.3226		131.066330
ANGLE	H49	C8	C9			32.3226		131.066330
ANGLE	H50	C28	C33			32.3226		131.066330
ANGLE	H51	C31	C32			32.3226		131.066330
ANGLE	H52	C14	C15			32.3226		131.066330
ANGLE	H53	C29	C30			32.3226		131.066330
ANGLE	C10	N2	Fe1			145.8802		136.257347
ANGLE	C13	N4	Fe1			145.8802		136.257347
ANGLE	C16	N6	Fe1			145.8802		136.257347
ANGLE	C24	N18	Fe1			145.8802		136.257347
ANGLE	C26	N19	Fe1			145.8802		136.257347
ANGLE	C27	N20	Fe1			145.8802		136.257347
dihedral	i1	i2	i3	i4			k divf	phi
DIHEDRAL	C10	C9	C8	N3	1	12.7484	1.0	0.000000
DIHEDRAL	C13	C12	C11	N5	1	12.7484	1.0	0.000000
DIHEDRAL	C16	C15	C14	N7	1	12.7484	1.0	0.000000
DIHEDRAL	C26	C32	C31	N25	1	12.7484	1.0	0.000000
DIHEDRAL	C24	C30	C29	N23	1	12.7484	1.0	0.000000
DIHEDRAL	C27	C33	C28	N22	1	12.7484	1.0	0.000000
DIHEDRAL	C11	C12	C13	N4	1	12.2571	1.0	0.000000
DIHEDRAL	C8	C9	C10	N2	1	12.2571	1.0	0.000000
DIHEDRAL	C14	C15	C16	N6	1	12.2571	1.0	0.000000
DIHEDRAL	C28	C33	C27	N20	1	12.2571	1.0	0.000000
DIHEDRAL	C29	C30	C24	N18	1	12.2571	1.0	0.000000
DIHEDRAL	C31	C32	C26	N19	1	12.2571	1.0	0.000000
DIHEDRAL	C8	N3	N2	C10	1	13.4638	1.0	0.000000
DIHEDRAL	C11	N5	N4	C13	1	13.4638	1.0	0.000000
DIHEDRAL	C14	N7	N6	C16	1	13.4638	1.0	0.000000
DIHEDRAL	C28	N22	N20	C27	1	13.4638	1.0	0.000000
DIHEDRAL	C29	N23	N18	C24	1	13.4638	1.0	0.000000
DIHEDRAL	C31	N25	N19	C26	1	13.4638	1.0	0.000000
DIHEDRAL	C9	C8	N3	N2	1	12.2631	1.0	0.000000
DIHEDRAL	C12	C11	N5	N4	1	12.2631	1.0	0.000000
DIHEDRAL	C15	C14	N7	N6	1	12.2631	1.0	0.000000
DIHEDRAL	C30	C29	N23	N18	1	12.2631	1.0	0.000000
DIHEDRAL	C32	C31	N25	N19	1	12.2631	1.0	0.000000
DIHEDRAL	C33	C28	N22	N20	1	12.2631	1.0	0.000000
DIHEDRAL	C9	C10	N2	N3	1	12.9817	1.0	0.000000
DIHEDRAL	C12	C13	N4	N5	1	12.9817	1.0	0.000000
DIHEDRAL	C15	C16	N6	N7	1	12.9817	1.0	0.000000
DIHEDRAL	C30	C24	N18	N23	1	12.9817	1.0	0.000000
DIHEDRAL	C32	C26	N19	N25	1	12.9817	1.0	0.000000
DIHEDRAL	C33	C27	N20	N22	1	12.9817	1.0	0.000000
DIHEDRAL	B17	N3	N2	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	B17	N22	N20	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	B17	N5	N4	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	B21	N23	N18	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	B21	N25	N19	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	B21	N7	N6	Fe1	1	10.8660	1.0	0.000000
DIHEDRAL	C28	N22	B17	H35	1	3.8593	1.0	0.000000

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DIHEDRAL	C29	N23	B21	H34	1	3.8593	1.0	0.000000
DIHEDRAL	C31	N25	B21	H34	1	3.8593	1.0	0.000000
DIHEDRAL	H34	B21	N7	C14	1	3.8593	1.0	0.000000
DIHEDRAL	H35	B17	N3	C8	1	3.8593	1.0	0.000000
DIHEDRAL	H35	B17	N5	C11	1	3.8593	1.0	0.000000
DIHEDRAL	H36	C32	C26	H46	1	2.0399	1.0	360.000000
DIHEDRAL	H37	C30	C24	H45	1	2.0399	1.0	360.000000
DIHEDRAL	H38	C33	C27	H44	1	2.0399	1.0	360.000000
DIHEDRAL	H42	C16	C15	H40	1	2.0399	1.0	360.000000
DIHEDRAL	H43	C10	C9	H39	1	2.0399	1.0	360.000000
DIHEDRAL	H47	C13	C12	H41	1	2.0399	1.0	360.000000
DIHEDRAL	H36	C32	C31	H51	1	1.8451	1.0	360.000000
DIHEDRAL	H37	C30	C29	H53	1	1.8451	1.0	360.000000
DIHEDRAL	H38	C33	C28	H50	1	1.8451	1.0	360.000000
DIHEDRAL	H39	C9	C8	H49	1	1.8451	1.0	360.000000
DIHEDRAL	H40	C15	C14	H52	1	1.8451	1.0	360.000000
DIHEDRAL	H41	C12	C11	H48	1	1.8451	1.0	360.000000
DIHEDRAL	H42	C16	N6	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H43	C10	N2	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H44	C27	N20	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H45	C24	N18	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H46	C26	N19	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H47	C13	N4	Fe1	1	3.1442	1.0	360.000000
DIHEDRAL	H48	C11	N5	B17	1	3.3589	1.0	360.000000
DIHEDRAL	H49	C8	N3	B17	1	3.3589	1.0	360.000000
DIHEDRAL	H50	C28	N22	B17	1	3.3589	1.0	360.000000
DIHEDRAL	H51	C31	N25	B21	1	3.3589	1.0	360.000000
DIHEDRAL	H52	C14	N7	B21	1	3.3589	1.0	360.000000
DIHEDRAL	H53	C29	N23	B21	1	3.3589	1.0	360.000000
DIHEDRAL	C13	N4	Fe1	N6	1	3.5433	1.0	42.736913
DIHEDRAL	C16	N6	Fe1	N4	1	3.5433	1.0	42.736913
DIHEDRAL	N19	Fe1	N2	C10	1	3.5433	1.0	42.736913
DIHEDRAL	C24	N18	Fe1	N20	1	3.5433	1.0	42.736913
DIHEDRAL	C26	N19	Fe1	N2	1	3.5433	1.0	42.736913
DIHEDRAL	C27	N20	Fe1	N18	1	3.5433	1.0	42.736913
DIHEDRAL	N19	Fe1	N6	N7	1	7.9079	1.0	42.736913
DIHEDRAL	N22	N20	Fe1	N2	1	7.9079	1.0	42.736913
DIHEDRAL	N23	N18	Fe1	N6	1	7.9079	1.0	42.736913
DIHEDRAL	N25	N19	Fe1	N18	1	7.9079	1.0	42.736913
DIHEDRAL	N3	N2	Fe1	N4	1	7.9079	1.0	42.736913
DIHEDRAL	N5	N4	Fe1	N20	1	7.9079	1.0	42.736913
DIHEDRAL	N19	N25	B21	N7	1	11.6485	1.0	60.291424
DIHEDRAL	N20	N22	B17	N5	1	11.6485	1.0	60.291424
DIHEDRAL	N22	B17	N3	N2	1	11.6485	1.0	60.291424
DIHEDRAL	N23	B21	N7	N6	1	11.6485	1.0	60.291424
DIHEDRAL	N25	B21	N23	N18	1	11.6485	1.0	60.291424
DIHEDRAL	N4	N5	B17	N3	1	11.6485	1.0	60.291424
DIHEDRAL	N22	B17	N5	C11	1	11.7635	1.0	119.708576
DIHEDRAL	N25	B21	N7	C14	1	11.7635	1.0	119.708576
DIHEDRAL	C28	N22	B17	N3	1	11.7635	1.0	119.708576
DIHEDRAL	C29	N23	B21	N7	1	11.7635	1.0	119.708576
DIHEDRAL	C31	N25	B21	N23	1	11.7635	1.0	119.708576
DIHEDRAL	N5	B17	N3	C8	1	11.7635	1.0	119.708576
DIHEDRAL	C10	N2	Fe1	N20	1	4.2135	1.0	137.263087
DIHEDRAL	C13	N4	Fe1	N2	1	4.2135	1.0	137.263087
DIHEDRAL	C16	N6	Fe1	N18	1	4.2135	1.0	137.263087
DIHEDRAL	N19	Fe1	N18	C24	1	4.2135	1.0	137.263087
DIHEDRAL	C26	N19	Fe1	N6	1	4.2135	1.0	137.263087
DIHEDRAL	C27	N20	Fe1	N4	1	4.2135	1.0	137.263087
DIHEDRAL	N22	N20	Fe1	N19	1	8.9050	1.0	137.263087
DIHEDRAL	N23	N18	Fe1	N4	1	8.9050	1.0	137.263087
DIHEDRAL	N25	N19	Fe1	N20	1	8.9050	1.0	137.263087
DIHEDRAL	N3	N2	Fe1	N6	1	8.9050	1.0	137.263087
DIHEDRAL	N5	N4	Fe1	N18	1	8.9050	1.0	137.263087
DIHEDRAL	N7	N6	Fe1	N2	1	8.9050	1.0	137.263087
DIHEDRAL	C10	C9	C8	H49	1	3.5267	1.0	180.000000
DIHEDRAL	H51	C31	C32	C26	1	3.5267	1.0	180.000000
DIHEDRAL	C13	C12	C11	H48	1	3.5267	1.0	180.000000
DIHEDRAL	C16	C15	C14	H52	1	3.5267	1.0	180.000000
DIHEDRAL	H50	C28	C33	C27	1	3.5267	1.0	180.000000
DIHEDRAL	H53	C29	C30	C24	1	3.5267	1.0	180.000000
DIHEDRAL	C11	N5	N4	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C14	N7	N6	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C28	N22	N20	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C29	N23	N18	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C31	N25	N19	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C8	N3	N2	Fe1	1	15.1662	1.0	180.000000
DIHEDRAL	C12	C11	N5	B17	1	15.3220	1.0	180.000000
DIHEDRAL	C9	C8	N3	B17	1	15.3220	1.0	180.000000
DIHEDRAL	C15	C14	N7	B21	1	15.3220	1.0	180.000000

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DIHEDRAL	C30	C29	N23	B21	1	15.3220	1.0	180.000000
DIHEDRAL	C32	C31	N25	B21	1	15.3220	1.0	180.000000
DIHEDRAL	C33	C28	N22	B17	1	15.3220	1.0	180.000000
DIHEDRAL	C12	C13	N4	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	C15	C16	N6	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	C30	C24	N18	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	C32	C26	N19	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	C33	C27	N20	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	C9	C10	N2	Fe1	1	8.1759	1.0	180.000000
DIHEDRAL	B17	N3	N2	C10	1	17.6121	1.0	180.000000
DIHEDRAL	B17	N5	N4	C13	1	17.6121	1.0	180.000000
DIHEDRAL	B21	N23	N18	C24	1	17.6121	1.0	180.000000
DIHEDRAL	B21	N25	N19	C26	1	17.6121	1.0	180.000000
DIHEDRAL	B21	N7	N6	C16	1	17.6121	1.0	180.000000
DIHEDRAL	C27	N20	N22	B17	1	17.6121	1.0	180.000000
DIHEDRAL	N20	N22	B17	H35	1	5.7732	1.0	180.000000
DIHEDRAL	H34	B21	N23	N18	1	5.7732	1.0	180.000000
DIHEDRAL	H34	B21	N25	N19	1	5.7732	1.0	180.000000
DIHEDRAL	H34	B21	N7	N6	1	5.7732	1.0	180.000000
DIHEDRAL	H35	B17	N3	N2	1	5.7732	1.0	180.000000
DIHEDRAL	H35	B17	N5	N4	1	5.7732	1.0	180.000000
DIHEDRAL	C28	C33	C27	H44	1	4.0944	1.0	180.000000
DIHEDRAL	C29	C30	C24	H45	1	4.0944	1.0	180.000000
DIHEDRAL	C31	C32	C26	H46	1	4.0944	1.0	180.000000
DIHEDRAL	H42	C16	C15	C14	1	4.0944	1.0	180.000000
DIHEDRAL	H43	C10	C9	C8	1	4.0944	1.0	180.000000
DIHEDRAL	H47	C13	C12	C11	1	4.0944	1.0	180.000000
DIHEDRAL	H36	C32	C26	N19	1	3.4380	1.0	180.000000
DIHEDRAL	H37	C30	C24	N18	1	3.4380	1.0	180.000000
DIHEDRAL	H38	C33	C27	N20	1	3.4380	1.0	180.000000
DIHEDRAL	H39	C9	C10	N2	1	3.4380	1.0	180.000000
DIHEDRAL	H40	C15	C16	N6	1	3.4380	1.0	180.000000
DIHEDRAL	H41	C12	C13	N4	1	3.4380	1.0	180.000000
DIHEDRAL	H36	C32	C31	N25	1	3.5614	1.0	180.000000
DIHEDRAL	H37	C30	C29	N23	1	3.5614	1.0	180.000000
DIHEDRAL	H38	C33	C28	N22	1	3.5614	1.0	180.000000
DIHEDRAL	H39	C9	C8	N3	1	3.5614	1.0	180.000000
DIHEDRAL	H40	C15	C14	N7	1	3.5614	1.0	180.000000
DIHEDRAL	H41	C12	C11	N5	1	3.5614	1.0	180.000000
DIHEDRAL	H42	C16	N6	N7	1	4.7141	1.0	180.000000
DIHEDRAL	H45	C24	N18	N23	1	4.7141	1.0	180.000000
DIHEDRAL	H48	C11	N5	N4	1	4.7141	1.0	180.000000
DIHEDRAL	H49	C8	N3	N2	1	4.7141	1.0	180.000000
DIHEDRAL	H50	C28	N22	N20	1	4.7141	1.0	180.000000
DIHEDRAL	H51	C31	N25	N19	1	4.7141	1.0	180.000000
DIHEDRAL	H43	C10	N2	N3	1	4.9576	1.0	180.000000
DIHEDRAL	H44	C27	N20	N22	1	4.9576	1.0	180.000000
DIHEDRAL	H46	C26	N19	N25	1	4.9576	1.0	180.000000
DIHEDRAL	H47	C13	N4	N5	1	4.9576	1.0	180.000000
DIHEDRAL	H52	C14	N7	N6	1	4.9576	1.0	180.000000
DIHEDRAL	H53	C29	N23	N18	1	4.9576	1.0	180.000000
DIHEDRAL	C10	N2	Fe1	N4	1	4.2130	1.0	222.736913
DIHEDRAL	C13	N4	Fe1	N20	1	4.2130	1.0	222.736913
DIHEDRAL	N19	Fe1	N6	C16	1	4.2130	1.0	222.736913
DIHEDRAL	C24	N18	Fe1	N6	1	4.2130	1.0	222.736913
DIHEDRAL	C26	N19	Fe1	N18	1	4.2130	1.0	222.736913
DIHEDRAL	C27	N20	Fe1	N2	1	4.2130	1.0	222.736913
DIHEDRAL	N19	Fe1	N2	N3	1	8.9054	1.0	222.736913
DIHEDRAL	N22	N20	Fe1	N18	1	8.9054	1.0	222.736913
DIHEDRAL	N23	N18	Fe1	N20	1	8.9054	1.0	222.736913
DIHEDRAL	N25	N19	Fe1	N2	1	8.9054	1.0	222.736913
DIHEDRAL	N5	N4	Fe1	N6	1	8.9054	1.0	222.736913
DIHEDRAL	N7	N6	Fe1	N4	1	8.9054	1.0	222.736913
DIHEDRAL	C11	N5	B17	N3	1	11.7621	1.0	240.291424
DIHEDRAL	N22	B17	N3	C8	1	11.7621	1.0	240.291424
DIHEDRAL	N23	B21	N7	C14	1	11.7621	1.0	240.291424
DIHEDRAL	C28	N22	B17	N5	1	11.7621	1.0	240.291424
DIHEDRAL	C29	N23	B21	N25	1	11.7621	1.0	240.291424
DIHEDRAL	C31	N25	B21	N7	1	11.7621	1.0	240.291424
DIHEDRAL	N18	N23	B21	N7	1	11.6482	1.0	299.708576
DIHEDRAL	N20	N22	B17	N3	1	11.6482	1.0	299.708576
DIHEDRAL	N22	B17	N5	N4	1	11.6482	1.0	299.708576
DIHEDRAL	N23	B21	N25	N19	1	11.6482	1.0	299.708576
DIHEDRAL	N25	B21	N7	N6	1	11.6482	1.0	299.708576
DIHEDRAL	N5	B17	N3	N2	1	11.6482	1.0	299.708576
DIHEDRAL	C10	N2	Fe1	N6	1	3.5431	1.0	317.263087
DIHEDRAL	C13	N4	Fe1	N18	1	3.5431	1.0	317.263087
DIHEDRAL	C16	N6	Fe1	N2	1	3.5431	1.0	317.263087
DIHEDRAL	C24	N18	Fe1	N4	1	3.5431	1.0	317.263087
DIHEDRAL	C26	N19	Fe1	N20	1	3.5431	1.0	317.263087

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DIHEDRAL	C27	N20	Fe1	N19	1	3.5431	1.0	317.263087
DIHEDRAL	N19	Fe1	N18	N23	1	7.9076	1.0	317.263087
DIHEDRAL	N22	N20	Fe1	N4	1	7.9076	1.0	317.263087
DIHEDRAL	N25	N19	Fe1	N6	1	7.9076	1.0	317.263087
DIHEDRAL	N5	N4	Fe1	N2	1	7.9076	1.0	317.263087
DIHEDRAL	N7	N6	Fe1	N18	1	7.9076	1.0	317.263087
DIHEDRAL	N3	N2	Fe1	N20	1	7.9076	1.0	317.263087
improper	i1	i2	i3	i4				k divf phi
IMPROPER	C10	Fe1	N2	N3	1	6.3484	2.0	180.000000
IMPROPER	C13	Fe1	N4	N5	1	6.3484	2.0	180.000000
IMPROPER	C16	Fe1	N6	N7	1	6.3484	2.0	180.000000
IMPROPER	C24	Fe1	N18	N23	1	6.3484	2.0	180.000000
IMPROPER	C26	Fe1	N19	N25	1	6.3484	2.0	180.000000
IMPROPER	C27	Fe1	N20	N22	1	6.3484	2.0	180.000000
IMPROPER	B17	N2	N3	C8	1	10.4360	2.0	180.000000
IMPROPER	B17	N4	N5	C11	1	10.4360	2.0	180.000000
IMPROPER	B17	N20	N22	C28	1	10.4360	2.0	180.000000
IMPROPER	B21	N6	N7	C14	1	10.4360	2.0	180.000000
IMPROPER	B21	N18	N23	C29	1	10.4360	2.0	180.000000
IMPROPER	B21	N19	N25	C31	1	10.4360	2.0	180.000000
IMPROPER	H49	C9	C8	N3	1	3.5273	2.0	180.000000
IMPROPER	H48	C12	C11	N5	1	3.5273	2.0	180.000000
IMPROPER	H52	C15	C14	N7	1	3.5273	2.0	180.000000
IMPROPER	H50	C33	C28	N22	1	3.5273	2.0	180.000000
IMPROPER	H53	C30	C29	N23	1	3.5273	2.0	180.000000
IMPROPER	H51	C32	C31	N25	1	3.5273	2.0	180.000000
IMPROPER	H39	C10	C9	C8	1	3.6459	2.0	180.000000
IMPROPER	H41	C13	C12	C11	1	3.6459	2.0	180.000000
IMPROPER	H40	C16	C15	C14	1	3.6459	2.0	180.000000
IMPROPER	H37	C24	C30	C29	1	3.6459	2.0	180.000000
IMPROPER	H36	C26	C32	C31	1	3.6459	2.0	180.000000
IMPROPER	H38	C27	C33	C28	1	3.6459	2.0	180.000000
IMPROPER	H43	N2	C10	C9	1	5.6038	2.0	180.000000
IMPROPER	H47	N4	C13	C12	1	5.6038	2.0	180.000000
IMPROPER	H42	N6	C16	C15	1	5.6038	2.0	180.000000
IMPROPER	H45	N18	C24	C30	1	5.6038	2.0	180.000000
IMPROPER	H46	N19	C26	C32	1	5.6038	2.0	180.000000
IMPROPER	H44	N20	C27	C33	1	5.6038	2.0	180.000000