

Two polymorphs of luminescent (2-fluoro-3-pyridyl)(2,2'-biphenyl)borinic 8-oxyquinolate – structures and properties

Supplementary Information

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Table of content:

1. Crystallographic data.....	S2-S25
2. DSC data	S26-S28
2. Energies of interactions and CT properties	S29-S31
3. Energy scan (Θ - constrained)	S32-S134

Table S1. Refinement details

	I-ortho	II-tric
Chemical formula	C ₂₆ H ₁₈ BF ₁ N ₂ O	C ₂₆ H ₁₈ BF ₁ N ₂ O
M_r	808.50	808.50
space group	<i>Pca</i> 2 ₁	<i>P</i> -1
Cell settings:	12.3765(7)	11.18331(13)
a, b, c (Å)	14.9478(9)	12.02706(13)
	21.9246(13)	15.06878(16)
α, β, γ (°)	90.000	91.5953(9)
	90.000	91.9937(9)
	90.000	96.6478(9)
V (Å ³)	4056.1(4)	2010.90(4)
Z	8	4
d (Mg·m ⁻³)	1.32	1.34
No. of measured, independent and observed [$F^2 > 2\sigma(F^2)$]	45654 6388 6073	61584 12260 10932
R_{int} (%)	5.6	1.9
θ_{max}	30.66	30.51
$R[F^2 > 2\sigma(F^2)]$,	0.045	0.047
$wR(F^2)$,	0.103	0.079
GooF	1.00	1.00
No. of parameters	559	559
Reflection used [cutoff $I > -3 \sigma(I)$]	6370	12226
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e·Å ⁻³)	0.46, -0.25	0.46, -0.26

X-ray powder diffraction. The powder X-ray diffraction patterns were collected at room temperature. Collected data were compared with each other and with simulated patterns. The relative shifts of some parts of simulated patterns can be shifted with respect to experimental data since simulated X-ray powder diffraction patterns were calculated on the basis of crystal structures measured at 100 K. Even though main features of the experimental patterns were reproduced by theoretical data. Both forms can be distinguished from each other on the basis of the X-ray powder diffraction patterns.

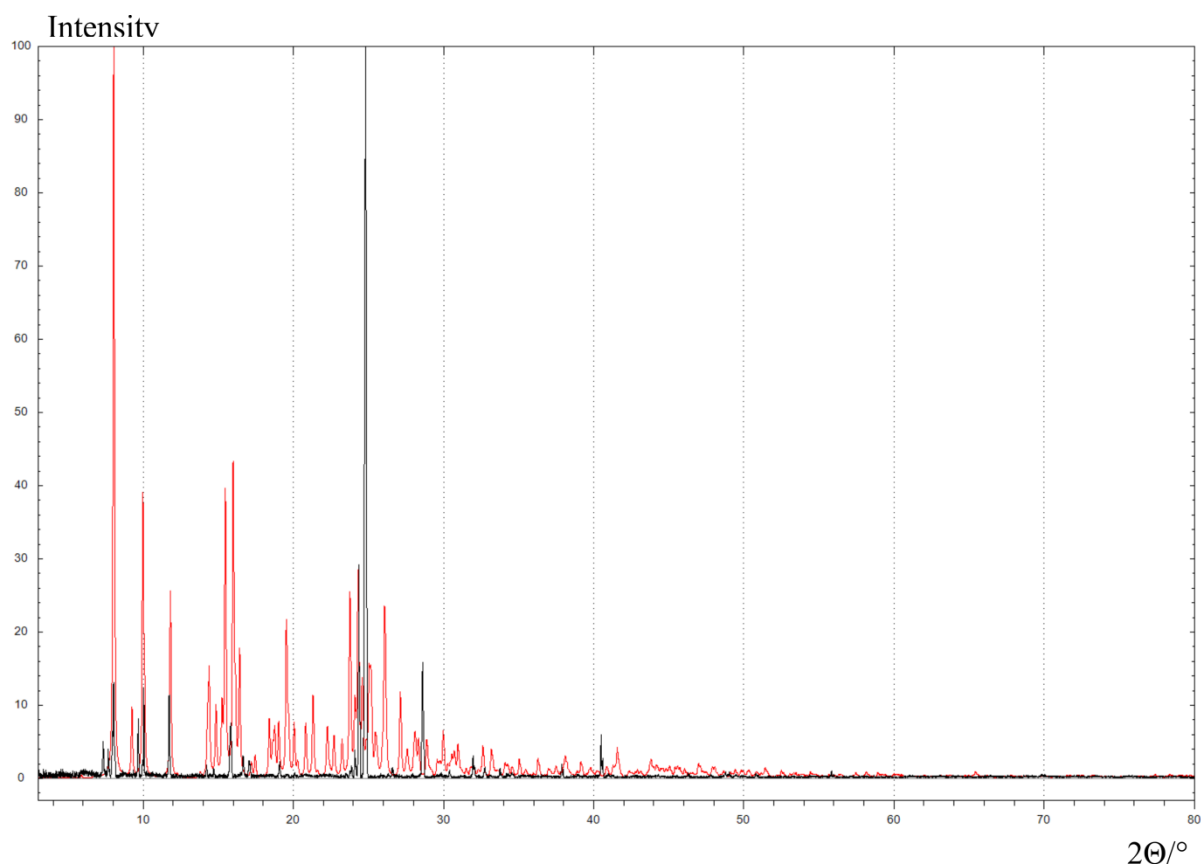


Figure S1. Experimental (black solid line) and simulated (red solid line) powder X-ray diffraction patterns of form **I-ortho**.

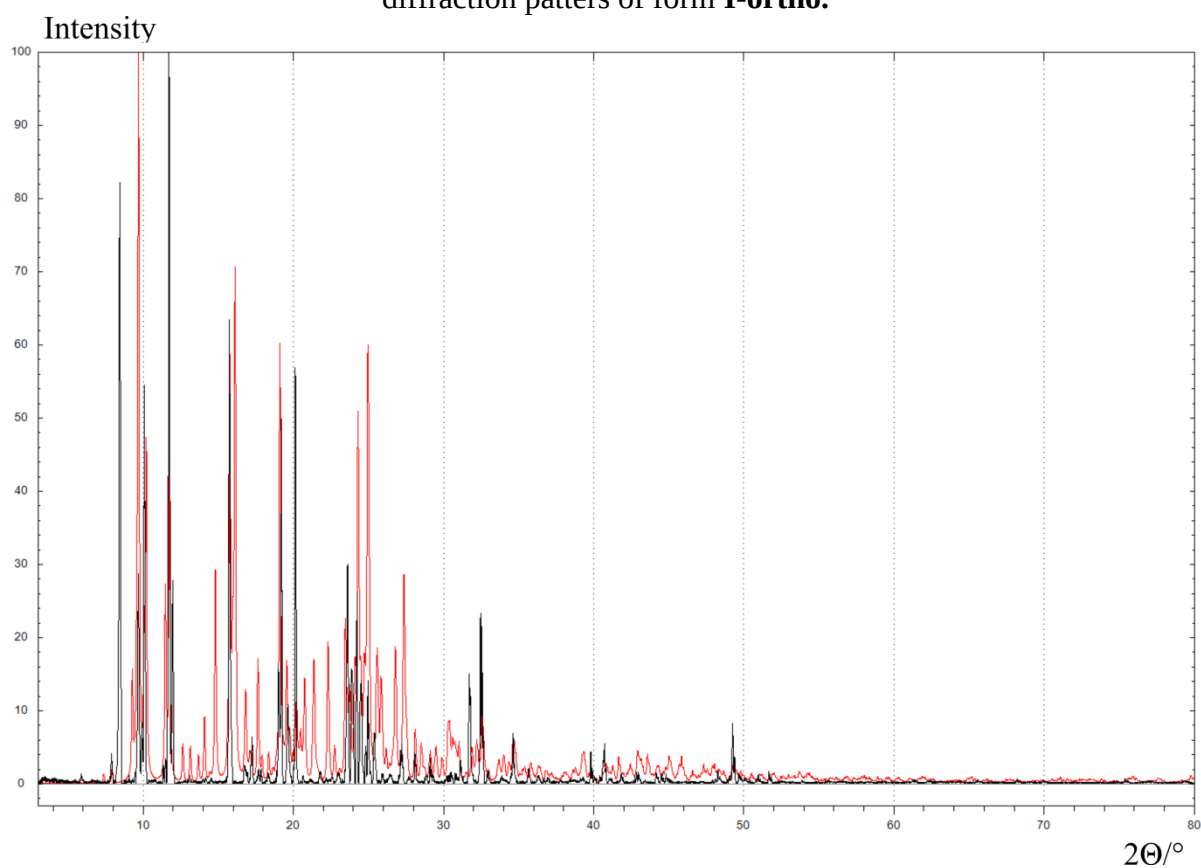


Figure S2. Experimental (black solid line) and simulated (red solid line) powder X-ray diffraction patterns of form **II-tric**.

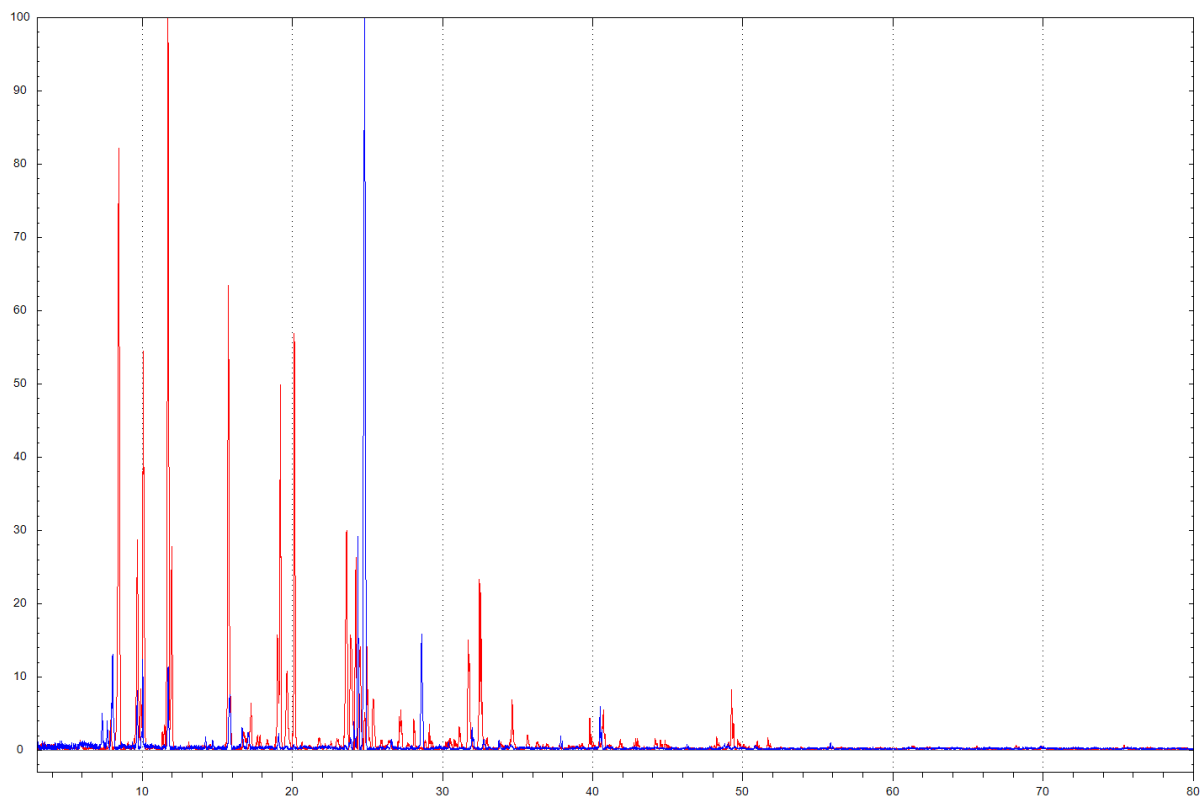


Figure S3. Experimental (blue solid line) and experimental (red solid line) powder X-ray diffraction patterns of form **I-ortho** and **II-tric**, respectively.

Table S2. Cartesian coordinates for **I-ortho**.

Number	Label	X	Y	Z
1	H5	0.1338	0.1203	0.4361
2	H6	−0.0411	0.1727	0.4418
3	H7	−0.0852	0.3255	0.4302
4	N1	0.24884(13)	0.40121(10)	0.40756(8)
5	N2	0.28902(16)	0.53844(12)	0.23315(9)
6	O1	0.06635(11)	0.45532(9)	0.41341(7)
7	F1	0.35648(11)	0.55966(10)	0.32676(7)
8	B1	0.17646(17)	0.49086(14)	0.39607(10)
9	H1	0.4045	0.4303	0.3990
10	H2	0.4647	0.2818	0.4080
11	H3	0.3432	0.1657	0.4222
12	H12	0.0327	0.4527	0.3005
13	H13	0.0536	0.4616	0.1945
14	H14	0.2158	0.5145	0.1543
15	H17	0.2886	0.6558	0.5685
16	H18	0.2425	0.7931	0.5243
17	H19	0.1751	0.7965	0.4243
18	H20	0.1528	0.6636	0.3705

19	H22	0.4430	0.5189	0.5220
20	H23	0.5007	0.3859	0.5684
21	H24	0.3746	0.2843	0.6058
22	H25	0.1901	0.3129	0.5943
23	H26	0.1318	0.4419	0.5439
24	C1	0.35393(16)	0.38323(14)	0.40459(10)
25	C2	0.38958(16)	0.29462(15)	0.41007(11)
26	C3	0.31773(17)	0.22546(14)	0.41893(11)
27	C4	0.20578(16)	0.24325(12)	0.42202(9)
28	C5	0.11956(17)	0.18247(13)	0.43177(10)
29	C6	0.01538(17)	0.21454(13)	0.43481(10)
30	C7	−0.01213(16)	0.30614(13)	0.42828(9)
31	C8	0.07046(15)	0.36575(12)	0.41890(9)
32	C9	0.17691(15)	0.33344(12)	0.41609(9)
33	C10	0.27215(16)	0.53249(13)	0.29173(10)
34	C11	0.18076(15)	0.50206(12)	0.32262(9)
35	C12	0.09814(17)	0.47485(13)	0.28367(10)
36	C13	0.11033(19)	0.47973(14)	0.22093(11)
37	C14	0.2068(2)	0.51162(15)	0.19728(10)
38	C15	0.20457(15)	0.57738(12)	0.43638(9)
39	C16	0.24655(17)	0.57717(13)	0.49631(10)
40	C17	0.26049(19)	0.65750(15)	0.52820(10)
41	C18	0.23342(18)	0.73925(14)	0.50188(11)
42	C19	0.19346(18)	0.74116(14)	0.44291(11)
43	C20	0.17984(16)	0.66117(13)	0.41103(10)
44	C21	0.28145(18)	0.49320(15)	0.52752(9)
45	C22	0.3915(2)	0.47642(17)	0.53582(11)
46	C23	0.4258(2)	0.3982(2)	0.56418(12)
47	C24	0.3512(3)	0.33738(18)	0.58594(12)
48	C25	0.2416(3)	0.35426(15)	0.57883(11)
49	C26	0.2068(2)	0.43134(15)	0.54947(11)
50	H31	−0.0679	0.6292	0.2290
51	H32	0.1118	0.6627	0.2460
52	H33	0.1702	0.8084	0.2739
53	H38	0.0510	0.9582	0.4006
54	H39	0.0123	0.9655	0.5053
55	H40	−0.1604	1.0073	0.5364
56	H43	−0.0905	1.1596	0.1162
57	H44	−0.1112	1.2963	0.1668
58	H45	−0.1107	1.2996	0.2734
59	H46	−0.0993	1.1671	0.3283
60	H48	0.0954	0.9827	0.1742
61	H49	0.1192	0.8487	0.1201
62	H50	−0.0259	0.7856	0.0673

63	H51	−0.1951	0.8539	0.0707
64	H52	−0.2198	0.9872	0.1249
65	N3	−0.15454(13)	0.91175(11)	0.27490(8)
66	N4	−0.22019(15)	1.03276(12)	0.45441(9)
67	O2	0.03282(11)	0.94768(9)	0.28927(7)
68	F2	−0.27148(10)	1.05753(9)	0.35811(6)
69	B2	−0.07502(16)	0.99286(14)	0.29803(10)
70	H27	−0.3064	0.9540	0.2733
71	H28	−0.3811	0.8159	0.2443
72	H29	−0.2718	0.6923	0.2292
73	C27	−0.26043(16)	0.90395(13)	0.26717(10)
74	C28	−0.30519(17)	0.82112(15)	0.24962(11)
75	C29	−0.24066(17)	0.74785(14)	0.24079(10)
76	C30	−0.12739(16)	0.75465(13)	0.24881(10)
77	C31	−0.04705(18)	0.68782(14)	0.24092(10)
78	C32	0.05969(18)	0.70889(14)	0.25066(11)
79	C33	0.09578(16)	0.79543(14)	0.26815(10)
80	C34	0.01914(15)	0.86095(13)	0.27578(9)
81	C35	−0.09010(15)	0.83931(12)	0.26631(9)
82	C36	−0.19255(15)	1.03016(13)	0.39683(10)
83	C37	−0.09503(15)	1.00285(12)	0.37057(9)
84	C38	−0.01809(16)	0.97766(12)	0.41396(9)
85	C39	−0.04119(18)	0.98079(14)	0.47603(10)
86	C40	−0.14345(19)	1.00739(15)	0.49413(10)
87	C41	−0.08596(15)	1.08161(12)	0.25675(9)
88	C42	−0.08182(17)	1.08097(13)	0.19244(10)
89	C43	−0.0919(2)	1.16098(15)	0.15951(11)
90	C44	−0.1036(2)	1.24246(15)	0.18943(12)
91	C45	−0.10484(17)	1.24413(13)	0.25247(12)
92	C46	−0.09705(16)	1.16477(13)	0.28507(10)
93	C47	−0.06534(18)	0.99687(14)	0.15640(9)
94	C48	0.03587(19)	0.95608(15)	0.15374(10)
95	C49	0.0505(2)	0.87701(16)	0.12118(11)
96	C50	−0.0357(2)	0.83921(16)	0.08991(11)
97	C51	−0.1359(2)	0.88045(18)	0.09141(11)
98	C52	−0.1510(2)	0.95903(16)	0.12449(10)

Table S3. Atomic displacement parameters for **I-ortho**.

Label	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
N1	0.0107(6)	0.0128(6)	0.0153(7)	0.0009(6)	0.0014(5)	0.0004(5)
N2	0.0263(9)	0.0169(8)	0.0201(9)	0.0020(6)	0.0070(7)	0.0023(7)
N3	0.0107(6)	0.0122(7)	0.0119(6)	−0.0013(5)	0.0001(5)	0.0004(5)
N4	0.0173(8)	0.0200(8)	0.0185(8)	−0.0038(6)	0.0041(6)	−0.0040(6)

O1	0.0109(6)	0.0114(6)	0.0185(6)	0.0012(5)	0.0012(5)	−0.0003(4)
O2	0.0094(5)	0.0121(6)	0.0171(6)	−0.0019(5)	−0.0003(5)	0.0006(4)
F1	0.0146(5)	0.0297(7)	0.0261(7)	0.0057(6)	0.0009(5)	−0.0062(5)
F2	0.0109(5)	0.0254(6)	0.0211(6)	−0.0044(5)	−0.0013(4)	0.0036(4)
B1	0.0094(8)	0.0109(8)	0.0167(9)	0.0015(7)	−0.0006(7)	−0.0007(6)
B2	0.0085(8)	0.0106(8)	0.0146(8)	−0.0005(7)	−0.0009(7)	0.0003(6)
C1	0.0120(8)	0.0173(8)	0.0192(9)	0.0004(7)	−0.0003(7)	−0.0002(6)
C2	0.0133(8)	0.0201(9)	0.0240(10)	0.0011(8)	0.0003(7)	0.0035(7)
C3	0.0175(9)	0.0165(8)	0.0221(9)	−0.0004(7)	−0.0011(7)	0.0051(7)
C4	0.0187(8)	0.0110(7)	0.0141(8)	0.0003(6)	−0.0008(7)	0.0010(6)
C5	0.0213(9)	0.0119(7)	0.0191(9)	0.0014(7)	−0.0003(7)	−0.0024(7)
C6	0.0206(9)	0.0150(8)	0.0168(9)	0.0016(7)	−0.0004(7)	−0.0057(7)
C7	0.0140(8)	0.0156(8)	0.0155(8)	0.0011(7)	0.0001(7)	−0.0025(6)
C8	0.0136(8)	0.0135(7)	0.0123(8)	0.0002(6)	0.0007(6)	−0.0007(6)
C9	0.0141(8)	0.0121(7)	0.0114(7)	−0.0002(6)	−0.0002(6)	0.0004(6)
C10	0.0155(8)	0.0126(8)	0.0192(9)	0.0025(7)	0.0025(7)	0.0010(6)
C11	0.0114(7)	0.0113(7)	0.0162(8)	0.0010(6)	0.0013(6)	0.0014(6)
C12	0.0181(9)	0.0137(8)	0.0189(9)	0.0000(7)	−0.0003(7)	0.0006(7)
C13	0.0259(10)	0.0187(9)	0.0201(9)	−0.0040(8)	−0.0054(8)	0.0043(7)
C14	0.0345(12)	0.0178(9)	0.0143(8)	−0.0010(7)	0.0029(8)	0.0078(8)
C15	0.0120(7)	0.0124(7)	0.0177(9)	0.0006(7)	0.0012(7)	−0.0009(6)
C16	0.0163(8)	0.0154(8)	0.0169(8)	0.0023(7)	0.0007(7)	−0.0012(7)
C17	0.0241(10)	0.0216(9)	0.0181(9)	−0.0042(8)	0.0003(8)	−0.0020(8)
C18	0.0225(10)	0.0158(8)	0.0270(11)	−0.0055(8)	0.0014(8)	−0.0019(7)
C19	0.0189(9)	0.0123(8)	0.0300(11)	−0.0003(8)	0.0023(8)	0.0009(7)
C20	0.0153(8)	0.0143(8)	0.0213(9)	0.0011(7)	−0.0010(7)	0.0012(6)
C21	0.0217(9)	0.0203(9)	0.0115(7)	−0.0007(7)	−0.0027(7)	−0.0007(7)
C22	0.0229(11)	0.0308(11)	0.0229(10)	0.0059(9)	0.0003(8)	0.0025(9)
C23	0.0357(13)	0.0366(13)	0.0243(11)	0.0052(10)	−0.0038(10)	0.0124(11)
C24	0.0511(16)	0.0245(11)	0.0200(10)	0.0030(8)	−0.0070(10)	0.0095(11)
C25	0.0470(15)	0.0192(10)	0.0205(10)	0.0017(8)	−0.0094(10)	−0.0076(10)
C26	0.0279(10)	0.0222(10)	0.0175(9)	0.0006(8)	−0.0046(8)	−0.0061(8)
C27	0.0123(8)	0.0180(8)	0.0172(8)	−0.0024(7)	−0.0007(7)	0.0007(6)
C28	0.0143(8)	0.0215(9)	0.0225(10)	−0.0040(8)	−0.0015(7)	−0.0052(7)
C29	0.0201(9)	0.0163(8)	0.0204(9)	−0.0034(7)	−0.0010(7)	−0.0052(7)
C30	0.0189(8)	0.0120(7)	0.0165(8)	−0.0026(7)	−0.0005(7)	0.0001(6)
C31	0.0253(10)	0.0118(8)	0.0224(10)	−0.0031(7)	−0.0010(8)	0.0022(7)
C32	0.0233(10)	0.0153(8)	0.0235(10)	−0.0026(8)	−0.0022(8)	0.0076(7)
C33	0.0137(8)	0.0179(8)	0.0217(9)	−0.0017(7)	−0.0016(7)	0.0053(7)
C34	0.0129(7)	0.0132(8)	0.0134(8)	0.0001(6)	−0.0002(6)	0.0007(6)
C35	0.0130(7)	0.0131(7)	0.0120(7)	−0.0006(6)	0.0000(6)	0.0008(6)
C36	0.0116(8)	0.0137(8)	0.0186(9)	−0.0032(6)	−0.0024(7)	−0.0011(6)
C37	0.0108(7)	0.0111(7)	0.0135(7)	−0.0015(6)	0.0008(6)	−0.0017(6)
C38	0.0125(8)	0.0130(7)	0.0178(8)	0.0011(7)	−0.0022(7)	−0.0022(6)

C39	0.0222(9)	0.0182(9)	0.0149(8)	0.0015(7)	−0.0043(7)	−0.0053(7)
C40	0.0259(10)	0.0225(10)	0.0152(8)	−0.0030(7)	0.0033(8)	−0.0075(8)
C41	0.0107(7)	0.0122(7)	0.0159(8)	−0.0001(6)	−0.0009(6)	0.0005(6)
C42	0.0174(8)	0.0143(8)	0.0163(8)	0.0009(7)	−0.0013(7)	−0.0010(7)
C43	0.0292(11)	0.0200(9)	0.0204(9)	0.0082(8)	−0.0008(8)	0.0004(8)
C44	0.0291(11)	0.0158(9)	0.0301(12)	0.0081(8)	−0.0001(9)	0.0023(8)
C45	0.0191(9)	0.0100(8)	0.0333(11)	0.0004(8)	0.0004(8)	0.0019(7)
C46	0.0140(8)	0.0139(8)	0.0209(9)	−0.0009(7)	0.0012(7)	0.0017(6)
C47	0.0229(9)	0.0161(8)	0.0118(7)	0.0015(7)	0.0013(7)	−0.0031(7)
C48	0.0248(10)	0.0221(10)	0.0147(8)	−0.0008(7)	0.0044(8)	−0.0010(8)
C49	0.0331(12)	0.0260(11)	0.0175(10)	0.0007(8)	0.0094(9)	0.0034(9)
C50	0.0460(14)	0.0206(10)	0.0176(10)	−0.0024(8)	0.0053(10)	−0.0029(10)
C51	0.0386(13)	0.0281(12)	0.0189(10)	−0.0040(9)	−0.0020(9)	−0.0095(10)
C52	0.0253(10)	0.0269(11)	0.0171(9)	0.0001(8)	−0.0019(8)	−0.0038(8)

Table S4. Bond lengths for **I-ortho**.

Number	Atom(1)	Atom(2)	Length (Å)
1	H5	C5	0.951(2)
2	H6	C6	0.950(2)
3	H7	C7	0.950(2)
4	N1	B1	1.631(3)
5	N1	C1	1.330(3)
6	N1	C9	1.362(2)
7	N2	C10	1.304(3)
8	N2	C14	1.347(3)
9	O1	B1	1.511(3)
10	O1	C8	1.345(2)
11	F1	C10	1.358(2)
12	B1	C11	1.620(3)
13	B1	C15	1.605(3)
14	H1	C1	0.950(2)
15	H2	C2	0.950(2)
16	H3	C3	0.950(2)
17	H12	C12	0.950(2)
18	H13	C13	0.950(2)
19	H14	C14	0.950(2)
20	H17	C17	0.950(2)
21	H18	C18	0.950(2)
22	H19	C19	0.950(2)
23	H20	C20	0.950(2)
24	H22	C22	0.949(2)
25	H23	C23	0.950(2)
26	H24	C24	0.950(3)

27	H25	C25	0.951(3)
28	H26	C26	0.949(2)
29	C1	C2	1.401(3)
30	C2	C3	1.377(3)
31	C3	C4	1.412(3)
32	C4	C5	1.418(3)
33	C4	C9	1.401(3)
34	C5	C6	1.377(3)
35	C6	C7	1.418(3)
36	C7	C8	1.372(3)
37	C8	C9	1.405(3)
38	C10	C11	1.395(3)
39	C11	C12	1.393(3)
40	C12	C13	1.386(3)
41	C13	C14	1.386(3)
42	C15	C16	1.413(3)
43	C15	C20	1.404(3)
44	C16	C17	1.400(3)
45	C16	C21	1.493(3)
46	C17	C18	1.392(3)
47	C18	C19	1.385(3)
48	C19	C20	1.395(3)
49	C21	C22	1.397(3)
50	C21	C26	1.393(3)
51	C22	C23	1.391(4)
52	C23	C24	1.381(4)
53	C24	C25	1.389(5)
54	C25	C26	1.388(3)
55	H31	C31	0.950(2)
56	H32	C32	0.950(2)
57	H33	C33	0.950(2)
58	H38	C38	0.950(2)
59	H39	C39	0.950(2)
60	H40	C40	0.950(2)
61	H43	C43	0.950(2)
62	H44	C44	0.950(2)
63	H45	C45	0.950(2)
64	H46	C46	0.949(2)
65	H48	C48	0.950(2)
66	H49	C49	0.950(2)
67	H50	C50	0.950(2)
68	H51	C51	0.949(3)
69	H52	C52	0.950(2)
70	N3	B2	1.642(3)

71	N3	C27	1.327(3)
72	N3	C35	1.358(2)
73	N4	C36	1.309(3)
74	N4	C40	1.343(3)
75	O2	B2	1.508(2)
76	O2	C34	1.340(2)
77	F2	C36	1.357(2)
78	B2	C37	1.616(3)
79	B2	C41	1.612(3)
80	H27	C27	0.949(2)
81	H28	C28	0.950(2)
82	H29	C29	0.950(2)
83	C27	C28	1.410(3)
84	C28	C29	1.369(3)
85	C29	C30	1.417(3)
86	C30	C31	1.420(3)
87	C30	C35	1.401(3)
88	C31	C32	1.375(3)
89	C32	C33	1.421(3)
90	C33	C34	1.374(3)
91	C34	C35	1.406(3)
92	C36	C37	1.398(3)
93	C37	C38	1.398(3)
94	C38	C39	1.391(3)
95	C39	C40	1.385(3)
96	C41	C42	1.411(3)
97	C41	C46	1.396(3)
98	C42	C43	1.403(3)
99	C42	C47	1.499(3)
100	C43	C44	1.391(3)
101	C44	C45	1.382(4)
102	C45	C46	1.388(3)
103	C47	C48	1.394(3)
104	C47	C52	1.390(3)
105	C48	C49	1.393(3)
106	C49	C50	1.388(3)
107	C50	C51	1.385(4)
108	C51	C52	1.393(4)

Table S5. Bond angles for **I-ortho**.

Number	Atom(1)	Atom(2)	Atom(3)	Angle (°)
1	B1	N1	C1	134.1(2)
2	B1	N1	C9	105.9(1)

3	C1	N1	C9	119.7(2)
4	C10	N2	C14	115.7(2)
5	B1	O1	C8	109.8(1)
6	N1	B1	O1	99.6(1)
7	N1	B1	C11	102.7(1)
8	N1	B1	C15	117.3(2)
9	O1	B1	C11	108.4(2)
10	O1	B1	C15	109.9(2)
11	C11	B1	C15	117.2(2)
12	N1	C1	H1	120.1(2)
13	N1	C1	C2	119.7(2)
14	H1	C1	C2	120.3(2)
15	H2	C2	C1	119.6(2)
16	H2	C2	C3	119.1(2)
17	C1	C2	C3	121.2(2)
18	H3	C3	C2	120.1(2)
19	H3	C3	C4	119.9(2)
20	C2	C3	C4	119.9(2)
21	C3	C4	C5	128.7(2)
22	C3	C4	C9	115.3(2)
23	C5	C4	C9	116.0(2)
24	H5	C5	C4	120.1(2)
25	H5	C5	C6	120.6(2)
26	C4	C5	C6	119.3(2)
27	H6	C6	C5	117.9(2)
28	H6	C6	C7	118.4(2)
29	C5	C6	C7	123.8(2)
30	H7	C7	C6	121.2(2)
31	H7	C7	C8	121.2(2)
32	C6	C7	C8	117.6(2)
33	O1	C8	C7	129.2(2)
34	O1	C8	C9	111.9(2)
35	C7	C8	C9	118.8(2)
36	N1	C9	C4	124.2(2)
37	N1	C9	C8	111.3(2)
38	C4	C9	C8	124.5(2)
39	N2	C10	F1	114.4(2)
40	N2	C10	C11	129.1(2)
41	F1	C10	C11	116.5(2)
42	B1	C11	C10	122.9(2)
43	B1	C11	C12	123.7(2)
44	C10	C11	C12	113.1(2)
45	H12	C12	C11	119.3(2)
46	H12	C12	C13	119.8(2)

47	C11	C12	C13	120.9(2)
48	H13	C13	C12	120.7(2)
49	H13	C13	C14	120.4(2)
50	C12	C13	C14	118.9(2)
51	N2	C14	H14	118.5(2)
52	N2	C14	C13	122.3(2)
53	H14	C14	C13	119.2(2)
54	B1	C15	C16	126.2(2)
55	B1	C15	C20	117.0(2)
56	C16	C15	C20	116.8(2)
57	C15	C16	C17	120.5(2)
58	C15	C16	C21	122.3(2)
59	C17	C16	C21	117.2(2)
60	H17	C17	C16	119.1(2)
61	H17	C17	C18	119.8(2)
62	C16	C17	C18	121.1(2)
63	H18	C18	C17	120.1(2)
64	H18	C18	C19	120.5(2)
65	C17	C18	C19	119.4(2)
66	H19	C19	C18	120.3(2)
67	H19	C19	C20	120.1(2)
68	C18	C19	C20	119.6(2)
69	H20	C20	C15	118.8(2)
70	H20	C20	C19	118.6(2)
71	C15	C20	C19	122.7(2)
72	C16	C21	C22	119.5(2)
73	C16	C21	C26	121.6(2)
74	C22	C21	C26	118.9(2)
75	H22	C22	C21	119.5(2)
76	H22	C22	C23	120.0(2)
77	C21	C22	C23	120.5(2)
78	H23	C23	C22	120.3(3)
79	H23	C23	C24	119.4(3)
80	C22	C23	C24	120.3(3)
81	H24	C24	C23	120.3(3)
82	H24	C24	C25	120.1(3)
83	C23	C24	C25	119.7(3)
84	H25	C25	C24	119.8(3)
85	H25	C25	C26	119.8(3)
86	C24	C25	C26	120.4(3)
87	H26	C26	C21	119.6(2)
88	H26	C26	C25	120.1(2)
89	C21	C26	C25	120.4(2)
90	B2	N3	C27	134.1(2)

91	B2	N3	C35	106.2(1)
92	C27	N3	C35	119.5(2)
93	C36	N4	C40	115.6(2)
94	B2	O2	C34	110.5(1)
95	N3	B2	O2	99.2(1)
96	N3	B2	C37	106.3(1)
97	N3	B2	C41	112.6(2)
98	O2	B2	C37	107.6(2)
99	O2	B2	C41	111.8(2)
100	C37	B2	C41	117.6(2)
101	N3	C27	H27	120.3(2)
102	N3	C27	C28	120.0(2)
103	H27	C27	C28	119.7(2)
104	H28	C28	C27	119.6(2)
105	H28	C28	C29	119.6(2)
106	C27	C28	C29	120.8(2)
107	H29	C29	C28	120.0(2)
108	H29	C29	C30	119.8(2)
109	C28	C29	C30	120.2(2)
110	C29	C30	C31	128.9(2)
111	C29	C30	C35	115.1(2)
112	C31	C30	C35	116.0(2)
113	H31	C31	C30	119.5(2)
114	H31	C31	C32	121.0(2)
115	C30	C31	C32	119.5(2)
116	H32	C32	C31	118.0(2)
117	H32	C32	C33	118.5(2)
118	C31	C32	C33	123.5(2)
119	H33	C33	C32	121.8(2)
120	H33	C33	C34	120.5(2)
121	C32	C33	C34	117.7(2)
122	O2	C34	C33	129.0(2)
123	O2	C34	C35	112.1(2)
124	C33	C34	C35	118.8(2)
125	N3	C35	C30	124.4(2)
126	N3	C35	C34	111.2(2)
127	C30	C35	C34	124.4(2)
128	N4	C36	F2	114.0(2)
129	N4	C36	C37	129.2(2)
130	F2	C36	C37	116.9(2)
131	B2	C37	C36	124.4(2)
132	B2	C37	C38	122.7(2)
133	C36	C37	C38	112.7(2)
134	H38	C38	C37	119.1(2)

135	H38	C38	C39	119.8(2)
136	C37	C38	C39	121.1(2)
137	H39	C39	C38	120.6(2)
138	H39	C39	C40	120.8(2)
139	C38	C39	C40	118.5(2)
140	H40	C40	N4	118.5(2)
141	H40	C40	C39	118.7(2)
142	N4	C40	C39	122.8(2)
143	B2	C41	C42	123.5(2)
144	B2	C41	C46	119.4(2)
145	C42	C41	C46	117.0(2)
146	C41	C42	C43	120.4(2)
147	C41	C42	C47	122.5(2)
148	C43	C42	C47	117.1(2)
149	H43	C43	C42	119.6(2)
150	H43	C43	C44	119.5(2)
151	C42	C43	C44	120.9(2)
152	H44	C44	C43	120.4(2)
153	H44	C44	C45	120.4(2)
154	C43	C44	C45	119.2(2)
155	H45	C45	C44	120.0(2)
156	H45	C45	C46	120.1(2)
157	C44	C45	C46	119.9(2)
158	H46	C46	C41	118.7(2)
159	H46	C46	C45	118.7(2)
160	C41	C46	C45	122.6(2)
161	C42	C47	C48	120.7(2)
162	C42	C47	C52	120.2(2)
163	C48	C47	C52	119.1(2)
164	H48	C48	C47	119.6(2)
165	H48	C48	C49	119.8(2)
166	C47	C48	C49	120.6(2)
167	H49	C49	C48	120.5(2)
168	H49	C49	C50	119.6(2)
169	C48	C49	C50	119.9(2)
170	H50	C50	C49	120.2(2)
171	H50	C50	C51	120.1(2)
172	C49	C50	C51	119.7(2)
173	H51	C51	C50	119.6(2)
174	H51	C51	C52	119.9(2)
175	C50	C51	C52	120.5(2)
176	H52	C52	C47	119.9(2)
177	H52	C52	C51	119.9(2)
178	C47	C52	C51	120.2(2)

Table S6. Cartesian coordinates for **II-tric**.

Number	Label	X	Y	Z
1	O1	0.58635(7)	0.26484(6)	0.67144(5)
2	H7	0.5378	0.1579	0.5099
3	H26	0.8112	0.1953	0.6894
4	H25	0.9060	0.1797	0.5544
5	C22	0.94994(10)	0.44912(10)	0.68641(8)
6	C23	1.00599(11)	0.43959(11)	0.60586(8)
7	C24	0.98963(11)	0.33930(12)	0.55670(8)
8	C25	0.91719(11)	0.24843(11)	0.58794(8)
9	C26	0.86112(10)	0.25772(10)	0.66853(8)
10	F1	0.53804(6)	0.56739(6)	0.82873(5)
11	H1	0.7095	0.6036	0.7286
12	H2	0.7488	0.7084	0.6014
13	H3	0.7112	0.6262	0.4602
14	H5	0.6385	0.4342	0.3660
15	H6	0.5640	0.2483	0.3738
16	H12	0.3701	0.2528	0.7038
17	H13	0.1777	0.3081	0.7263
18	H14	0.1631	0.4827	0.7919
19	H17	0.9842	0.3817	0.8753
20	H18	0.9100	0.3915	1.0182
21	H19	0.7016	0.3705	1.0367
22	H20	0.5704	0.3573	0.9122
23	H22	0.9615	0.5180	0.7197
24	H23	1.0548	0.5023	0.5843
25	H24	1.0288	0.3329	0.5021
26	B1	0.60125(10)	0.36658(9)	0.73385(7)
27	N1	0.65067(8)	0.46154(7)	0.66359(6)
28	N2	0.33788(9)	0.52977(9)	0.81259(6)
29	C1	0.69415(9)	0.56883(9)	0.67128(7)
30	C2	0.71774(10)	0.63152(9)	0.59503(8)
31	C3	0.69670(10)	0.58279(10)	0.51126(8)
32	C4	0.65278(10)	0.46784(9)	0.50174(7)
33	C5	0.62601(11)	0.40199(11)	0.42230(7)
34	C6	0.58334(11)	0.29057(11)	0.42759(8)
35	C7	0.56618(11)	0.23546(10)	0.50914(8)
36	C8	0.59197(9)	0.29744(9)	0.58679(7)
37	C9	0.63229(9)	0.41216(9)	0.58123(7)
38	C10	0.44243(10)	0.49397(9)	0.79880(7)
39	C11	0.46699(9)	0.39453(9)	0.75741(7)
40	C12	0.36267(10)	0.32374(9)	0.73101(7)

41	C13	0.24830(10)	0.35618(11)	0.74442(8)
42	C14	0.24058(11)	0.45966(11)	0.78415(8)
43	C15	0.69560(10)	0.36193(8)	0.81670(7)
44	C16	0.82150(10)	0.36612(9)	0.80737(7)
45	C17	0.89981(11)	0.37729(10)	0.88264(8)
46	C18	0.85596(12)	0.38125(10)	0.96785(8)
47	C19	0.73274(12)	0.37166(10)	0.97883(7)
48	C20	0.65464(11)	0.36278(9)	0.90396(7)
49	C21	0.87673(9)	0.35794(9)	0.71879(7)
50	O2	0.86289(7)	0.75988(6)	0.79059(5)
51	H27	0.9159	1.1093	0.8364
52	H28	0.8709	1.1651	0.9813
53	H29	0.8041	1.0331	1.0835
54	F2	1.06402(6)	1.08138(6)	0.72250(5)
55	H31	0.7495	0.8132	1.1130
56	H32	0.7361	0.6343	1.0519
57	H33	0.7893	0.5963	0.9046
58	H38	1.0757	0.7278	0.7776
59	H39	1.2846	0.7481	0.7580
60	H40	1.3796	0.9208	0.7193
61	H43	0.5795	0.9942	0.5962
62	H44	0.6761	0.9856	0.4617
63	H45	0.8697	0.9285	0.4596
64	H46	0.9675	0.8910	0.5925
65	H48	0.6272	1.1071	0.7666
66	H49	0.5042	1.1007	0.8894
67	H50	0.4367	0.9287	0.9500
68	H51	0.4942	0.7628	0.8890
69	H52	0.6196	0.7692	0.7677
70	B2	0.90546(10)	0.87848(9)	0.76320(7)
71	N3	0.87909(8)	0.94682(7)	0.85404(6)
72	N4	1.23628(9)	1.00379(9)	0.71911(6)
73	C27	0.88959(10)	1.05455(9)	0.87796(7)
74	C28	0.86222(11)	1.08769(10)	0.96469(8)
75	C29	0.82312(10)	1.00968(10)	1.02550(7)
76	C30	0.81126(10)	0.89443(10)	1.00131(7)
77	C31	0.77103(12)	0.80180(11)	1.05325(8)
78	C32	0.76377(13)	0.69527(11)	1.01624(8)
79	C33	0.79502(11)	0.67113(10)	0.92759(8)
80	C34	0.83390(9)	0.76021(9)	0.87645(7)
81	C35	0.84178(9)	0.86923(9)	0.91427(7)
82	C36	1.12010(10)	0.98740(9)	0.73183(7)
83	C37	1.04968(9)	0.88914(9)	0.75288(7)
84	C38	1.11581(10)	0.79842(10)	0.76267(8)

85	C39	1.23983(11)	0.80996(11)	0.75077(8)
86	C40	1.29551(10)	0.91318(11)	0.72863(8)
87	C41	0.83164(9)	0.91259(8)	0.67605(6)
88	C42	0.71257(9)	0.94138(8)	0.67496(7)
89	C43	0.65774(10)	0.97078(10)	0.59533(7)
90	C44	0.71525(11)	0.96645(11)	0.51515(7)
91	C45	0.83034(10)	0.93420(10)	0.51413(7)
92	C46	0.88741(9)	0.90999(9)	0.59373(7)
93	C47	0.63767(9)	0.93882(9)	0.75544(7)
94	C48	0.60142(10)	1.03726(9)	0.79172(7)
95	C49	0.52722(11)	1.03334(10)	0.86430(8)
96	C50	0.48744(10)	0.93124(10)	0.90064(7)
97	C51	0.52179(9)	0.83269(9)	0.86463(7)
98	C52	0.59629(9)	0.83670(9)	0.79227(7)

Table S7. Atomic displacement parameters for **II-tric**.

Label	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
O1	0.0264(4)	0.0139(3)	0.0162(3)	0.0001(3)	0.0011(3)	0.0021(3)
O2	0.0211(3)	0.0151(3)	0.0161(3)	0.0005(3)	0.0011(3)	0.0003(3)
C22	0.0202(5)	0.0223(5)	0.0248(5)	0.0034(4)	0.0001(4)	0.0014(4)
C23	0.0229(5)	0.0323(6)	0.0290(6)	0.0086(5)	0.0055(4)	0.0011(4)
C24	0.0254(6)	0.0395(7)	0.0249(5)	0.0042(5)	0.0079(4)	0.0075(5)
C25	0.0272(6)	0.0298(6)	0.0258(6)	−0.0024(4)	0.0045(4)	0.0067(5)
C26	0.0232(5)	0.0209(5)	0.0243(5)	0.0011(4)	0.0034(4)	0.0027(4)
F1	0.0241(3)	0.0204(3)	0.0280(3)	−0.0052(3)	0.0022(3)	0.0001(3)
F2	0.0223(3)	0.0212(3)	0.0353(4)	0.0084(3)	0.0021(3)	0.0023(3)
B1	0.0195(5)	0.0146(5)	0.0146(5)	0.0010(4)	0.0017(4)	0.0009(4)
B2	0.0165(5)	0.0151(5)	0.0143(4)	−0.0002(4)	0.0013(4)	0.0014(4)
N1	0.0166(4)	0.0149(4)	0.0144(4)	0.0004(3)	0.0009(3)	0.0015(3)
N2	0.0239(4)	0.0284(5)	0.0171(4)	0.0039(3)	0.0051(3)	0.0071(4)
N3	0.0147(4)	0.0162(4)	0.0146(4)	0.0007(3)	−0.0003(3)	0.0016(3)
N4	0.0175(4)	0.0321(5)	0.0193(4)	0.0027(4)	0.0009(3)	−0.0010(4)
C1	0.0194(4)	0.0163(4)	0.0195(5)	−0.0001(4)	0.0016(4)	0.0010(4)
C2	0.0233(5)	0.0178(5)	0.0258(5)	0.0041(4)	0.0047(4)	−0.0005(4)
C3	0.0240(5)	0.0240(5)	0.0217(5)	0.0081(4)	0.0057(4)	0.0022(4)
C4	0.0198(5)	0.0242(5)	0.0159(4)	0.0027(4)	0.0030(4)	0.0041(4)
C5	0.0291(6)	0.0336(6)	0.0143(4)	0.0009(4)	0.0028(4)	0.0054(5)
C6	0.0313(6)	0.0324(6)	0.0163(5)	−0.0062(4)	−0.0001(4)	0.0057(5)
C7	0.0279(5)	0.0209(5)	0.0211(5)	−0.0050(4)	−0.0002(4)	0.0031(4)
C8	0.0195(4)	0.0171(4)	0.0171(4)	−0.0004(3)	0.0013(3)	0.0034(3)
C9	0.0169(4)	0.0173(4)	0.0145(4)	−0.0005(3)	0.0011(3)	0.0025(3)
C10	0.0208(5)	0.0205(5)	0.0150(4)	0.0023(4)	0.0023(3)	0.0014(4)
C11	0.0201(5)	0.0175(4)	0.0144(4)	0.0026(3)	0.0021(3)	0.0009(4)

C12	0.0229(5)	0.0221(5)	0.0178(4)	0.0036(4)	0.0010(4)	−0.0018(4)
C13	0.0199(5)	0.0347(6)	0.0211(5)	0.0064(4)	0.0007(4)	−0.0026(4)
C14	0.0206(5)	0.0391(7)	0.0196(5)	0.0073(4)	0.0042(4)	0.0069(5)
C15	0.0218(5)	0.0147(4)	0.0152(4)	0.0011(3)	0.0010(3)	0.0023(3)
C16	0.0218(5)	0.0160(4)	0.0173(4)	0.0019(3)	−0.0005(4)	0.0019(4)
C17	0.0238(5)	0.0244(5)	0.0224(5)	0.0028(4)	−0.0042(4)	0.0010(4)
C18	0.0356(6)	0.0229(5)	0.0187(5)	0.0014(4)	−0.0074(4)	0.0028(4)
C19	0.0381(6)	0.0208(5)	0.0152(4)	0.0014(4)	0.0008(4)	0.0059(4)
C20	0.0274(5)	0.0191(5)	0.0169(4)	0.0023(4)	0.0029(4)	0.0047(4)
C21	0.0166(4)	0.0210(5)	0.0191(4)	0.0035(4)	−0.0003(3)	0.0030(4)
C27	0.0219(5)	0.0175(4)	0.0199(5)	0.0001(4)	−0.0002(4)	0.0023(4)
C28	0.0268(5)	0.0217(5)	0.0221(5)	−0.0056(4)	−0.0004(4)	0.0054(4)
C29	0.0236(5)	0.0305(6)	0.0171(5)	−0.0043(4)	−0.0007(4)	0.0053(4)
C30	0.0206(5)	0.0274(5)	0.0147(4)	0.0008(4)	−0.0004(4)	0.0020(4)
C31	0.0355(6)	0.0358(6)	0.0155(5)	0.0056(4)	0.0026(4)	−0.0014(5)
C32	0.0410(7)	0.0316(6)	0.0206(5)	0.0108(5)	0.0006(5)	−0.0047(5)
C33	0.0300(6)	0.0208(5)	0.0218(5)	0.0064(4)	−0.0032(4)	−0.0022(4)
C34	0.0176(4)	0.0183(4)	0.0167(4)	0.0023(3)	−0.0018(3)	0.0012(3)
C35	0.0154(4)	0.0183(4)	0.0148(4)	0.0022(3)	−0.0012(3)	0.0012(3)
C36	0.0185(5)	0.0221(5)	0.0169(4)	0.0022(4)	−0.0002(3)	0.0024(4)
C37	0.0166(4)	0.0189(4)	0.0151(4)	−0.0003(3)	0.0000(3)	0.0019(3)
C38	0.0200(5)	0.0217(5)	0.0243(5)	−0.0012(4)	0.0006(4)	0.0040(4)
C39	0.0199(5)	0.0304(6)	0.0309(6)	−0.0027(5)	0.0007(4)	0.0085(4)
C40	0.0162(5)	0.0392(7)	0.0236(5)	−0.0012(5)	0.0007(4)	0.0039(4)
C41	0.0163(4)	0.0150(4)	0.0146(4)	0.0004(3)	0.0010(3)	−0.0004(3)
C42	0.0166(4)	0.0155(4)	0.0153(4)	0.0013(3)	0.0011(3)	−0.0001(3)
C43	0.0187(5)	0.0304(6)	0.0190(5)	0.0055(4)	−0.0008(4)	0.0030(4)
C44	0.0245(5)	0.0367(6)	0.0160(5)	0.0065(4)	−0.0020(4)	0.0008(5)
C45	0.0239(5)	0.0279(5)	0.0148(4)	0.0020(4)	0.0034(4)	−0.0020(4)
C46	0.0181(4)	0.0206(5)	0.0165(4)	0.0003(4)	0.0027(3)	−0.0006(4)
C47	0.0134(4)	0.0187(4)	0.0154(4)	0.0011(3)	−0.0004(3)	0.0015(3)
C48	0.0225(5)	0.0173(5)	0.0216(5)	0.0007(4)	0.0024(4)	0.0015(4)
C49	0.0268(5)	0.0226(5)	0.0234(5)	−0.0042(4)	0.0045(4)	0.0049(4)
C50	0.0217(5)	0.0284(5)	0.0180(5)	−0.0015(4)	0.0043(4)	0.0023(4)
C51	0.0182(4)	0.0222(5)	0.0184(4)	0.0037(4)	0.0023(4)	0.0004(4)
C52	0.0165(4)	0.0172(4)	0.0178(4)	0.0012(3)	0.0009(3)	0.0026(3)

Table S8. Bond lengths for **II-tric**.

Number	Atom(1)	Atom(2)	Length (Å)
1	O1	B1	1.512(1)
2	O1	C8	1.346(1)
3	H7	C7	0.950(1)
4	H26	C26	0.950(1)

5	H25	C25	0.950(1)
6	C22	C23	1.393(2)
7	C22	H22	0.950(1)
8	C22	C21	1.400(2)
9	C23	C24	1.388(2)
10	C23	H23	0.950(1)
11	C24	C25	1.387(2)
12	C24	H24	0.951(1)
13	C25	C26	1.394(2)
14	C26	C21	1.396(2)
15	F1	C10	1.361(1)
16	H1	C1	0.950(1)
17	H2	C2	0.950(1)
18	H3	C3	0.950(1)
19	H5	C5	0.950(1)
20	H6	C6	0.950(1)
21	H12	C12	0.950(1)
22	H13	C13	0.950(1)
23	H14	C14	0.950(1)
24	H17	C17	0.950(1)
25	H18	C18	0.950(1)
26	H19	C19	0.950(1)
27	H20	C20	0.949(1)
28	B1	N1	1.641(1)
29	B1	C11	1.625(2)
30	B1	C15	1.613(2)
31	N1	C1	1.326(1)
32	N1	C9	1.359(1)
33	N2	C10	1.313(2)
34	N2	C14	1.347(2)
35	C1	C2	1.408(2)
36	C2	C3	1.378(2)
37	C3	C4	1.414(2)
38	C4	C5	1.420(2)
39	C4	C9	1.401(2)
40	C5	C6	1.375(2)
41	C6	C7	1.421(2)
42	C7	C8	1.373(2)
43	C8	C9	1.407(1)
44	C10	C11	1.393(2)
45	C11	C12	1.401(1)
46	C12	C13	1.399(2)
47	C13	C14	1.379(2)
48	C15	C16	1.415(2)

49	C15	C20	1.408(2)
50	C16	C17	1.402(2)
51	C16	C21	1.496(2)
52	C17	C18	1.392(2)
53	C18	C19	1.386(2)
54	C19	C20	1.397(2)
55	O2	B2	1.523(1)
56	O2	C34	1.345(1)
57	H27	C27	0.950(1)
58	H28	C28	0.950(1)
59	H29	C29	0.949(1)
60	F2	C36	1.363(1)
61	H31	C31	0.950(1)
62	H32	C32	0.950(1)
63	H33	C33	0.950(1)
64	H38	C38	0.950(1)
65	H39	C39	0.950(1)
66	H40	C40	0.950(1)
67	H43	C43	0.950(1)
68	H44	C44	0.950(1)
69	H45	C45	0.950(1)
70	H46	C46	0.950(1)
71	H48	C48	0.949(1)
72	H49	C49	0.951(1)
73	H50	C50	0.950(1)
74	H51	C51	0.950(1)
75	H52	C52	0.950(1)
76	B2	N3	1.630(1)
77	B2	C37	1.616(2)
78	B2	C41	1.615(1)
79	N3	C27	1.326(1)
80	N3	C35	1.361(1)
81	N4	C36	1.313(1)
82	N4	C40	1.348(2)
83	C27	C28	1.410(2)
84	C28	C29	1.375(2)
85	C29	C30	1.413(2)
86	C30	C31	1.419(2)
87	C30	C35	1.401(2)
88	C31	C32	1.376(2)
89	C32	C33	1.423(2)
90	C33	C34	1.376(2)
91	C34	C35	1.407(2)
92	C36	C37	1.393(1)

93	C37	C38	1.395(2)
94	C38	C39	1.396(2)
95	C39	C40	1.378(2)
96	C41	C42	1.414(1)
97	C41	C46	1.409(1)
98	C42	C43	1.401(2)
99	C42	C47	1.497(1)
100	C43	C44	1.391(2)
101	C44	C45	1.387(2)
102	C45	C46	1.393(2)
103	C47	C48	1.398(2)
104	C47	C52	1.398(1)
105	C48	C49	1.394(2)
106	C49	C50	1.391(2)
107	C50	C51	1.390(2)
108	C51	C52	1.394(1)

Table S9. Bond angles for **II-tric**.

Number	Atom(1)	Atom(2)	Atom(3)	Angle (°)
1	B1	O1	C8	109.73(8)
2	C23	C22	H22	119.8(1)
3	C23	C22	C21	120.6(1)
4	H22	C22	C21	119.7(1)
5	C22	C23	C24	120.2(1)
6	C22	C23	H23	119.8(1)
7	C24	C23	H23	120.0(1)
8	C23	C24	C25	119.8(1)
9	C23	C24	H24	119.9(1)
10	C25	C24	H24	120.3(1)
11	H25	C25	C24	119.9(1)
12	H25	C25	C26	120.0(1)
13	C24	C25	C26	120.1(1)
14	H26	C26	C25	119.7(1)
15	H26	C26	C21	119.5(1)
16	C25	C26	C21	120.8(1)
17	O1	B1	N1	98.99(7)
18	O1	B1	C11	107.22(8)
19	O1	B1	C15	115.51(8)
20	N1	B1	C11	105.40(8)
21	N1	B1	C15	111.38(8)
22	C11	B1	C15	116.50(8)
23	B1	N1	C1	134.44(9)
24	B1	N1	C9	106.28(8)

25	C1	N1	C9	119.14(9)
26	C10	N2	C14	115.5(1)
27	H1	C1	N1	119.8(1)
28	H1	C1	C2	119.8(1)
29	N1	C1	C2	120.4(1)
30	H2	C2	C1	119.6(1)
31	H2	C2	C3	119.6(1)
32	C1	C2	C3	120.9(1)
33	H3	C3	C2	120.2(1)
34	H3	C3	C4	120.2(1)
35	C2	C3	C4	119.6(1)
36	C3	C4	C5	128.5(1)
37	C3	C4	C9	115.5(1)
38	C5	C4	C9	116.0(1)
39	H5	C5	C4	120.5(1)
40	H5	C5	C6	120.2(1)
41	C4	C5	C6	119.3(1)
42	H6	C6	C5	118.2(1)
43	H6	C6	C7	118.3(1)
44	C5	C6	C7	123.6(1)
45	H7	C7	C6	120.9(1)
46	H7	C7	C8	121.0(1)
47	C6	C7	C8	118.1(1)
48	O1	C8	C7	129.5(1)
49	O1	C8	C9	112.21(9)
50	C7	C8	C9	118.3(1)
51	N1	C9	C4	124.5(1)
52	N1	C9	C8	110.80(9)
53	C4	C9	C8	124.7(1)
54	F1	C10	N2	113.41(9)
55	F1	C10	C11	117.46(9)
56	N2	C10	C11	129.1(1)
57	B1	C11	C10	124.20(9)
58	B1	C11	C12	122.62(9)
59	C10	C11	C12	113.0(1)
60	H12	C12	C11	119.3(1)
61	H12	C12	C13	119.9(1)
62	C11	C12	C13	120.9(1)
63	H13	C13	C12	120.7(1)
64	H13	C13	C14	120.9(1)
65	C12	C13	C14	118.4(1)
66	H14	C14	N2	118.3(1)
67	H14	C14	C13	118.6(1)
68	N2	C14	C13	123.1(1)

69	B1	C15	C16	123.28(9)
70	B1	C15	C20	119.76(9)
71	C16	C15	C20	116.8(1)
72	C15	C16	C17	120.3(1)
73	C15	C16	C21	122.42(9)
74	C17	C16	C21	117.3(1)
75	H17	C17	C16	119.4(1)
76	H17	C17	C18	119.5(1)
77	C16	C17	C18	121.2(1)
78	H18	C18	C17	120.4(1)
79	H18	C18	C19	120.1(1)
80	C17	C18	C19	119.6(1)
81	H19	C19	C18	120.4(1)
82	H19	C19	C20	120.3(1)
83	C18	C19	C20	119.3(1)
84	H20	C20	C15	118.6(1)
85	H20	C20	C19	118.7(1)
86	C15	C20	C19	122.7(1)
87	C22	C21	C26	118.5(1)
88	C22	C21	C16	120.7(1)
89	C26	C21	C16	120.7(1)
90	B2	O2	C34	110.18(8)
91	O2	B2	N3	99.24(7)
92	O2	B2	C37	108.34(8)
93	O2	B2	C41	111.83(8)
94	N3	B2	C37	107.95(8)
95	N3	B2	C41	114.32(8)
96	C37	B2	C41	114.04(8)
97	B2	N3	C27	133.84(9)
98	B2	N3	C35	107.04(8)
99	C27	N3	C35	119.10(9)
100	C36	N4	C40	115.4(1)
101	H27	C27	N3	119.7(1)
102	H27	C27	C28	120.2(1)
103	N3	C27	C28	120.2(1)
104	H28	C28	C27	119.4(1)
105	H28	C28	C29	119.6(1)
106	C27	C28	C29	121.0(1)
107	H29	C29	C28	120.2(1)
108	H29	C29	C30	120.1(1)
109	C28	C29	C30	119.7(1)
110	C29	C30	C31	128.4(1)
111	C29	C30	C35	115.4(1)
112	C31	C30	C35	116.2(1)

113	H31	C31	C30	120.4(1)
114	H31	C31	C32	120.3(1)
115	C30	C31	C32	119.3(1)
116	H32	C32	C31	118.1(1)
117	H32	C32	C33	118.1(1)
118	C31	C32	C33	123.8(1)
119	H33	C33	C32	121.2(1)
120	H33	C33	C34	121.2(1)
121	C32	C33	C34	117.5(1)
122	O2	C34	C33	128.9(1)
123	O2	C34	C35	112.31(9)
124	C33	C34	C35	118.8(1)
125	N3	C35	C30	124.7(1)
126	N3	C35	C34	110.90(9)
127	C30	C35	C34	124.4(1)
128	F2	C36	N4	113.44(9)
129	F2	C36	C37	117.64(9)
130	N4	C36	C37	128.9(1)
131	B2	C37	C36	124.25(9)
132	B2	C37	C38	122.54(9)
133	C36	C37	C38	113.2(1)
134	H38	C38	C37	119.4(1)
135	H38	C38	C39	119.6(1)
136	C37	C38	C39	121.0(1)
137	H39	C39	C38	120.7(1)
138	H39	C39	C40	121.0(1)
139	C38	C39	C40	118.4(1)
140	H40	C40	N4	118.4(1)
141	H40	C40	C39	118.5(1)
142	N4	C40	C39	123.1(1)
143	B2	C41	C42	125.04(9)
144	B2	C41	C46	118.19(8)
145	C42	C41	C46	116.73(9)
146	C41	C42	C43	120.10(9)
147	C41	C42	C47	123.17(9)
148	C43	C42	C47	116.70(9)
149	H43	C43	C42	119.2(1)
150	H43	C43	C44	119.3(1)
151	C42	C43	C44	121.5(1)
152	H44	C44	C43	120.3(1)
153	H44	C44	C45	120.4(1)
154	C43	C44	C45	119.3(1)
155	H45	C45	C44	120.2(1)
156	H45	C45	C46	120.4(1)

157	C44	C45	C46	119.4(1)
158	H46	C46	C41	118.5(1)
159	H46	C46	C45	118.6(1)
160	C41	C46	C45	122.9(1)
161	C42	C47	C48	120.84(9)
162	C42	C47	C52	120.29(9)
163	C48	C47	C52	118.7(1)
164	H48	C48	C47	119.8(1)
165	H48	C48	C49	119.8(1)
166	C47	C48	C49	120.4(1)
167	H49	C49	C48	120.0(1)
168	H49	C49	C50	119.8(1)
169	C48	C49	C50	120.2(1)
170	H50	C50	C49	120.1(1)
171	H50	C50	C51	119.9(1)
172	C49	C50	C51	120.0(1)
173	H51	C51	C50	120.1(1)
174	H51	C51	C52	120.1(1)
175	C50	C51	C52	119.8(1)
176	H52	C52	C47	119.5(1)
177	H52	C52	C51	119.6(1)
178	C47	C52	C51	120.9(1)

DSC measurements. Differential scanning calorimetric (DSC) measurements were performed on a DSC Q200 from TA Instruments. For the DSC measurements the same samples were used as for the X-ray powder diffraction data collection ($m_{\text{I-ortho}} = 1.800\text{mg}$; $m_{\text{II-tric}} = 2.2400\text{ mg}$). Data were collected in two cycles of heating and cooling with rate of heating equal $10^\circ\text{C}/\text{min}$. Crystals of both polymorph have identical melting points ($219.9^\circ\text{C} / 217.3^\circ\text{C}$ and $219.4^\circ\text{C} / 217.2^\circ\text{C}$ for **I-ortho** and **II-tric**, respectively). These results are consistent with the calculated lattice energies which are also close in terms of absolute value (**Table 5**). **I-ortho** form crystallized during the first cycle of cooling at 141.9°C , and the **II-tric** form crystallized during the second cycle of heating (at 113.2°C).

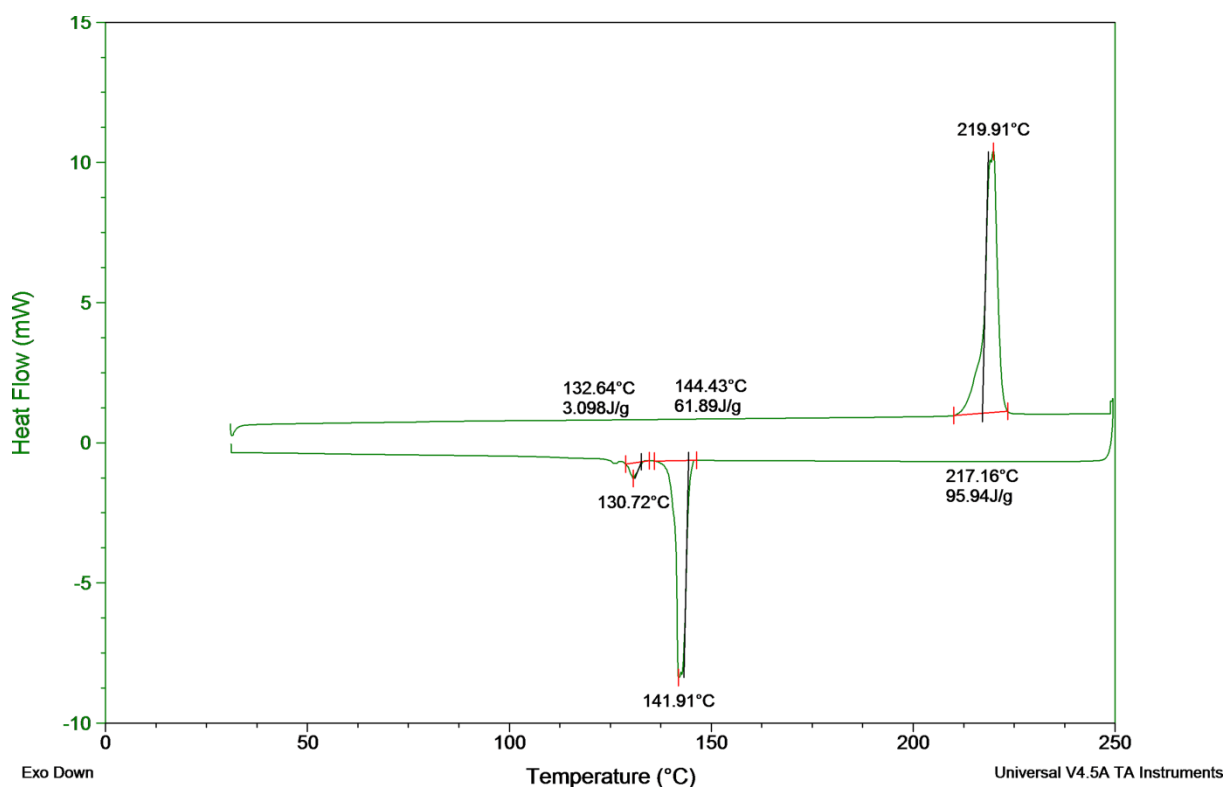


Figure S4. The first cycle of heating for **I-ortho** form.

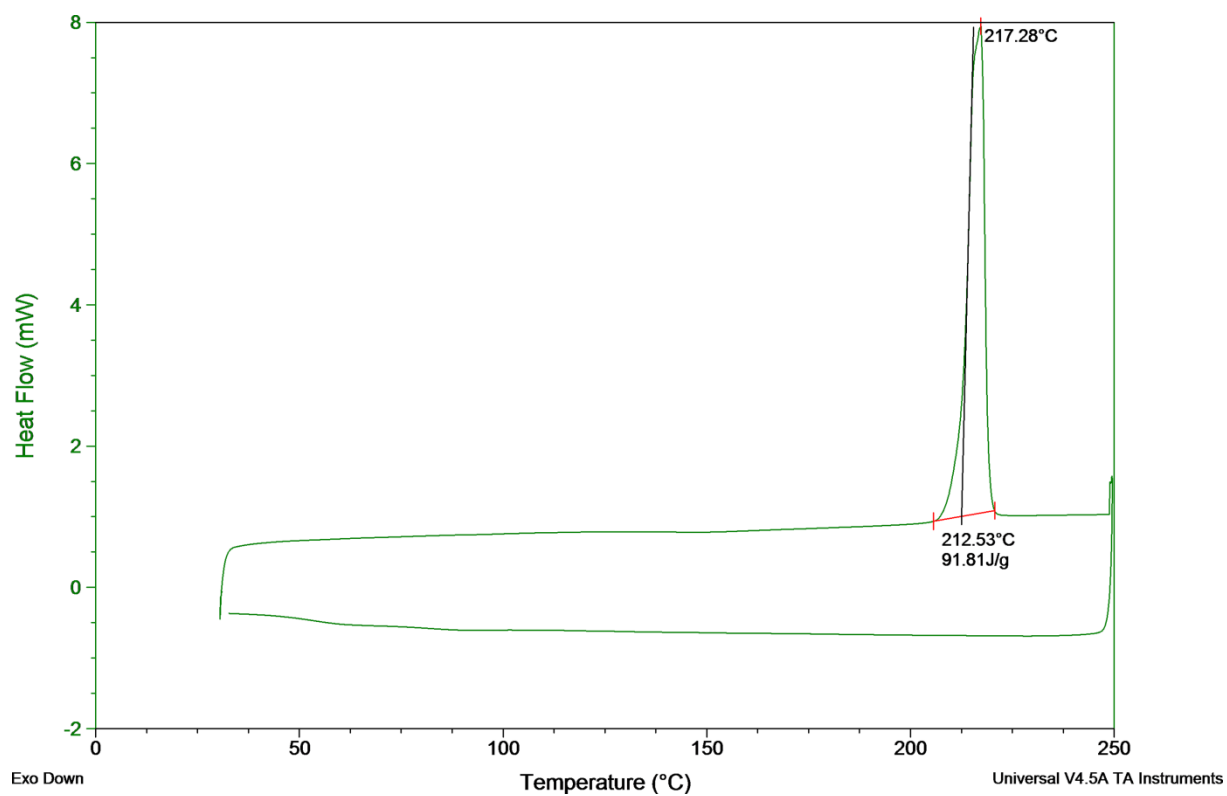


Figure S5. The second cycle of heating for **I-ortho** form.

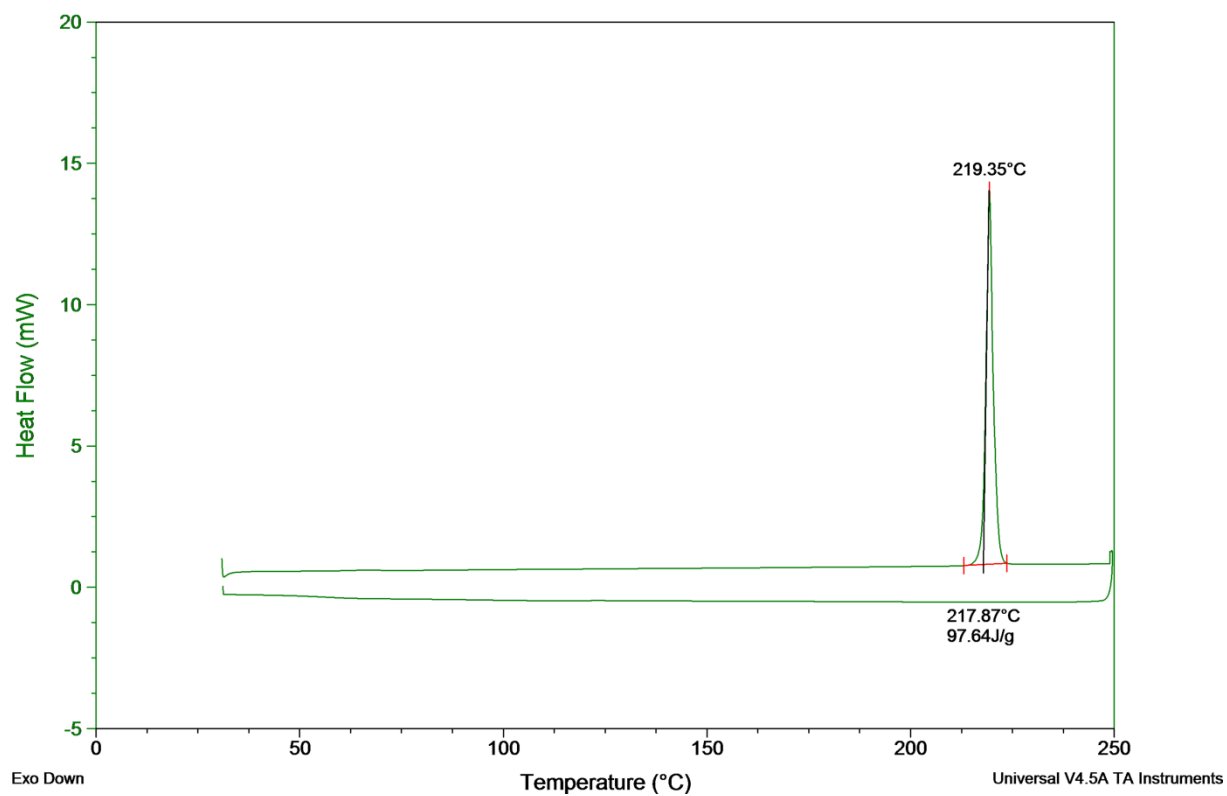


Figure S6. The first cycle of heating for **II-tric** form.

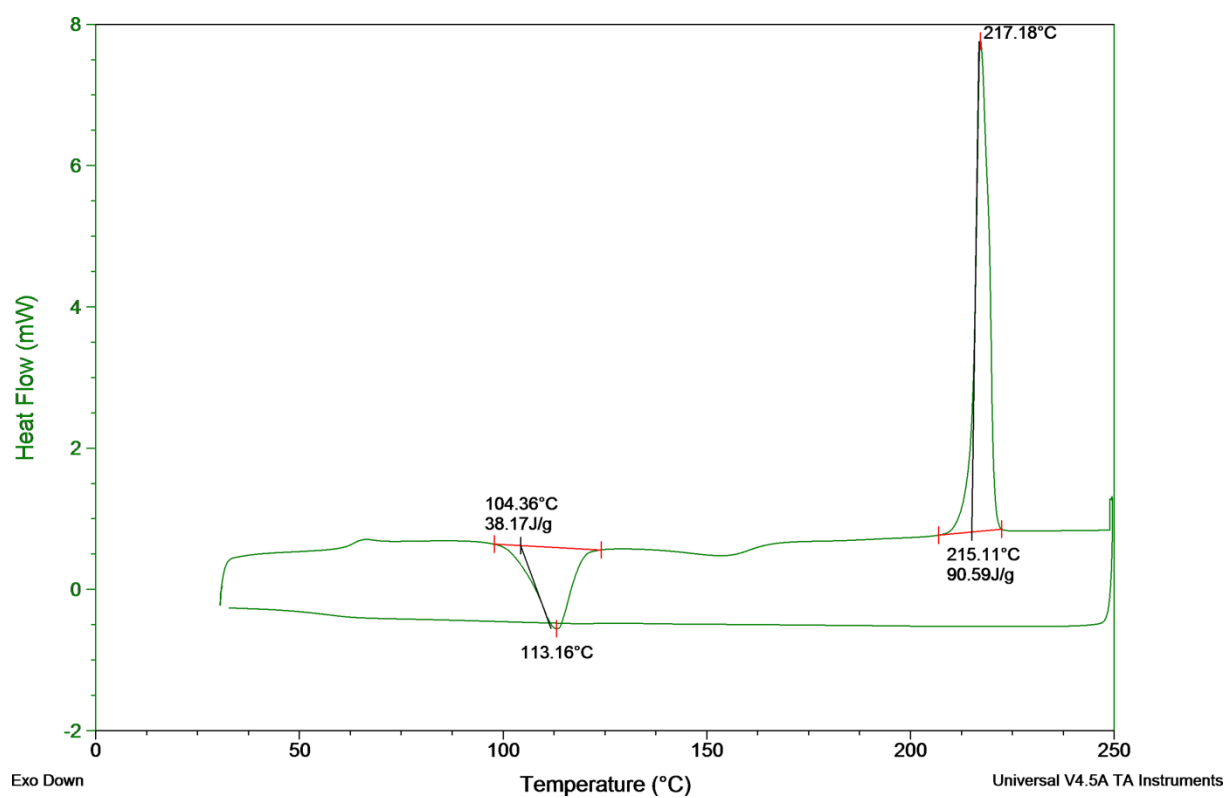


Figure S7. The second cycle of heating for **II-tric** form.

Energies of interactions and CT properties.

Table S10. Energies of interactions (E_{tot}) and their contribution from electrostatic (E_{elstat}), polarization (E_{pol}), dispersion (E_{disp}), and repulsion (E_{rep}) terms. Calculated by *PIXEL* module.

		Form I-ortho						
		Energy (kJ mol ⁻¹)						Symmetry
Motifs		d (Å)	E_{elstat}	E_{pol}	E_{disp}	E_{rep}	E_{tot}	
A...A	1	10.984	-9.5	-5.3	-23.0	22.6	-15.1	0.5-x, y, z±0.5
	2	6.419	-45.4	-19.1	-65.0	52.7	-76.8	x±0.5, 1-y, z
A...B	3	9.256	-13.7	-6.6	-32.6	26.9	-25.9	x,y,z
	4	11.391	-0.4	-0.4	-7.1	1.2	-6.7	0.5-x, y, 0.5+z
	5	9.155	-11.9	-6.0	-33.7	25.2	-26.3	x, y-1, z
	6	9.426	-12.3	-4.3	-33.1	20.0	-29.7	-x, 1-y, 0.5+z
	7	11.746	-1.0	-0.3	-6.9	1.5	-6.6	-x, 2-y, 0.5+z
	8	11.309	-1.7	-0.6	-7.2	1.7	-7.9	0.5-x, y-1, 0.5+z
	9	7.306	-27.1	-10.9	-55.5	32.4	-61.1	0.5+x, 1-y, z
	10	10.125	-12.5	-6.4	-25.4	19.3	-25.1	0.5+x, 2-y, z
	11	11.892	-3.0	-0.3	-1.0	0.0	-4.3	1+x, y-1, z
	12	11.970	-2.8	-0.3	-0.8	0.0	-3.9	1+x, y, z
B...B	13	11.298	-6.8	-2.4	-16.1	10.5	-14.8	-x, 2-y, z±0.5
	14	6.387	-42.2	-16.2	-59.0	45.1	-72.3	x±0.5, 2-y, z
	15	11.655	1.6	-1.8	-9.1	5.1	-4.2	-0.5-x, y, z±0.5

		Form II-tric						
		Energy (kJ mol ⁻¹)						Symmetry
Motifs		d (Å)	E_{elstat}	E_{pol}	E_{disp}	E_{rep}	E_{tot}	
A...A	1	11.183	-7.6	-3.3	-20.0	15.0	-15.9	x±1, y, z
	2	7.382	-28.0	-11.8	-69.0	45.1	-63.6	1-x, 1-y, 1-z
	3	10.670	-13.0	-6.6	-18.1	18.6	-19.1	1-x, 1-y, 2-z
	4	9.506	-13.4	-4.3	-34.8	20.3	-32.2	2-x, 1-y, 1-z
	5	11.747	-1.1	-0.2	-6.6	1.1	-6.8	2-x, 1-y, 2-z
A...B	6	6.335	-42.4	-19.1	-64.0	48.7	-76.9	x, y, z
	7	10.795	-3.6	-2.0	-7.3	1.6	-11.3	x-1, y-1, z
	8	12.003	-5.2	-1.6	-6.8	2.9	-10.7	x-1, y, z
	9	6.615	-28	-14.5	-63.6	44.7	-61.4	x, y-1, z
	10	9.500	-5.0	-2.6	-18.5	9.5	-16.7	1-x, 1-y, 1-z
	11	10.174	-9.9	-3.8	-22.5	14.6	-21.6	1-x, 1-y, 2-z
	12	10.247	-2.4	-2.2	-20.2	9.2	-15.6	2-x, 1-y, 1-z
	13	10.321	-0.4	-0.3	-9.2	1.1	-8.9	2-x, 1-y, 2-z
	14	12.309	-3.5	-0.3	-0.9	0.0	-4.8	2-x, 2-y, 1-z

Table S11. Charge transport properties evaluated through Marcus theory at B97D/6-31+(d,p) level of theory.

Form I-ortho			
Motifs	H_{AB} (10^{-4} eV)		charge transport
	hole	electron	
1	193.609	199.324	electron
2	152.112	341.775	electron
3	1666.834	1833.776	electron
4	803.281	1014.849	electron
5	1805.068	1443.429	hole
6	172.384	574.569	electron
7	166.398	405.722	electron
8	990.495	733.211	hole
9	575.521	315.108	hole
10	171.976	456.607	electron
11	1035.394	974.032	hole
12	954.712	1399.754	electron
13	166.398	405.722	electron
14	171.976	456.607	electron
15	789.675	1037.707	electron
	9815.833	11592.192	electron

Form II-tric			
Motifs	H_{AB} (10^{-4} eV)		charge transport
	hole	electron	
1	165.990	102.587	hole
2	113.063	774.028	electron
3	28.028	8.844	hole
4	31.293	127.758	electron
5	9.252	0.544	hole
6	563.684	1081.925	electron
7	966.549	938.929	hole
8	568.310	451.981	hole
9	996.345	1172.675	electron
10	1533.907	1524.655	hole
11	1527.376	1522.614	hole
12	987.774	1000.971	electron
13	673.346	609.807	hole
14	1246.962	1482.477	electron
	9411.879	10799.795	electron

Table S12. Energy difference between single point calculations of every molecules present in the asymmetric part of the unit cell and optimized geometry.

	E_x-E_{opt} (kJ mol ⁻¹)	
	A	B
I-ortho	30.9	25.1
II-tric	23.3	19.5

Constrained energy scan

Table S13. Energies calculated for the constrained Θ – scan.

step	θ	E(a.u.)	E(kJ mol ⁻¹)	ΔE (kJ mol ⁻¹)
1	167.78	-1310.249365	-3440059.4	0.26656699
2	171.38	-1310.249143	-3440058.8	0.85039937
3	174.98	-1310.248851	-3440058	1.61759665
4	178.58	-1310.248506	-3440057.1	2.52213382
5	182.18	-1310.248103	-3440056.1	3.58097162
6	185.78	-1310.247699	-3440055	4.64230363
7	189.38	-1310.247282	-3440053.9	5.73771464
8	192.98	-1310.247019	-3440053.2	6.42630446
9	196.58	-1310.246802	-3440052.6	6.99593288
10	200.18	-1310.246492	-3440051.8	7.81049418
11	203.78	-1310.246075	-3440050.7	8.9062465
12	207.38	-1310.245565	-3440049.4	10.2445162
13	210.98	-1310.244978	-3440047.9	11.7862622
14	214.58	-1310.244296	-3440046.1	13.576853
15	218.18	-1310.243515	-3440044	15.6258718
16	221.78	-1310.242703	-3440041.9	17.7595367
17	225.38	-1310.241875	-3440039.7	19.9335817
18	228.98	-1310.241092	-3440037.7	21.987799
19	232.58	-1310.240456	-3440036	23.6589558
20	236.18	-1310.239927	-3440034.6	25.0469788
21	239.78	-1310.239462	-3440033.4	26.2670485
22	243.38	-1310.238957	-3440032.1	27.5932147
23	246.98	-1310.239195	-3440032.7	26.9687921
24	250.58	-1310.239634	-3440033.8	25.8153838
25	254.18	-1310.240151	-3440035.2	24.4580004
26	257.78	-1310.240602	-3440036.4	23.2752128
27	261.38	-1310.241033	-3440037.5	22.1446201
28	264.98	-1310.241372	-3440038.4	21.2541293
29	268.58	-1310.241627	-3440039.1	20.5828941
30	272.18	-1310.241816	-3440039.6	20.0869372
31	275.78	-1310.241963	-3440039.9	19.7021964
32	279.38	-1310.242096	-3440040.3	19.3527162
33	282.98	-1310.242211	-3440040.6	19.0502586
34	286.58	-1310.242377	-3440041	18.6145832
35	290.18	-1310.242907	-3440042.4	17.2225695
36	293.78	-1310.243741	-3440044.6	15.0324301
37	297.38	-1310.244551	-3440046.7	12.9065367
38	300.98	-1310.245264	-3440048.6	11.034214
39	304.58	-1310.245921	-3440050.3	9.3097333
40	308.18	-1310.246456	-3440051.7	7.90456584
41	311.78	-1310.246862	-3440052.8	6.83971565

42	315.38	-1310.247104	-3440053.4	6.20392463
43	318.98	-1310.247159	-3440053.6	6.05831441
44	322.58	-1310.247036	-3440053.3	6.38295746
45	326.18	-1310.246805	-3440052.7	6.98852897
46	329.78	-1310.246481	-3440051.8	7.83882332
47	333.38	-1310.24608	-3440050.8	8.89332904
48	336.98	-1310.245712	-3440049.8	9.8597755
49	340.58	-1310.245336	-3440048.8	10.8449418
50	344.18	-1310.244939	-3440047.8	11.889103
51	347.78	-1310.244568	-3440046.8	12.8632422
52	351.38	-1310.244259	-3440046	13.6740228
53	354.98	-1310.243979	-3440045.2	14.4085588
54	358.58	-1310.243648	-3440044.4	15.2767853
55	2.18	-1310.243254	-3440043.3	16.3134377
56	5.78	-1310.23962	-3440033.8	25.8520883
57	9.38	-1310.23991	-3440034.6	25.0923212
58	12.98	-1310.240135	-3440035.1	24.5021876
59	16.58	-1310.239765	-3440034.2	25.4725986
60	20.18	-1310.240053	-3440034.9	24.7163496
61	23.78	-1310.240306	-3440035.6	24.0516256
62	27.38	-1310.240558	-3440036.3	23.3891857
63	30.98	-1310.240791	-3440036.9	22.7797285
64	34.58	-1310.240981	-3440037.4	22.2798333
65	38.18	-1310.241145	-3440037.8	21.8487
66	41.78	-1310.24132	-3440038.3	21.388975
67	45.38	-1310.241584	-3440038.9	20.6962106
68	48.98	-1310.242016	-3440040.1	19.5615747
69	52.58	-1310.243094	-3440042.9	16.7330713
70	56.18	-1310.243941	-3440045.1	14.5075927
71	59.78	-1310.244616	-3440046.9	12.736378
72	63.38	-1310.245125	-3440048.2	11.3999199
73	66.98	-1310.245497	-3440049.2	10.4240742
74	70.58	-1310.245738	-3440049.9	9.79019976
75	74.18	-1310.245844	-3440050.1	9.51221184
76	77.78	-1310.245822	-3440050.1	9.56994658
77	81.38	-1310.245626	-3440049.6	10.0844133
78	84.98	-1310.245373	-3440048.9	10.7489798
79	88.58	-1310.244995	-3440047.9	11.7422588
80	92.18	-1310.244505	-3440046.6	13.0283074
81	95.78	-1310.243917	-3440045.1	14.5722587
82	99.38	-1310.242426	-3440041.2	18.4863275
83	102.98	-1310.242988	-3440042.6	17.0093264
84	106.58	-1310.243553	-3440044.1	15.5259453
85	110.18	-1310.244116	-3440045.6	14.048419
86	113.78	-1310.244688	-3440047.1	12.5463969
87	117.38	-1310.245244	-3440048.6	11.0878005

88	120.98	-1310.245746	-3440049.9	9.77037723
89	124.58	-1310.246215	-3440051.1	8.53744255
90	128.18	-1310.246666	-3440052.3	7.35344718
91	131.78	-1310.247112	-3440053.5	6.18415462
92	135.38	-1310.247563	-3440054.6	4.99782256
93	138.98	-1310.247929	-3440055.6	4.0390163
94	142.58	-1310.248212	-3440056.4	3.29502844
95	146.18	-1310.24851	-3440057.1	2.51173684
96	149.78	-1310.248784	-3440057.9	1.79429278
97	153.38	-1310.248965	-3440058.3	1.31744952
98	156.98	-1310.249245	-3440059.1	0.58204704
99	160.58	-1310.249425	-3440059.5	0.11071733
100	164.18	-1310.249467	-3440059.6	0
ortho_A	206.45	-1310.237591	-3440028.5	31.1803825
ortho_B	186.85	-1310.239928	-3440034.6	25.0432506
tric_A	195.98	-1310.240527	-3440036.2	23.4712064
tric_B	198.98	-1310.241885	-3440039.7	19.9066704

Cartesian coordinates of step 1

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62473900
C	1.36007900	0.00000000	-0.88807200
C	1.12413700	0.04276400	2.49819900
C	-1.28131800	0.13691100	2.21573800
N	-0.91783200	1.29331700	-0.51757000
O	-0.91147200	-1.13330400	-0.52464600
C	1.65371200	-1.02378000	-1.80972300
C	2.33874300	1.01254400	-0.85297300
C	0.93178000	0.27546000	3.88199200
C	2.51585900	-0.24605200	2.05225600
C	-1.47004700	0.33825100	3.58923700
H	-2.16309200	0.09742600	1.57162800
C	-1.94230200	0.78256000	-1.25391900
C	-0.82341600	2.61476400	-0.33990000
C	-1.91295100	-0.63884600	-1.25132900
C	2.84028400	-1.00229200	-2.56199000
H	0.95093400	-1.85039000	-1.91510600
N	3.46441800	1.09029900	-1.53381000
F	2.12296700	2.07682700	-0.00701900
C	-0.34753200	0.43017900	4.42890000
H	1.80765100	0.29606800	4.53286500
C	3.58179700	0.61444300	2.38899500
C	2.80249800	-1.42413900	1.33087600
H	-2.47788800	0.43169900	3.99823800
C	-2.93544500	1.56555400	-1.90234700
C	-1.76351800	3.48183100	-0.95121800
H	-0.00595000	2.97058200	0.27941900
C	-2.91212500	-1.31535700	-1.95423600
C	3.71897300	0.07242800	-2.38514100
H	3.07794700	-1.80070400	-3.26561400

H	-0.46773900	0.59761500	5.50079700
C	4.89494900	0.31851300	1.99444100
H	3.36778800	1.53639600	2.93135300
C	4.11478800	-1.72508200	0.93859400
H	1.98376200	-2.09839100	1.07934100
C	-2.80284300	2.97388600	-1.72909100
C	-3.93891000	0.85093100	-2.61921500
H	-1.65757300	4.55464800	-0.79749900
C	-3.90359000	-0.54602700	-2.62976700
H	-2.93814700	-2.40388000	-1.97752400
H	4.65803300	0.13616500	-2.93965900
C	5.16597200	-0.85230000	1.26655900
H	5.70322700	1.00870100	2.24135800
H	4.31483600	-2.63716700	0.37410800
H	-3.52235600	3.64869100	-2.19556100
H	-4.72487800	1.39382800	-3.14364000
H	-4.67901400	-1.08366100	-3.17771800
H	6.18600600	-1.07882700	0.95214100
Cartesian coordinates of step 2			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63031600
C	1.38717200	0.00000000	-0.84548800
C	1.11135400	0.11246700	2.51266600
C	-1.26719400	-0.24503500	2.21827200
N	-1.05633300	1.16172500	-0.49455100
O	-0.78755600	-1.24502900	-0.50778700
C	2.14473600	-1.19106700	-0.84357900
C	1.95073600	1.00691300	-1.64782300
C	0.92433300	-0.05705900	3.90709300
C	2.49580200	0.43397200	2.06167100
C	-1.45255300	-0.38922900	3.59873800
H	-2.13683700	-0.35081000	1.56574000
C	-2.05717900	0.54183700	-1.17727700
C	-1.10952600	2.48164600	-0.29616800
C	-1.86903100	-0.86753900	-1.18459700
C	3.33183700	-1.30282300	-1.58202500
H	1.79306500	-2.03307500	-0.24610800
N	3.04885700	0.95528600	-2.37841000
F	1.33050000	2.23864200	-1.68469600
C	-0.34022000	-0.30455800	4.45284200
H	1.79139200	0.03664700	4.56343900
C	2.76970700	1.60460800	1.32742900
C	3.57282200	-0.40882600	2.40963800
H	-2.44906400	-0.57687900	4.00293700
C	-3.16810900	1.21099300	-1.75940100
C	-2.17666000	3.23976500	-0.83409100
H	-0.29811900	2.92753100	0.27209500
C	-2.81816600	-1.64937400	-1.84745300
C	3.74081600	-0.20220100	-2.34501500
H	3.92338200	-2.21835400	-1.56689000
H	-0.45773300	-0.41927600	5.53190000

C	4.07608000	1.91347000	0.92263500
H	1.94743400	2.26968900	1.06355900
C	4.88327700	-0.10194000	2.01121700
H	3.37094400	-1.31958500	2.97613800
C	-3.19038000	2.62239300	-1.56665700
C	-4.11878600	0.39026500	-2.43319200
H	-2.18794500	4.31560600	-0.66701900
C	-3.92252800	-0.99329300	-2.46467000
H	-2.72124900	-2.73342900	-1.88229600
H	4.65083900	-0.23527400	-2.94854900
C	5.13864200	1.05871800	1.26173200
H	4.26085600	2.81262100	0.33360400
H	5.70180300	-0.77341900	2.27677800
H	-4.00730100	3.21472200	-1.98184700
H	-4.98926700	0.84185900	-2.90835100
H	-4.65799000	-1.61236900	-2.98095500
H	6.15476900	1.29417800	0.94165400
Cartesian coordinates of step 3			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63289100
C	1.40069700	0.00000000	-0.81897600
C	1.09788700	0.18133200	2.52257100
C	-1.25451500	-0.31350100	2.21543000
N	-1.03895300	1.17906400	-0.48249200
O	-0.79532000	-1.22927200	-0.52485900
C	2.27052600	-1.08955600	-0.59909400
C	1.88081600	0.90170300	-1.78362700
C	0.90886600	0.01327200	3.91739900
C	2.46491900	0.58046300	2.08178200
C	-1.44192900	-0.45728200	3.59573300
H	-2.11151200	-0.47463700	1.55797600
C	-2.04558400	0.57987700	-1.17346300
C	-1.06692300	2.49930000	-0.28275600
C	-1.87343400	-0.83158300	-1.19686400
C	3.48894200	-1.20109700	-1.28278100
H	1.98715800	-1.84368300	0.13638400
N	3.01376400	0.84893500	-2.46089900
F	1.12362500	2.01579800	-2.07812400
C	-0.34289900	-0.30234000	4.45680300
H	1.76302200	0.16417100	4.57989300
C	2.67510400	1.71919800	1.27837800
C	3.59094500	-0.16364100	2.49463600
H	-2.42925500	-0.69834000	3.99409100
C	-3.14312900	1.27018200	-1.75593700
C	-2.11803000	3.27824600	-0.82162400
H	-0.24951600	2.92985900	0.28983500
C	-2.83060200	-1.59421200	-1.86987300
C	3.81999800	-0.20177100	-2.20676700
H	4.16814600	-2.03313300	-1.09719400
H	-0.46124000	-0.41436400	5.53603500
C	3.96361400	2.08655900	0.86690900

H	1.81606400	2.31148700	0.96361700
C	4.88450700	0.20382600	2.09305500
H	3.44104800	-1.05057500	3.11268900
C	-3.14131000	2.68091400	-1.55783800
C	-4.10278100	0.46837500	-2.43974400
H	-2.10991300	4.35387100	-0.65297100
C	-3.92490200	-0.91733300	-2.48308000
H	-2.74658000	-2.67884500	-1.91770300
H	4.75857300	-0.23284500	-2.76508100
C	5.07490800	1.32720100	1.27143600
H	4.09860100	2.95788400	0.22473800
H	5.74080400	-0.39369800	2.41086100
H	-3.94593700	3.28922600	-1.97385300
H	-4.96458800	0.93594400	-2.91524900
H	-4.66664000	-1.52162800	-3.00783200
H	6.07791600	1.60792400	0.94673500
Cartesian coordinates of step 4			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63255100
C	1.40352400	0.00000000	-0.81318700
C	1.08649200	0.25040800	2.52006800
C	-1.24038500	-0.35845100	2.21907300
N	-1.04272500	1.17636500	-0.48532900
O	-0.79033000	-1.23130800	-0.52672000
C	2.29575300	-1.06263900	-0.55616100
C	1.86453100	0.87923600	-1.80759400
C	0.90077500	0.10411900	3.91786800
C	2.44138300	0.68518300	2.07412700
C	-1.42457000	-0.48191800	3.60187800
H	-2.08701600	-0.57180900	1.56344100
C	-2.04606200	0.57285800	-1.17767300
C	-1.07542300	2.49727700	-0.29051800
C	-1.86874700	-0.83784200	-1.20053800
C	3.51684700	-1.17062500	-1.23586600
H	2.02820000	-1.79697000	0.20490300
N	2.99973700	0.82933900	-2.48130300
F	1.08169400	1.96437500	-2.14021200
C	-0.33690600	-0.25650300	4.46163500
H	1.74556900	0.30620300	4.57871600
C	2.62191700	1.80914800	1.24340100
C	3.58764800	-0.01531200	2.50761400
H	-2.40070000	-0.76056800	4.00331300
C	-3.14435300	1.25842200	-1.76449200
C	-2.12761900	3.27174600	-0.83360900
H	-0.26135100	2.93322000	0.28239000
C	-2.82117200	-1.60463400	-1.87547800
C	3.82779000	-0.19505900	-2.19168600
H	4.21346900	-1.98151500	-1.02316300
H	-0.45309300	-0.35037300	5.54283300
C	3.90041400	2.20358800	0.82589600
H	1.74834800	2.36898700	0.91110000

C	4.87131900	0.37946200	2.10044200
H	3.46158900	-0.89129300	3.14620800
C	-3.14763200	2.66958100	-1.57017900
C	-4.09940100	0.45257500	-2.44994700
H	-2.12262200	4.34784900	-0.66788300
C	-3.91655600	-0.93248100	-2.49175700
H	-2.73226400	-2.68889100	-1.92295800
H	4.76787800	-0.22424400	-2.74756400
C	5.03204500	1.48719700	1.25175200
H	4.01176800	3.06201700	0.16220200
H	5.74333400	-0.18532700	2.43494100
H	-3.95309000	3.27427300	-1.98982400
H	-4.96132500	0.91685400	-2.92845400
H	-4.65459100	-1.53987300	-3.01815000
H	6.02746400	1.78865100	0.92236200
Cartesian coordinates of step 5			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62697200
C	1.41281100	0.00000000	-0.80472800
C	1.09735400	0.32668900	2.46816600
C	-1.18811900	-0.44794100	2.25619100
N	-1.03336100	1.18675300	-0.50388100
O	-0.79574200	-1.22339500	-0.52539300
C	2.07132600	-1.24008900	-0.95612100
C	2.09833300	1.06386700	-1.41799800
C	0.99115800	0.16755400	3.86873400
C	2.36927400	0.92029000	1.94872900
C	-1.30052900	-0.58488600	3.64644100
H	-2.04242900	-0.71954100	1.63284800
C	-2.04360200	0.58162800	-1.18728000
C	-1.06947000	2.50766600	-0.30540200
C	-1.87363600	-0.82935800	-1.20029100
C	3.29096500	-1.34165000	-1.64172200
H	1.61296800	-2.13127200	-0.52579300
N	3.23960400	1.02807400	-2.08172700
F	1.54328600	2.32072400	-1.35160000
C	-0.19512600	-0.28708300	4.46063800
H	1.85096700	0.42230200	4.49139300
C	2.42818800	2.29583300	1.65253400
C	3.53588900	0.14436900	1.79990000
H	-2.23532600	-0.93382600	4.08942000
C	-3.14551200	1.26544800	-1.76894200
C	-2.12743900	3.27968600	-0.84312800
H	-0.25207900	2.94098600	0.26311800
C	-2.83082300	-1.59821900	-1.86563800
C	3.83856900	-0.17534900	-2.18974200
H	3.80084400	-2.29925500	-1.75127100
H	-0.25763600	-0.39990900	5.54451700
C	3.61733300	2.88266700	1.19306800
H	1.53211600	2.90474500	1.78508500
C	4.72529900	0.72635900	1.33656000

H	3.49599900	-0.92217600	2.02478000
C	-3.14974000	2.67696700	-1.57543800
C	-4.10630900	0.45820500	-2.44525600
H	-2.12416900	4.35555800	-0.67537700
C	-3.92764200	-0.92731000	-2.48090800
H	-2.74610600	-2.68319700	-1.90445800
H	4.78416500	-0.19306300	-2.73690400
C	4.76832600	2.09685200	1.02780600
H	3.64016800	3.94572400	0.94927800
H	5.61472200	0.10808900	1.20399700
H	-3.95903400	3.28009500	-1.99004500
H	-4.97085500	0.92218800	-2.91937800
H	-4.67052000	-1.53589500	-2.99900500
H	5.68867100	2.54557600	0.65186900
Cartesian coordinates of step 6			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62712300
C	1.41627900	0.00000000	-0.79826800
C	1.07804700	0.39618600	2.46339800
C	-1.16808000	-0.48935300	2.26267800
N	-1.03086100	1.18956500	-0.50043400
O	-0.79545600	-1.22072500	-0.53026600
C	2.08479100	-1.23738700	-0.92490800
C	2.09724800	1.05901300	-1.42512800
C	0.97277200	0.26750100	3.86703600
C	2.33124600	1.02083300	1.93368700
C	-1.27886500	-0.59977800	3.65557800
H	-2.00670600	-0.81282600	1.64309500
C	-2.04415700	0.58748100	-1.18198400
C	-1.06333700	2.51032900	-0.30030700
C	-1.87572400	-0.82353000	-1.19987700
C	3.31015300	-1.34086000	-1.59989700
H	1.63010900	-2.12480500	-0.48281200
N	3.24368500	1.02090400	-2.07986500
F	1.53191100	2.31190500	-1.38515600
C	-0.19336700	-0.22834200	4.46602800
H	1.81769700	0.57525600	4.48613800
C	2.36288200	2.39965300	1.64951800
C	3.50957200	0.26688000	1.76407100
H	-2.19751700	-0.98325000	4.10377400
C	-3.14666100	1.27433000	-1.75880800
C	-2.12171300	3.28510900	-0.83313700
H	-0.24249200	2.94098600	0.26525800
C	-2.83560700	-1.58937300	-1.86471000
C	3.85301900	-0.17924600	-2.16271400
H	3.82789300	-2.29623700	-1.69050000
H	-0.25519800	-0.31777400	5.55212800
C	3.53648200	3.01116700	1.18123500
H	1.45880800	2.99267000	1.80035500
C	4.68337600	0.87348300	1.29335500
H	3.49047500	-0.80212800	1.97913400

C	-3.14779300	2.68547100	-1.56268600
C	-4.11058400	0.47009100	-2.43431800
H	-2.11568200	4.36076000	-0.66402500
C	-3.93369100	-0.91549700	-2.47448500
H	-2.75192700	-2.67428700	-1.90753700
H	4.80284300	-0.19869400	-2.70248300
C	4.69891400	2.24716900	0.99604400
H	3.53851600	4.07686100	0.94786100
H	5.58180300	0.27205000	1.14540800
H	-3.95736600	3.29078500	-1.97354200
H	-4.97591800	0.93645300	-2.90465300
H	-4.67881500	-1.52171400	-2.99212600
H	5.60691900	2.71510800	0.61363300
Cartesian coordinates of step 7			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62758500
C	1.42047000	0.00000000	-0.79012600
C	1.05476400	0.46473500	2.45863900
C	-1.14491400	-0.53329900	2.26956300
N	-1.02760000	1.19430600	-0.49556600
O	-0.79608700	-1.21637400	-0.53528500
C	2.09948400	-1.23415900	-0.88814400
C	2.09791400	1.05289700	-1.43116000
C	0.94845500	0.36468900	3.86432100
C	2.28649400	1.12397000	1.91942300
C	-1.25532200	-0.61972200	3.66443600
H	-1.96494400	-0.90865200	1.65460500
C	-2.04746200	0.59598200	-1.17054400
C	-1.05392400	2.51512400	-0.29482600
C	-1.88186000	-0.81524800	-1.19412000
C	3.33280200	-1.33987500	-1.54810000
H	1.64722700	-2.11705600	-0.43439000
N	3.25207500	1.01220000	-2.07213700
F	1.52112700	2.30052700	-1.42303600
C	-0.19470500	-0.17454800	4.47031200
H	1.77524800	0.72544200	4.47932500
C	2.28965900	2.50770500	1.65882500
C	3.47529400	0.39419000	1.71833200
H	-2.15532900	-1.03963600	4.11780300
C	-3.15233200	1.28662500	-1.73808000
C	-2.11414900	3.29343700	-0.81875300
H	-0.22633200	2.94260000	0.26324400
C	-2.84786900	-1.57744700	-1.85403100
C	3.87271700	-0.18376300	-2.12513900
H	3.85881200	-2.29258400	-1.61665200
H	-0.25723100	-0.24229600	5.55794000
C	3.44429500	3.14729800	1.17985100
H	1.37971200	3.08338700	1.83958700
C	4.62990500	1.02879100	1.23816800
H	3.47842800	-0.67817500	1.91579400
C	-3.14799800	2.69752200	-1.54030700

C	-4.12299900	0.48607100	-2.40837800
H	-2.10315700	4.36902300	-0.64941300
C	-3.94932200	-0.89970200	-2.45355700
H	-2.76618700	-2.66233800	-1.90115400
H	4.82890400	-0.20495800	-2.65355400
C	4.61612000	2.40697900	0.96187200
H	3.42446700	4.21697100	0.96593700
H	5.53595800	0.44580400	1.06556500
H	-3.95898600	3.30558600	-1.94425600
H	-4.99069100	0.95549600	-2.87127400
H	-4.69945100	-1.50303300	-2.96732100
H	5.50890500	2.89659800	0.57095700
Cartesian coordinates of step 8			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62827300
C	1.42877000	0.00000000	-0.77351400
C	1.02786300	0.53230600	2.45354500
C	-1.11064400	-0.59326500	2.27728400
N	-1.02824500	1.19015200	-0.50044000
O	-0.78853000	-1.21977100	-0.53667800
C	2.13410600	-1.22271200	-0.80304200
C	2.09200000	1.03544800	-1.45591300
C	0.92818900	0.44213700	3.86011100
C	2.22364700	1.24915900	1.90571600
C	-1.21369400	-0.67231600	3.67347800
H	-1.90797400	-1.02188800	1.66768400
C	-2.05273200	0.58639600	-1.16376600
C	-1.05204200	2.51301500	-0.31302600
C	-1.88312600	-0.82430500	-1.18449400
C	3.37873300	-1.33374500	-1.44020000
H	1.69368500	-2.09184300	-0.31218300
N	3.25637200	0.98851600	-2.07829900
F	1.49050800	2.26947000	-1.51390500
C	-0.18126300	-0.15647700	4.47335000
H	1.73372600	0.85562600	4.47014800
C	2.16778400	2.63457200	1.65945000
C	3.43990100	0.57177300	1.68537500
H	-2.08679100	-1.14032900	4.13234500
C	-3.16269200	1.27207500	-1.72725700
C	-2.11728100	3.28650100	-0.83381100
H	-0.21753900	2.94577000	0.23016200
C	-2.85198200	-1.59164500	-1.83409300
C	3.90286400	-0.19466700	-2.06422800
H	3.92533300	-2.27715700	-1.45607600
H	-0.23894900	-0.21634100	5.56170100
C	3.28861900	3.32487900	1.16951600
H	1.24128000	3.17314600	1.86791400
C	4.56086200	1.25691900	1.19577300
H	3.49083000	-0.50065300	1.87461800
C	-3.15803500	2.68434900	-1.53997800
C	-4.13682100	0.46632200	-2.38625600

H	-2.10409400	4.36366700	-0.67493400
C	-3.96026800	-0.91916900	-2.42698200
H	-2.76681500	-2.67635400	-1.87920800
H	4.86710500	-0.22045600	-2.57765700
C	4.48654400	2.63511600	0.92896600
H	3.22313400	4.39537800	0.96866500
H	5.48773600	0.71306800	1.00733100
H	-3.97290100	3.28871800	-1.94166000
H	-5.00879600	0.93189300	-2.84498700
H	-4.71282200	-1.52643500	-2.93249300
H	5.35309500	3.16380900	0.53006800
Cartesian coordinates of step 9			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62939700
C	1.43451400	0.00000000	-0.76125600
C	0.99467600	0.59715500	2.45221600
C	-1.07909400	-0.64478500	2.28211500
N	-1.02864700	1.18686300	-0.50230200
O	-0.78359900	-1.22221900	-0.53792500
C	2.16201100	-1.20941600	-0.73259400
C	2.08241500	1.01699400	-1.48474300
C	0.89179600	0.52292500	3.85917500
C	2.16037300	1.35923100	1.89918100
C	-1.18363200	-0.71147800	3.67924300
H	-1.84962600	-1.12284700	1.67529900
C	-2.06084300	0.57957500	-1.15030000
C	-1.04755700	2.51155900	-0.32646100
C	-1.88909400	-0.83083100	-1.16942900
C	3.41182100	-1.32592800	-1.35854800
H	1.73563500	-2.06293300	-0.20313700
N	3.25088400	0.96387700	-2.09871300
F	1.46232000	2.23846800	-1.59376800
C	-0.18662900	-0.12702600	4.47626600
H	1.67124700	0.98683000	4.46685700
C	2.06110300	2.74598200	1.67373900
C	3.39318600	0.72184800	1.65293700
H	-2.03159800	-1.22148000	4.14051100
C	-3.17739500	1.26224200	-1.70448400
C	-2.11853600	3.28197900	-0.83965400
H	-0.20406400	2.94738600	0.19976700
C	-2.86506900	-1.60168900	-1.80429300
C	3.91848100	-0.20574600	-2.02974700
H	3.97592000	-2.25866100	-1.32946300
H	-0.24634000	-0.17454900	5.56511300
C	3.15312700	3.47482300	1.17358900
H	1.12500600	3.25583400	1.91005400
C	4.48587600	1.44551200	1.15519400
H	3.47957300	-0.35036900	1.82853600
C	-3.16962600	2.67563700	-1.52672400
C	-4.15912000	0.45293500	-2.34757700
H	-2.10179300	4.36048600	-0.69043000

C	-3.98170300	-0.93261000	-2.38506900
H	-2.77839800	-2.68635400	-1.84790100
H	4.88567100	-0.23642900	-2.53731900
C	4.36679000	2.82376400	0.90521600
H	3.05383000	4.54594800	0.99017700
H	5.42530900	0.93136000	0.94708600
H	-3.98920000	3.27790900	-1.92190700
H	-5.03710700	0.91579100	-2.79748200
H	-4.74004700	-1.54234900	-2.87882500
H	5.21107600	3.38248200	0.49956100
Cartesian coordinates of step 10			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62931100
C	1.42968300	0.00000000	-0.77071100
C	0.95562900	0.65871600	2.45179400
C	-1.06147200	-0.67356800	2.28207300
N	-1.02592100	1.19396900	-0.49081900
O	-0.78896700	-1.21580700	-0.54313600
C	2.15473400	-1.21102300	-0.75764900
C	2.07742100	1.02400600	-1.48482700
C	0.82523400	0.62612100	3.85817300
C	2.11057000	1.43786600	1.89956100
C	-1.18839900	-0.70612900	3.67862300
H	-1.80231400	-1.19629400	1.67543800
C	-2.05995100	0.59463900	-1.14334700
C	-1.04117600	2.51698300	-0.30299100
C	-1.89319400	-0.81609300	-1.17234800
C	3.40279600	-1.32282400	-1.38838700
H	1.72805700	-2.06966100	-0.23671400
N	3.24216100	0.97434100	-2.10605400
F	1.46335200	2.24963700	-1.57215800
C	-0.23603500	-0.05157100	4.47534700
H	1.57276300	1.14029700	4.46553000
C	2.01284000	2.83290900	1.72992700
C	3.33414600	0.80561300	1.59926900
H	-2.02173000	-1.24002500	4.13956600
C	-3.17446600	1.28493400	-1.69179500
C	-2.11043800	3.29443800	-0.80948400
H	-0.19685700	2.94565100	0.22825200
C	-2.87162000	-1.57907500	-1.81267800
C	3.90824700	-0.19694800	-2.05104900
H	3.96570600	-2.25655400	-1.37042500
H	-0.31564200	-0.06798900	5.56384100
C	3.09648300	3.57574400	1.23142400
H	1.08385600	3.33693900	2.00478100
C	4.41894600	1.54346500	1.10552100
H	3.41955800	-0.27246000	1.73266900
C	-3.16273200	2.69682300	-1.50220200
C	-4.15883100	0.48358600	-2.34087500
H	-2.09104700	4.37147700	-0.65023600
C	-3.98594200	-0.90213500	-2.38870200

H	-2.78815100	-2.66361400	-1.86498500
H	4.87301800	-0.22445400	-2.56345700
C	4.30059200	2.93060800	0.91072100
H	2.99820500	4.65356200	1.09135000
H	5.35108900	1.03393400	0.85760400
H	-3.98080900	3.30442800	-1.89233000
H	-5.03539100	0.95275700	-2.78704300
H	-4.74608200	-1.50587700	-2.88704800
H	5.13847500	3.50104500	0.50806900
Cartesian coordinates of step 11			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63093400
C	1.43132600	0.00000000	-0.76704400
C	0.91300800	0.71791400	2.45346800
C	-1.03176800	-0.71778300	2.28411700
N	-1.02292700	1.19649500	-0.48658500
O	-0.78945100	-1.21332300	-0.54519500
C	2.17669100	-1.19717600	-0.70747600
C	2.06142600	1.00617400	-1.52113100
C	0.76724000	0.70146900	3.85866300
C	2.03873300	1.54201800	1.90574600
C	-1.17187700	-0.73621200	3.67980500
H	-1.73972000	-1.28459600	1.67818300
C	-2.06511100	0.59960600	-1.12819800
C	-1.02943800	2.52041000	-0.30432600
C	-1.90104300	-0.81128600	-1.16071800
C	3.42773000	-1.31188600	-1.33168100
H	1.76471100	-2.04185900	-0.15265900
N	3.23006100	0.95380200	-2.13527100
F	1.42545700	2.21559100	-1.66081500
C	-0.26488500	-0.01973600	4.47591700
H	1.48206200	1.26068700	4.46560800
C	1.90786300	2.94096900	1.79470000
C	3.26975200	0.95084000	1.55681300
H	-1.98097900	-1.30652600	4.14032100
C	-3.18234400	1.29280400	-1.66688100
C	-2.10074200	3.30057800	-0.80218000
H	-0.17559500	2.94756800	0.21303500
C	-2.88677200	-1.57178200	-1.79222400
C	3.91635600	-0.20257700	-2.03387800
H	4.00602500	-2.23477600	-1.27829100
H	-0.35592800	-0.02263100	5.56362400
C	2.96416200	3.72709600	1.30318200
H	0.97404200	3.41272600	2.10836900
C	4.32720000	1.73154600	1.06941800
H	3.38428300	-0.12829600	1.65038800
C	-3.16335400	2.70506300	-1.48087200
C	-4.17485600	0.49378100	-2.30663200
H	-2.07408100	4.37828700	-0.64859400
C	-4.00569100	-0.89217400	-2.35658300
H	-2.80592000	-2.65642200	-1.84655100

H	4.88367000	-0.23231300	-2.54136200
C	4.17443500	3.12193700	0.93044600
H	2.84045200	4.80754100	1.21087800
H	5.26477500	1.25283500	0.78385900
H	-3.98276400	3.31496200	-1.86458500
H	-5.05416500	0.96512000	-2.74505300
H	-4.77183800	-1.49405700	-2.84790800
H	4.99125000	3.72634100	0.53400200
Cartesian coordinates of step 12			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63183600
C	1.43621500	0.00000000	-0.75781100
C	0.86789900	0.77540700	2.45243300
C	-0.98081800	-0.78295300	2.28825500
N	-1.02396500	1.19129000	-0.49633300
O	-0.78141700	-1.21779800	-0.54526300
C	2.19677700	-1.18469900	-0.65716800
C	2.05635400	0.99041900	-1.54022100
C	0.72641800	0.74911300	3.85806000
C	1.93314100	1.67945500	1.90868600
C	-1.11438000	-0.81207400	3.68470100
H	-1.65384400	-1.39181100	1.68367900
C	-2.06375500	0.58761800	-1.13602600
C	-1.03196300	2.51712700	-0.32755300
C	-1.89494000	-0.82264500	-1.16203100
C	3.45155200	-1.30347100	-1.27360000
H	1.79433800	-2.01596500	-0.07557600
N	3.22744100	0.93313500	-2.14956500
F	1.41025000	2.18990400	-1.71142600
C	-0.25362400	-0.03881400	4.47845000
H	1.40469800	1.35357400	4.46355000
C	1.72667200	3.07431300	1.87551300
C	3.18451200	1.17521000	1.50066500
H	-1.88343100	-1.43398600	4.14703000
C	-3.18119400	1.27443000	-1.68218800
C	-2.10411500	3.29108100	-0.83326900
H	-0.17884800	2.95102800	0.18532900
C	-2.87678000	-1.58968700	-1.79152700
C	3.92755200	-0.21122100	-2.01069600
H	4.04182000	-2.21629200	-1.18821200
H	-0.34008000	-0.04852900	5.56648500
C	2.72590000	3.94062500	1.39988000
H	0.77730600	3.47740300	2.23491900
C	4.18625800	2.03670200	1.03089100
H	3.36121300	0.10143600	1.53675300
C	-3.16530600	2.68826600	-1.50749800
C	-4.17022000	0.46889800	-2.31930400
H	-2.07841300	4.37021200	-0.68977800
C	-3.99706300	-0.91675300	-2.36137300
H	-2.79167600	-2.67423000	-1.84107200
H	4.89615800	-0.24514300	-2.51544800

C	3.95677300	3.42164000	0.96762600
H	2.54338600	5.01633400	1.36956100
H	5.14078900	1.62472500	0.70124800
H	-3.98518600	3.29346600	-1.89762100
H	-5.04970200	0.93536700	-2.76255200
H	-4.76034900	-1.52356000	-2.85108700
H	4.73088800	4.08910400	0.58685000
Cartesian coordinates of step 13			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63356800
C	1.44627700	0.00000000	-0.73597500
C	0.81756800	0.82844400	2.45673700
C	-0.88980300	-0.88381900	2.29115100
N	-1.02283100	1.18479800	-0.51365400
O	-0.76901900	-1.22345500	-0.54649300
C	2.24889900	-1.14223400	-0.52740200
C	2.03670800	0.94312000	-1.59517800
C	0.71525700	0.74934100	3.86400200
C	1.75696700	1.87075400	1.92532600
C	-0.98314400	-0.96377100	3.68922400
H	-1.52175700	-1.53346600	1.68508600
C	-2.06225100	0.57133300	-1.14546000
C	-1.02909200	2.51408700	-0.37177400
C	-1.88802400	-0.83826900	-1.16035900
C	3.51409400	-1.26575900	-1.12154400
H	1.87267900	-1.93336200	0.12384300
N	3.21935400	0.88156000	-2.18237400
F	1.34692500	2.09654300	-1.87489900
C	-0.17115000	-0.14217600	4.48472900
H	1.34988900	1.39771400	4.47133900
C	1.40914400	3.23519000	2.03581600
C	3.02194500	1.54302300	1.39746500
H	-1.68268800	-1.66359800	4.15046900
C	-3.18037300	1.24880000	-1.70169000
C	-2.10266000	3.27884700	-0.88837100
H	-0.17611000	2.96021200	0.13078900
C	-2.86686000	-1.61502800	-1.78217400
C	3.95911800	-0.22041600	-1.94187400
H	4.13711300	-2.14472500	-0.95383100
H	-0.22488200	-0.19131300	5.57378600
C	2.27913900	4.24252500	1.58517100
H	0.44792900	3.49964200	2.48172500
C	3.89446600	2.54609300	0.94866700
H	3.31637600	0.49774500	1.32873200
C	-3.16571200	2.66501700	-1.54927200
C	-4.16745900	0.43353500	-2.32949300
H	-2.07509200	4.36037700	-0.76463200
C	-3.99017700	-0.95181700	-2.35742100
H	-2.77635100	-2.69949300	-1.82337500
H	4.93562900	-0.25847000	-2.43078600
C	3.52279700	3.89837400	1.02997700

H	1.98754700	5.29096500	1.67124600
H	4.86033900	2.26848900	0.52509100
H	-3.98632100	3.26332100	-1.94840700
H	-5.04780400	0.89302200	-2.77831600
H	-4.75143800	-1.56604900	-2.84097300
H	4.19796400	4.67570700	0.66954100
Cartesian coordinates of step 14			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63765800
C	1.46538200	0.00000000	-0.69518100
C	0.76073700	0.87446800	2.47068700
C	-0.75822400	-1.00446500	2.28756300
N	-1.00158400	1.19123900	-0.53618300
O	-0.76961600	-1.21828200	-0.54719100
C	2.34408800	-1.03358300	-0.30553400
C	2.00895900	0.85338300	-1.67185200
C	0.73195000	0.71776800	3.87479900
C	1.50360900	2.07604200	1.96296700
C	-0.78032200	-1.15808300	3.68288500
H	-1.33918900	-1.69470000	1.67572800
C	-2.05812600	0.58108000	-1.14272800
C	-0.97402800	2.52496300	-0.44610000
C	-1.89905000	-0.83009300	-1.14185300
C	3.63673000	-1.13547500	-0.84195500
H	2.00769500	-1.74829600	0.44793500
N	3.22058700	0.81601600	-2.20026900
F	1.23432000	1.87889200	-2.15336400
C	-0.02134300	-0.29508700	4.48552400
H	1.31520100	1.40693300	4.48880000
C	0.97608800	3.35750800	2.24608000
C	2.72981700	1.99784600	1.27240400
H	-1.38095900	-1.94984600	4.13483200
C	-3.16962700	1.26373500	-1.70496100
C	-2.03945500	3.29508300	-0.97159100
H	-0.10600300	2.97249600	0.02678200
C	-2.89415200	-1.60484600	-1.73910800
C	4.03490500	-0.17493900	-1.78158700
H	4.31872400	-1.92885500	-0.53520000
H	-0.01650400	-0.40164000	5.57176700
C	1.62433400	4.52258800	1.80457800
H	0.03948000	3.42872200	2.80228900
C	3.37966100	3.16078300	0.82726600
H	3.17802800	1.02562200	1.08342000
C	-3.12614900	2.68320700	-1.59428300
C	-4.17538700	0.45049200	-2.30548300
H	-1.98496100	4.37924000	-0.88576600
C	-4.01709700	-0.93723300	-2.31039300
H	-2.81474100	-2.69056900	-1.76842000
H	5.03428100	-0.19257500	-2.22301500
C	2.82533900	4.42623000	1.08046200
H	1.19319100	5.50072500	2.02626700

H	4.31741700	3.07311400	0.27734200
H	-3.94014800	3.28549400	-2.00094100
H	-5.05335700	0.91393400	-2.75493300
H	-4.79165900	-1.54970900	-2.77466900
H	3.32808500	5.32725000	0.72593800
Cartesian coordinates of step 15			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64008600
C	1.47627200	0.00000000	-0.67088400
C	0.70580600	0.92244100	2.47018000
C	-0.58442500	-1.11630900	2.28706700
N	-0.94375100	1.24075700	-0.55326400
O	-0.82016200	-1.17723200	-0.54112000
C	2.50417200	-0.74277200	-0.05271800
C	1.87537200	0.60287500	-1.87956900
C	0.79803600	0.70585100	3.86215200
C	1.19012200	2.25240200	1.97204700
C	-0.49214900	-1.32859400	3.67259800
H	-1.11522300	-1.84973600	1.68019600
C	-2.07275000	0.67154000	-1.06187300
C	-0.81275100	2.57104800	-0.57306700
C	-1.98098000	-0.74509100	-1.04179800
C	3.79549900	-0.80033700	-0.60083300
H	2.28426400	-1.25420800	0.88584400
N	3.07947900	0.60874000	-2.42657300
F	0.93807900	1.28954600	-2.60964400
C	0.21862100	-0.41899500	4.46743500
H	1.32940900	1.44008500	4.47114200
C	0.45421800	3.39892200	2.35295100
C	2.32445500	2.43008200	1.15394400
H	-0.96291000	-2.20535800	4.12153800
C	-3.17578400	1.39545900	-1.58639000
C	-1.86224700	3.38194200	-1.07065400
H	0.12207400	2.98901500	-0.21701300
C	-3.05131600	-1.48259800	-1.54786600
C	4.03946700	-0.08923500	-1.78324700
H	4.59205000	-1.36866200	-0.12004700
H	0.31437900	-0.57247000	5.54378300
C	0.80843000	4.67623100	1.89076000
H	-0.41868000	3.27169500	2.99518400
C	2.67642000	3.70638200	0.68163600
H	2.93364600	1.57338400	0.88147500
C	-3.03497800	2.81317000	-1.56290100
C	-4.26288300	0.62064500	-2.08801800
H	-1.72439100	4.46198200	-1.06665800
C	-4.17841300	-0.77302700	-2.05732200
H	-3.02317000	-2.57120200	-1.56133600
H	5.03035800	-0.07555500	-2.24346000
C	1.91425900	4.83244600	1.03664100
H	0.21811900	5.54429100	2.18977700
H	3.54892200	3.81659800	0.03591000

H	-3.83698300	3.44576800	-1.94686400
H	-5.14154300	1.11784500	-2.49849500
H	-5.01304500	-1.35625800	-2.44959100
H	2.18697200	5.82068900	0.66308900
Cartesian coordinates of step 16			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64032100
C	1.47505100	0.00000000	-0.67318300
C	0.64615100	0.96442800	2.47073800
C	-0.53660700	-1.13855600	2.28988400
N	-0.95422000	1.22971600	-0.56045400
O	-0.81461600	-1.18714100	-0.53158900
C	2.52309300	-0.69680900	-0.03633300
C	1.85187000	0.56593300	-1.90696500
C	0.72572700	0.76798700	3.86668500
C	1.09994800	2.29982400	1.96194500
C	-0.45411000	-1.33249800	3.67859900
H	-1.02347500	-1.90185500	1.68315600
C	-2.08853600	0.64840800	-1.04444600
C	-0.82820700	2.55983700	-0.60746800
C	-1.98746300	-0.76724000	-1.01324000
C	3.81049300	-0.74950600	-0.59445400
H	2.32137300	-1.17699700	0.92264100
N	3.05048600	0.57463300	-2.46574400
F	0.89386300	1.20652600	-2.65180300
C	0.19377300	-0.37815500	4.47510300
H	1.21214000	1.53300200	4.47534900
C	0.33801100	3.43598800	2.32074100
C	2.23881300	2.48839600	1.15241100
H	-0.88548800	-2.22829700	4.12951900
C	-3.20278600	1.35999900	-1.56211700
C	-1.88886200	3.35894100	-1.10058100
H	0.11176200	2.98760100	-0.27843200
C	-3.06121800	-1.51624800	-1.49487100
C	4.02965700	-0.07983500	-1.80549900
H	4.62251400	-1.28330100	-0.10016500
H	0.27862900	-0.51519100	5.55456900
C	0.67315500	4.71392700	1.84617100
H	-0.53934800	3.30005600	2.95504600
C	2.57221900	3.76518700	0.66833700
H	2.86407300	1.63854000	0.89430500
C	-3.06795200	2.77848100	-1.56237600
C	-4.29341400	0.57385200	-2.03763600
H	-1.75407300	4.43923200	-1.11684600
C	-4.20070800	-0.81893800	-1.99304800
H	-3.02580100	-2.60471700	-1.49912500
H	5.01586700	-0.06495400	-2.27562200
C	1.78516300	4.88080700	1.00221500
H	0.06316100	5.57425300	2.12744000
H	3.44929900	3.88455600	0.03044100
H	-3.87894900	3.40182900	-1.94258400

H	-5.18074400	1.06185100	-2.44043400
H	-5.03798800	-1.41106500	-2.36585600
H	2.04340300	5.86962500	0.61999200
Cartesian coordinates of step 17			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64052400
C	1.47299800	0.00000000	-0.67707800
C	0.58341400	1.00154500	2.47299200
C	-0.49705300	-1.15578600	2.29116900
N	-0.96575600	1.21886400	-0.56561400
O	-0.80815600	-1.19690000	-0.52332300
C	2.53456300	-0.66573000	-0.02989900
C	1.83381300	0.53991700	-1.92732700
C	0.63816200	0.82517400	3.87314700
C	1.02102900	2.33775700	1.95584700
C	-0.43544800	-1.33129000	3.68327800
H	-0.93885500	-1.94473900	1.68287000
C	-2.10169800	0.62533600	-1.03206300
C	-0.84867700	2.54910200	-0.63145800
C	-1.99012200	-0.78917900	-0.99187200
C	3.81827000	-0.71697300	-0.59681000
H	2.34572000	-1.12367900	0.94258900
N	3.02767300	0.54835800	-2.49613800
F	0.86179600	1.15058100	-2.67910400
C	0.14510700	-0.33712600	4.48317400
H	1.07787800	1.61697800	4.48308500
C	0.24601600	3.47103000	2.29389400
C	2.16691400	2.52590200	1.15580800
H	-0.83343500	-2.24203900	4.13495400
C	-3.22609000	1.32439800	-1.54506400
C	-1.91959500	3.33607100	-1.12196100
H	0.09212800	2.98764700	-0.32014700
C	-3.06394800	-1.54965300	-1.45533300
C	4.01968700	-0.07721100	-1.82691300
H	4.64077200	-1.22736500	-0.09517500
H	0.20993200	-0.45763200	5.56598600
C	0.57639100	4.74607500	1.80823000
H	-0.63711600	3.33520200	2.92015200
C	2.49597500	3.79968900	0.66141100
H	2.79952500	1.67690500	0.91284700
C	-3.10051200	2.74356000	-1.56263500
C	-4.31661700	0.52694200	-2.00139400
H	-1.79091300	4.41678200	-1.15250500
C	-4.21398800	-0.86477500	-1.94595500
H	-3.02014800	-2.63782000	-1.45200700
H	5.00189600	-0.06333400	-2.30536300
C	1.69636300	4.91255500	0.97486100
H	-0.04350900	5.60468100	2.07255700
H	3.37902100	3.91942100	0.03183800
H	-3.91974500	3.35745400	-1.94057000
H	-5.21138200	1.00563700	-2.39887200

H	-5.05122700	-1.46577400	-2.30436600
H	1.95094800	5.89925100	0.58479200
Cartesian coordinates of step 18			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64083800
C	1.47000700	0.00000000	-0.68302400
C	0.51802600	1.03350700	2.47699600
C	-0.46087400	-1.17138300	2.29054600
N	-0.97611100	1.20918600	-0.57012300
O	-0.80248000	-1.20549000	-0.51614200
C	2.54669900	-0.63186400	-0.02741600
C	1.81164800	0.50988300	-1.95129800
C	0.54052000	0.87428000	3.88046600
C	0.94387800	2.37039900	1.95541500
C	-0.42692700	-1.33126100	3.68531600
H	-0.85522000	-1.98273200	1.67918000
C	-2.11155300	0.60494300	-1.02502300
C	-0.86738900	2.53943800	-0.65129700
C	-1.99064100	-0.80847800	-0.97699200
C	3.82536600	-0.68249300	-0.60598900
H	2.37301600	-1.06519800	0.95919300
N	2.99922200	0.51690600	-2.53302000
F	0.82348800	1.08684300	-2.70863200
C	0.08226500	-0.30221200	4.48987200
H	0.93084600	1.68961100	4.49304900
C	0.15926700	3.50198500	2.27531600
C	2.09804600	2.55709900	1.16675700
H	-0.79401900	-2.25534600	4.13606200
C	-3.24342400	1.29286500	-1.53688800
C	-1.94585800	3.31555000	-1.14251100
H	0.07245500	2.98770600	-0.35162500
C	-3.06280900	-1.57898500	-1.42777500
C	4.00585500	-0.07673300	-1.85633800
H	4.65962600	-1.16734200	-0.09843800
H	0.12106600	-0.40828800	5.57542900
C	0.48959100	4.77443600	1.78283300
H	-0.73070700	3.36695100	2.89197000
C	2.42764300	3.82824900	0.66646800
H	2.73482700	1.70763300	0.93673600
C	-3.12653900	2.71243100	-1.56861900
C	-4.33207800	0.48552600	-1.97993000
H	-1.82296400	4.39653300	-1.18464700
C	-4.22061400	-0.90506400	-1.91505900
H	-3.01156100	-2.66677500	-1.41767600
H	4.98283400	-0.06483700	-2.34542500
C	1.61905300	4.93973800	0.96203800
H	-0.13765600	5.63224800	2.03196400
H	3.31762600	3.94752800	0.04660800
H	-3.95195700	3.31789500	-1.94670700
H	-5.23214300	0.95598800	-2.37526000
H	-5.05644800	-1.51387300	-2.26342200

H	1.87376100	5.92468200	0.56765700
Cartesian coordinates of step 19			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64118000
C	1.46616200	0.00000000	-0.69110200
C	0.45080100	1.06091800	2.48144300
C	-0.42233300	-1.18722300	2.28875200
N	-0.98464000	1.20006800	-0.57625900
O	-0.79754000	-1.21338800	-0.50922900
C	2.56201900	-0.58774700	-0.02670000
C	1.78216200	0.46629000	-1.98276400
C	0.44114900	0.91422500	3.88671600
C	0.86244300	2.40038700	1.95838500
C	-0.41556300	-1.33593400	3.68499900
H	-0.76783000	-2.01814400	1.67424500
C	-2.11880600	0.58626800	-1.02245500
C	-0.88227800	2.52985300	-0.67354100
C	-1.99003200	-0.82597600	-0.96578700
C	3.83312500	-0.64122200	-0.62194800
H	2.40858800	-0.98620900	0.97787300
N	2.96053000	0.46759400	-2.58275300
F	0.77362000	0.99908200	-2.74559400
C	0.02002600	-0.27690000	4.49399100
H	0.78018200	1.75007100	4.50217800
C	0.06481200	3.52751600	2.25989700
C	2.02587300	2.59001500	1.18399300
H	-0.74976100	-2.27333500	4.13382700
C	-3.25549700	1.26397100	-1.53752600
C	-1.96558400	3.29602200	-1.16970900
H	0.05601700	2.98662700	-0.38224500
C	-3.05974000	-1.60547300	-1.40716900
C	3.98574500	-0.08411700	-1.89834000
H	4.68232700	-1.09249900	-0.10820900
H	0.03287700	-0.37233200	5.58115000
C	0.39343500	4.79905300	1.76385800
H	-0.83306100	3.38990700	2.86438600
C	2.35467500	3.86035100	0.68161900
H	2.66876900	1.74190200	0.96640900
C	-3.14529700	2.68358000	-1.58448600
C	-4.34158800	0.44780800	-1.97028900
H	-1.84701600	4.37693400	-1.22400200
C	-4.22288400	-0.94166800	-1.89497000
H	-3.00205700	-2.69284700	-1.39007700
H	4.95506800	-0.07815400	-2.40252900
C	1.53408500	4.96780500	0.95954200
H	-0.24371700	5.65389500	1.99756600
H	3.25275100	3.98267300	0.07410000
H	-3.97470300	3.28129100	-1.96617300
H	-5.24503200	0.91074600	-2.36678500
H	-5.05667800	-1.55745900	-2.23586200
H	1.78772800	5.95243200	0.56370400

Cartesian coordinates of step 20

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64173100
C	1.46395900	0.00000000	-0.69567200
C	0.38246500	1.08477100	2.48478800
C	-0.38245800	-1.20176500	2.28758300
N	-0.99369900	1.18934500	-0.58293300
O	-0.79098400	-1.22232400	-0.50191100
C	2.57337700	-0.55239900	-0.02384400
C	1.76320700	0.43536600	-2.00217900
C	0.34197000	0.94795800	3.89070300
C	0.77858300	2.42709800	1.96022800
C	-0.40201200	-1.34151300	3.68451400
H	-0.67846700	-2.05023000	1.67133700
C	-2.12640300	0.56500200	-1.01914200
C	-0.89924600	2.51859500	-0.69559500
C	-1.98845000	-0.84592300	-0.95345500
C	3.84008200	-0.60585700	-0.62883600
H	2.43335300	-0.92539300	0.99244000
N	2.93591700	0.43450300	-2.61294600
F	0.74091100	0.93515200	-2.76901800
C	-0.04046000	-0.25681200	4.49621600
H	0.62962600	1.80154600	4.50794300
C	-0.03396200	3.54817600	2.24236600
C	1.95147300	2.62168100	1.20119500
H	-0.70202700	-2.29104500	4.13200100
C	-3.26921900	1.23142900	-1.53555600
C	-1.98880500	3.27380000	-1.19485500
H	0.03771400	2.98414900	-0.41421600
C	-3.05540200	-1.63540800	-1.38393100
C	3.97403100	-0.08453500	-1.92230300
H	4.69982900	-1.03053500	-0.10995600
H	-0.05267800	-0.34399800	5.58407400
C	0.29101000	4.81926000	1.74265600
H	-0.93966300	3.40637900	2.83406300
C	2.27751700	3.89161600	0.69650200
H	2.60284500	1.77639500	0.99750000
C	-3.16728400	2.65106300	-1.59712300
C	-4.35238900	0.40546300	-1.95665000
H	-1.87590300	4.35465100	-1.26088900
C	-4.22501900	-0.98266900	-1.87095800
H	-2.99034600	-2.72222200	-1.35953600
H	4.93868700	-0.08123500	-2.43538800
C	1.44295100	4.99341800	0.95555600
H	-0.35752000	5.66980400	1.96021000
H	3.18364100	4.01846000	0.10196400
H	-4.00179700	3.24030600	-1.98085700
H	-5.26016600	0.85995800	-2.35301400
H	-5.05659000	-1.60615500	-2.20318000
H	1.69407800	5.97800000	0.55800700

Cartesian coordinates of step 21

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64210300
C	1.46278300	0.00000000	-0.69812700
C	0.31301200	1.10458400	2.48746300
C	-0.33757400	-1.21627000	2.28614300
N	-1.00143600	1.17789800	-0.59240500
O	-0.78417700	-1.23157800	-0.49436100
C	2.58645900	-0.50735500	-0.01508300
C	1.74580800	0.39705100	-2.02056400
C	0.24556200	0.97370900	3.89302900
C	0.68872500	2.45179900	1.96292300
C	-0.38010600	-1.35052000	3.68298900
H	-0.58219800	-2.08030300	1.66901500
C	-2.13128300	0.54307300	-1.02179500
C	-0.91356000	2.50611600	-0.72245400
C	-1.98477600	-0.86628300	-0.94521800
C	3.84994100	-0.55914800	-0.62738900
H	2.45922500	-0.84880200	1.01394600
N	2.91378600	0.39500500	-2.64008500
F	0.70926700	0.85468500	-2.79450400
C	-0.09365700	-0.24475000	4.49651800
H	0.48110300	1.84220800	4.51153400
C	-0.14502200	3.56194400	2.22397900
C	1.87216800	2.65864100	1.22341700
H	-0.64213000	-2.31183800	4.12916300
C	-3.27789900	1.19797000	-1.54463400
C	-2.00689700	3.25007300	-1.23023300
H	0.02118900	2.98000000	-0.44777300
C	-3.04771200	-1.66572000	-1.36755200
C	3.96549500	-0.08193100	-1.93947000
H	4.72083800	-0.94979200	-0.10040500
H	-0.12813100	-0.32709300	5.58426600
C	0.17174300	4.83502100	1.72401100
H	-1.05969500	3.41017600	2.79915600
C	2.19090900	3.93084000	0.72006900
H	2.53715300	1.82020400	1.03442600
C	-3.18305400	2.61722200	-1.62296000
C	-4.35692800	0.36221700	-1.95673400
H	-1.89877300	4.33047900	-1.30980000
C	-4.22170100	-1.02437100	-1.85854300
H	-2.97578900	-2.75185600	-1.33447700
H	4.92630200	-0.08048100	-2.45972500
C	1.33647700	5.02207100	0.95912800
H	-0.49285000	5.67734700	1.92430400
H	3.10624600	4.06804100	0.14215000
H	-4.02076400	3.19782800	-2.01284800
H	-5.26737500	0.80805700	-2.35676500
H	-5.05002500	-1.65555500	-2.18427500
H	1.58175000	6.00861300	0.56280300
Cartesian coordinates of step 22			
B	0.00000000	0.00000000	0.00000000

C	0.00000000	0.00000000	1.64226500
C	1.46088600	0.00000000	-0.70199800
C	0.24261500	1.12010900	2.48976900
C	-0.29082500	-1.22960100	2.28421600
N	-1.00887400	1.16584700	-0.60261900
O	-0.77715400	-1.24126800	-0.48583000
C	2.60093300	-0.45242800	-0.00829300
C	1.72420800	0.34856000	-2.04230300
C	0.14747700	0.99226800	3.89414100
C	0.59705100	2.47287700	1.96694100
C	-0.35652700	-1.36099800	3.68030800
H	-0.48246100	-2.10650500	1.66640500
C	-2.13455300	0.52028600	-1.02789300
C	-0.92770000	2.49289100	-0.74920000
C	-1.97952100	-0.88736100	-0.93941100
C	3.85994700	-0.50341500	-0.63020900
H	2.48926700	-0.75357800	1.03512900
N	2.88601300	0.34320800	-2.67311100
F	0.67119400	0.75509100	-2.82223600
C	-0.14724200	-0.23873400	4.49511900
H	0.32942500	1.87284000	4.51367600
C	-0.25802300	3.57068100	2.20866000
C	1.79124000	2.69464900	1.24895000
H	-0.57929300	-2.33282900	4.12500200
C	-3.28371300	1.16332400	-1.55994000
C	-2.02347600	3.22516500	-1.26858700
H	0.00358600	2.97517100	-0.47719400
C	-3.03734800	-1.69690700	-1.35570700
C	3.95344800	-0.08218400	-1.96288500
H	4.74370700	-0.85259600	-0.09558600
H	-0.20434900	-0.31876000	5.58208600
C	0.05031600	4.84703700	1.71175100
H	-1.18156600	3.40689400	2.76610100
C	2.10240000	3.97030600	0.74999200
H	2.46956600	1.86364200	1.07323300
C	-3.19593100	2.58194000	-1.65509200
C	-4.35742100	0.31769300	-1.96547000
H	-1.92028900	4.30496900	-1.36153600
C	-4.21456700	-1.06715200	-1.85377900
H	-2.95863100	-2.78223700	-1.31333300
H	4.90915200	-0.08488800	-2.49243800
C	1.22794300	5.04965900	0.97062800
H	-0.63051600	5.67998800	1.89604800
H	3.02688700	4.11983600	0.18993600
H	-4.03575700	3.15354500	-2.05365000
H	-5.26938000	0.75460800	-2.37184500
H	-5.03876000	-1.70608900	-2.17487100
H	1.46719300	6.03916600	0.57802900
Cartesian coordinates of step 23			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64196500

C	1.45815900	0.00000000	-0.70721800
C	0.17144800	1.13078600	2.49205700
C	-0.23888700	-1.24248100	2.28096500
N	-1.01242400	1.15550900	-0.61700100
O	-0.77217500	-1.24943800	-0.47674500
C	2.61903800	-0.37512800	-0.00301500
C	1.69610100	0.28102500	-2.06845000
C	0.05316900	1.00128400	3.89455900
C	0.49870400	2.49155600	1.97390400
C	-0.32378900	-1.37516000	3.67579100
H	-0.37764200	-2.12854300	1.66195700
C	-2.13250000	0.50111000	-1.04414100
C	-0.93422900	2.48081600	-0.78076400
C	-1.97244600	-0.90499700	-0.94115500
C	3.87234500	-0.42298800	-0.63724000
H	2.52810700	-0.62114100	1.05677900
N	2.84986600	0.27264900	-2.71354500
F	0.62199500	0.61328800	-2.85426900
C	-0.19196700	-0.24204500	4.49208800
H	0.18116200	1.89039500	4.51543200
C	-0.38607100	3.57015300	2.19190100
C	1.70567900	2.73812200	1.28570600
H	-0.50407500	-2.35668000	4.11839100
C	-3.27932600	1.13382800	-1.59356200
C	-2.02745300	3.20290900	-1.31941700
H	-0.00777500	2.97010600	-0.50456100
C	-3.02396800	-1.72304400	-1.35727100
C	3.93764800	-0.07888800	-1.99342400
H	4.77243800	-0.71361200	-0.09488300
H	-0.26829100	-0.32348400	5.57776800
C	-0.09269800	4.85227600	1.70072600
H	-1.31985800	3.38682300	2.72568600
C	2.00280900	4.01992000	0.79423100
H	2.40538400	1.92085100	1.12868400
C	-3.19493900	2.55125900	-1.70656400
C	-4.34675100	0.28000400	-1.99816200
H	-1.92654900	4.28166400	-1.42579800
C	-4.19961100	-1.10311200	-1.87058200
H	-2.94081400	-2.80754800	-1.30382700
H	4.88692800	-0.08444000	-2.53437600
C	1.09954100	5.08012600	0.99091400
H	-0.79623600	5.67031300	1.86543800
H	2.93843600	4.18939400	0.25888900
H	-4.03309300	3.11505000	-2.11952600
H	-5.25681300	0.70921500	-2.41679900
H	-5.01880600	-1.74858300	-2.19140100
H	1.32763200	6.07455100	0.60414500
Cartesian coordinates of step 24			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64206100
C	1.45672300	0.00000000	-0.70932000

C	0.10004700	1.13864000	2.49257400
C	-0.19245800	-1.25142600	2.27939600
N	-1.01898700	1.14396500	-0.62526700
O	-0.76667100	-1.25863800	-0.46754900
C	2.62626900	-0.33576900	0.00012000
C	1.68522600	0.25151700	-2.07802200
C	-0.04686000	1.00790500	3.89224300
C	0.40853700	2.50426200	1.97777800
C	-0.30176900	-1.38475800	3.67242200
H	-0.27817500	-2.14433600	1.66055500
C	-2.13681100	0.48040400	-1.04498600
C	-0.94730000	2.46794700	-0.80247500
C	-1.96953800	-0.92401100	-0.93094300
C	3.87795800	-0.37897000	-0.63788800
H	2.54292700	-0.55758400	1.06585300
N	2.83642600	0.24513600	-2.72759400
F	0.60257900	0.54734900	-2.86645200
C	-0.24776000	-0.24425800	4.48759400
H	0.02726400	1.90322500	4.51292900
C	-0.49466400	3.57091000	2.17624000
C	1.62553300	2.76534600	1.31231200
H	-0.44351400	-2.37289100	4.11426600
C	-3.28730100	1.10277900	-1.59876700
C	-2.04407000	3.17980600	-1.34737200
H	-0.02353100	2.96452400	-0.53024500
C	-3.01817600	-1.75058900	-1.33804100
C	3.93244600	-0.06967200	-2.00285100
H	4.78492700	-0.64000700	-0.09195900
H	-0.34734700	-0.32699800	5.57127900
C	-0.20826100	4.85588200	1.68820600
H	-1.43650000	3.37611100	2.69151000
C	1.91591500	4.05009000	0.82494600
H	2.33735300	1.95557500	1.16926600
C	-3.20919100	2.51933000	-1.72628000
C	-4.35147700	0.24060600	-1.99376100
H	-1.94799500	4.25789900	-1.46404700
C	-4.19760000	-1.14079000	-1.85429900
H	-2.92931200	-2.83419200	-1.27608700
H	4.87974000	-0.07386200	-2.54727400
C	0.99490400	5.09851800	1.00224900
H	-0.92567900	5.66486700	1.83688900
H	2.85955000	4.23117700	0.30778600
H	-4.05034600	3.07528800	-2.14373600
H	-5.26409900	0.66198200	-2.41475600
H	-5.01435800	-1.79278200	-2.16804600
H	1.21751500	6.09546300	0.61881600
Cartesian coordinates of step 25			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64212600
C	1.45623600	0.00000000	-0.70972700
C	0.02833200	1.14178300	2.49325000

C	-0.14373700	-1.25931500	2.27691500
N	-1.02369400	1.13346600	-0.63501000
O	-0.76129800	-1.26644700	-0.45934000
C	2.63300800	-0.29588200	0.00514700
C	1.67680300	0.21891300	-2.08547600
C	-0.14339700	1.00564300	3.88955700
C	0.31207000	2.51430000	1.98420600
C	-0.27469800	-1.39701700	3.66757200
H	-0.17605400	-2.15556300	1.65775900
C	-2.13803300	0.46169800	-1.05137300
C	-0.95735600	2.45612000	-0.82394900
C	-1.96472900	-0.94102000	-0.92654600
C	3.88341200	-0.33655500	-0.63590600
H	2.55612100	-0.49141200	1.07648200
N	2.82569900	0.21184200	-2.73889600
F	0.58699600	0.47862700	-2.87658100
C	-0.29721600	-0.25455000	4.48184700
H	-0.12288100	1.90364800	4.51043000
C	-0.61591900	3.56274400	2.16228000
C	1.53880100	2.79903100	1.34623900
H	-0.37599600	-2.39070200	4.10810000
C	-3.29030200	1.07466200	-1.61206900
C	-2.05587700	3.15873100	-1.37706300
H	-0.03653000	2.95902100	-0.55309300
C	-3.00940700	-1.77530500	-1.32836200
C	3.92867900	-0.06565400	-2.00927100
H	4.79621500	-0.56735400	-0.08608800
H	-0.41729900	-0.34188000	5.56309300
C	-0.34289500	4.85337700	1.68129600
H	-1.56559900	3.34944000	2.65538400
C	1.81615000	4.08948700	0.86683700
H	2.26762000	2.00163700	1.21734500
C	-3.21779600	2.49032500	-1.75166000
C	-4.35024600	0.20492200	-2.00158300
H	-1.96395800	4.23618700	-1.50236800
C	-4.19072300	-1.17470100	-1.85079800
H	-2.91590200	-2.85798300	-1.25770200
H	4.87419300	-0.07083000	-2.55677500
C	0.87124600	5.11981200	1.02378600
H	-1.07903800	5.64830800	1.81323500
H	2.76766800	4.28921200	0.37143500
H	-4.06066100	3.03924000	-2.17497300
H	-5.26389800	0.61909600	-2.42747100
H	-5.00428700	-1.83264100	-2.16043800
H	1.08361500	6.12143500	0.64677200
Cartesian coordinates of step 26			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64208200
C	1.45609800	0.00000000	-0.70945200
C	-0.04334700	1.13947900	2.49478300
C	-0.09303000	-1.26634500	2.27250900

N	-1.02643100	1.12321500	-0.64644700
O	-0.75659600	-1.27404100	-0.45106900
C	2.63980600	-0.24843400	0.01174400
C	1.66949900	0.18102200	-2.09194800
C	-0.23770400	0.99325600	3.88711600
C	0.21028600	2.52035500	1.99389100
C	-0.24391500	-1.41286000	3.66011500
H	-0.07132100	-2.16189100	1.65174900
C	-2.13626900	0.44405400	-1.06323500
C	-0.96342200	2.44424900	-0.84774300
C	-1.95844700	-0.95693400	-0.92661500
C	3.88934600	-0.28613500	-0.63154700
H	2.56870500	-0.41212700	1.08879200
N	2.81649700	0.17309300	-2.74846300
F	0.57300400	0.39902400	-2.88618700
C	-0.34254700	-0.27418900	4.47452700
H	-0.27131900	1.89003900	4.50919400
C	-0.74760800	3.54476500	2.14993300
C	1.44567000	2.83661800	1.38758700
H	-0.30356200	-2.41110800	4.09794400
C	-3.28744300	1.04824400	-1.63572900
C	-2.06063600	3.13815700	-1.41395600
H	-0.04660900	2.95303800	-0.57405000
C	-2.99834800	-1.79814700	-1.32677100
C	3.92606500	-0.06058300	-2.01327800
H	4.80783000	-0.48118100	-0.07734600
H	-0.48158300	-0.36969400	5.55280400
C	-0.49366000	4.84303100	1.67892800
H	-1.70430300	3.30705900	2.61771900
C	1.70406700	4.13487600	0.91909500
H	2.19584300	2.05625100	1.27406900
C	-3.21850400	2.46270000	-1.78832700
C	-4.34235900	0.17168900	-2.02340800
H	-1.97132600	4.21470800	-1.54826700
C	-4.17893400	-1.20609800	-1.86012600
H	-2.90133400	-2.87985700	-1.24688000
H	4.87014300	-0.06703800	-2.56324000
C	0.73040800	5.14125400	1.05446800
H	-1.25228000	5.61935800	1.79305500
H	2.66281100	4.35946600	0.44888700
H	-4.06074600	3.00499300	-2.22131000
H	-5.25495900	0.57913700	-2.45793900
H	-4.98857000	-1.86942500	-2.16859200
H	0.92805500	6.14920200	0.68640700
Cartesian coordinates of step 27			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.64171000
C	1.45581500	0.00000000	-0.70965800
C	-0.11460500	1.13247800	2.49639800
C	-0.04322400	-1.27179300	2.26663600
N	-1.02920600	1.11345900	-0.65814700

O	-0.75159100	-1.28124000	-0.44323800
C	2.64566200	-0.20012100	0.01618700
C	1.66236400	0.14106500	-2.09793700
C	-0.33243900	0.97268600	3.88373300
C	0.11044500	2.52149700	2.00578800
C	-0.21485400	-1.43031400	3.65039700
H	0.03231100	-2.16324600	1.64398300
C	-2.13229700	0.42644800	-1.08006100
C	-0.97051900	2.43338600	-0.86873800
C	-1.94984100	-0.97279800	-0.93195800
C	3.89406800	-0.23655800	-0.62976700
H	2.58018100	-0.32904700	1.09833400
N	2.80725600	0.13052000	-2.75782700
F	0.55975400	0.31778600	-2.89380600
C	-0.38947700	-0.30061400	4.46499200
H	-0.41979900	1.86462900	4.50759100
C	-0.87185400	3.52423600	2.14762300
C	1.35140200	2.86709200	1.42672000
H	-0.23358600	-2.43171200	4.08467500
C	-3.28086000	1.02141800	-1.66752700
C	-2.06492500	3.11812400	-1.45095500
H	-0.05980000	2.94889400	-0.58731600
C	-2.98288700	-1.82129300	-1.33471600
C	3.92276600	-0.05881000	-2.01861600
H	4.81765000	-0.39499300	-0.07234500
H	-0.54801900	-0.40691400	5.53955500
C	-0.63448300	4.83070400	1.69069000
H	-1.83303400	3.26409600	2.59385000
C	1.59343700	4.17378400	0.97353500
H	2.11829300	2.10130300	1.32197500
C	-3.21638300	2.43481700	-1.83080800
C	-4.32864000	0.13765500	-2.05802500
H	-1.97901300	4.19401300	-1.59244700
C	-4.16106300	-1.23816500	-1.88291900
H	-2.88210800	-2.90193700	-1.24583300
H	4.86523700	-0.06824800	-2.57127900
C	0.59666100	5.15904800	1.09585000
H	-1.41132600	5.59045100	1.79335800
H	2.55714000	4.42165200	0.52561100
H	-4.05681400	2.97009100	-2.27587600
H	-5.23880700	0.53809500	-2.50401700
H	-4.96513100	-1.90719900	-2.19364900
H	0.78151500	6.17392300	0.74038500
Cartesian coordinates of step 28			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62898400
C	1.50347200	0.00000000	-0.62614500
C	-0.17820200	1.07893700	2.53455800
C	0.49623100	-1.21401300	2.16921800
N	-0.83201900	1.19024600	-0.77807800
O	-0.80009600	-1.21582400	-0.49705900

C	1.95622800	-1.01515200	-1.49217900
C	2.48081200	0.97502100	-0.34917400
C	0.16965800	0.93497900	3.89721400
C	-0.83983100	2.35855100	2.14577200
C	0.81273700	-1.36667000	3.52595500
H	0.65730100	-2.05870900	1.49619300
C	-1.87262600	0.58768600	-1.42007700
C	-0.63864500	2.50522600	-0.93212000
C	-1.84279000	-0.81929200	-1.22861100
C	3.26813900	-1.00288500	-1.99941400
H	1.26826400	-1.81891000	-1.75784900
N	3.72047400	1.04178600	-0.79596500
F	2.12888100	2.01438600	0.48235600
C	0.66818300	-0.27462700	4.39699500
H	0.01497100	1.78212500	4.56844900
C	-2.19257000	2.35334800	1.74198400
C	-0.16450500	3.59323000	2.23597600
H	1.18641500	-2.32341800	3.89555400
C	-2.83152600	1.26836100	-2.21726200
C	-1.53262800	3.26881800	-1.71915200
H	0.19981500	2.94791200	-0.40682300
C	-2.84959100	-1.58577400	-1.81744500
C	4.11424200	0.04677600	-1.62212600
H	3.62432400	-1.78739200	-2.66771800
H	0.92610000	-0.36650900	5.45344800
C	-2.84855400	3.54896100	1.41538600
H	-2.71950000	1.39994100	1.68250800
C	-0.81760400	4.79204400	1.90353100
H	0.88166300	3.60110700	2.54336300
C	-2.62363600	2.67179100	-2.34654800
C	-3.85235300	0.46467800	-2.80502200
H	-1.35512100	4.33880100	-1.80674300
C	-3.84163800	-0.91596300	-2.59172300
H	-2.87079000	-2.66785500	-1.69654800
H	5.14298600	0.10576200	-1.98474200
C	-2.16115700	4.77343300	1.49020500
H	-3.89383900	3.52595600	1.10231300
H	-0.27805800	5.73875300	1.96739700
H	-3.31376300	3.27105900	-2.94263200
H	-4.62207500	0.92832300	-3.42171200
H	-4.62573900	-1.52147700	-3.04905500
H	-2.67014300	5.70498100	1.23664500
Cartesian coordinates of step 29			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62828400
C	1.50347000	0.00000000	-0.62435800
C	-0.24578400	1.06642800	2.53252900
C	0.55077200	-1.18820500	2.17162000
N	-0.82721000	1.19450800	-0.77025700
O	-0.80467600	-1.21221700	-0.50025600
C	1.95519400	-1.00281500	-1.50466200

C	2.48171500	0.96927100	-0.33051000
C	0.09489600	0.93846900	3.89864000
C	-0.96515000	2.31191500	2.13574200
C	0.85855300	-1.32732400	3.53181600
H	0.76277400	-2.02170600	1.49853000
C	-1.87600200	0.60109600	-1.40613000
C	-0.62790300	2.50961300	-0.91621600
C	-1.85194600	-0.80712200	-1.22090700
C	3.26827900	-0.98529900	-2.00899800
H	1.26583700	-1.80110500	-1.78319500
N	3.72228900	1.04051900	-0.77386500
F	2.12906800	1.99635900	0.51619200
C	0.64860200	-0.24529900	4.40226300
H	-0.10974700	1.77548700	4.56921500
C	-2.30787600	2.23935700	1.70526100
C	-0.35597700	3.57918500	2.24310900
H	1.27617600	-2.26438400	3.90479900
C	-2.83863600	1.29177400	-2.18977000
C	-1.52635400	3.28307400	-1.68778800
H	0.21934200	2.94251700	-0.39696400
C	-2.86882300	-1.56472100	-1.80381900
C	4.11546600	0.05710800	-1.61430600
H	3.62458200	-1.76025000	-2.68830000
H	0.89912600	-0.32578200	5.46142400
C	-3.01832900	3.40124500	1.37176100
H	-2.78421800	1.26070300	1.63210300
C	-1.06418100	4.74461700	1.90473800
H	0.68257100	3.63950500	2.57096300
C	-2.62555800	2.69500200	-2.30988900
C	-3.86956100	0.49668000	-2.77178400
H	-1.34604700	4.35306800	-1.76905600
C	-3.86434800	-0.88502100	-2.56537400
H	-2.89575500	-2.64721300	-1.68786200
H	5.14497100	0.11957800	-1.97416500
C	-2.39708900	4.65924900	1.46659800
H	-4.05511700	3.32618200	1.03916700
H	-0.57574600	5.71761700	1.98365100
H	-3.31897000	3.30222300	-2.89397700
H	-4.64310900	0.96759400	-3.37809300
H	-4.65635300	-1.48383000	-3.01792100
H	-2.94890400	5.56467600	1.20819000
Cartesian coordinates of step 30			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62788900
C	1.50300400	0.00000000	-0.62579900
C	-0.31305900	1.05157500	2.52958200
C	0.62123300	-1.15109600	2.17379800
N	-0.82018900	1.20157200	-0.76290900
O	-0.80888600	-1.20664300	-0.50771300
C	1.95032000	-0.99341200	-1.51867800
C	2.48407500	0.96337400	-0.32173500

C	0.03629600	0.94830400	3.89576700
C	-1.11528100	2.24406500	2.13061300
C	0.93509100	-1.26876800	3.53469000
H	0.88689800	-1.97042900	1.50215200
C	-1.86554000	0.61672000	-1.41127300
C	-0.62238400	2.51928100	-0.88527600
C	-1.84805300	-0.79283000	-1.23533600
C	3.26262600	-0.97323400	-2.02512300
H	1.25829000	-1.78659700	-1.80518800
N	3.72405400	1.03663400	-0.76655400
F	2.13568200	1.98038900	0.53848400
C	0.66105400	-0.19836500	4.40194800
H	-0.22055700	1.77186400	4.56503800
C	-2.43246100	2.07462300	1.65075400
C	-0.61522700	3.55388200	2.28357500
H	1.40814400	-2.17799700	3.91035700
C	-2.82404800	1.31784000	-2.19028300
C	-1.51809200	3.30334600	-1.64901800
H	0.22292100	2.94390500	-0.35598100
C	-2.86482200	-1.54195800	-1.82937100
C	4.11303500	0.06234300	-1.61954700
H	3.61584700	-1.74093500	-2.71419700
H	0.91621000	-0.26071300	5.46122300
C	-3.22310700	3.18262600	1.31526500
H	-2.82597200	1.06302600	1.54281700
C	-1.40431300	4.66610100	1.94493900
H	0.40327600	3.69091300	2.64983800
C	-2.61174300	2.72272300	-2.28791400
C	-3.85416100	0.53101500	-2.78481000
H	-1.34071900	4.37508200	-1.71181700
C	-3.85394200	-0.85251900	-2.59060100
H	-2.89728500	-2.62508000	-1.72085300
H	5.14200300	0.12658800	-1.98065300
C	-2.71056700	4.48436600	1.45877900
H	-4.23796900	3.03094400	0.94359300
H	-0.99919600	5.67306300	2.06109900
H	-3.30324800	3.33821100	-2.86553600
H	-4.62424100	1.00971000	-3.38944600
H	-4.64586200	-1.44483300	-3.05176700
H	-3.32489900	5.34825100	1.19947100
Cartesian coordinates of step 31			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62765700
C	1.50314800	0.00000000	-0.62621200
C	-0.37898100	1.03123000	2.52800700
C	0.67951200	-1.11565000	2.17692500
N	-0.81497200	1.20498100	-0.76100500
O	-0.80910400	-1.20416200	-0.51397400
C	1.95007500	-0.98684400	-1.52622000
C	2.48422300	0.96096300	-0.31431100
C	-0.03622300	0.94390000	3.89725700

C	-1.23806000	2.18114800	2.12357000
C	0.98650300	-1.21937600	3.54048000
H	0.99826300	-1.91644100	1.50590100
C	-1.84800000	0.62282800	-1.43087800
C	-0.62403400	2.52549600	-0.86127100
C	-1.83330100	-0.78741800	-1.26095900
C	3.26289500	-0.96361000	-2.03141600
H	1.25772200	-1.77755200	-1.81879500
N	3.72472700	1.03661300	-0.75732000
F	2.13499400	1.97166300	0.55282500
C	0.64587900	-0.16786200	4.40693400
H	-0.34366200	1.75043200	4.56591800
C	-2.52908700	1.94547100	1.60232800
C	-0.81783100	3.51486900	2.30887700
H	1.50626500	-2.10156400	3.91882100
C	-2.79700300	1.32818500	-2.21731900
C	-1.51239000	3.31424100	-1.62875400
H	0.21150900	2.94721200	-0.31429900
C	-2.83993600	-1.53379800	-1.87549000
C	4.11362800	0.06825900	-1.61718600
H	3.61637600	-1.72636500	-2.72582700
H	0.89461100	-0.21855100	5.46835200
C	-3.37095400	3.01227400	1.25820900
H	-2.86180700	0.91529500	1.46979900
C	-1.65885500	4.58611500	1.96301400
H	0.18056600	3.70346400	2.70674900
C	-2.59101900	2.73522000	-2.29409500
C	-3.81603700	0.54399400	-2.83392000
H	-1.34150500	4.38793800	-1.67413300
C	-3.81696600	-0.84083800	-2.64890300
H	-2.87439700	-2.61735800	-1.77202100
H	5.14299900	0.13428400	-1.97682700
C	-2.93770100	4.33848800	1.43532700
H	-4.36411900	2.80922500	0.85396900
H	-1.31515900	5.61242600	2.10510100
H	-3.27707700	3.35420800	-2.87441600
H	-4.57772300	1.02584500	-3.44663300
H	-4.60080000	-1.43108600	-3.12623600
H	-3.59235300	5.17018500	1.16951700
Cartesian coordinates of step 32			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62719100
C	1.50318200	0.00000000	-0.62864600
C	-0.44389100	1.00745800	2.52572300
C	0.73684100	-1.07609400	2.18072800
N	-0.80481400	1.21273400	-0.75859800
O	-0.81135700	-1.19781500	-0.52437600
C	1.94582900	-0.97918000	-1.53886800
C	2.48587600	0.95796600	-0.31228500
C	-0.10678200	0.93709900	3.89760500
C	-1.36085300	2.10906700	2.11573700

C	1.03819300	-1.16489500	3.54661100
H	1.10739800	-1.85548200	1.51101500
C	-1.81890600	0.63675900	-1.46151200
C	-0.61992400	2.53590900	-0.82955600
C	-1.81105800	-0.77461600	-1.30065000
C	3.25675800	-0.95240400	-2.04898100
H	1.25193200	-1.76712200	-1.83525100
N	3.72479000	1.03648900	-0.75934600
F	2.14067500	1.96111900	0.56483900
C	0.63242800	-0.13537200	4.41138300
H	-0.46448700	1.72359600	4.56508400
C	-2.61651000	1.80732400	1.54416300
C	-1.03078900	3.46196600	2.34217000
H	1.60378700	-2.01703900	3.92802900
C	-2.75010500	1.34999200	-2.26159000
C	-1.49277100	3.33282500	-1.60644300
H	0.19992100	2.95162000	-0.25472300
C	-2.80252500	-1.51489400	-1.94648500
C	4.10965200	0.07539800	-1.62916200
H	3.60712900	-1.70942400	-2.75120200
H	0.87522700	-0.17369400	5.47468500
C	-3.50847700	2.82868900	1.18861500
H	-2.88202800	0.76220900	1.38088600
C	-1.92310700	4.48770200	1.98762200
H	-0.06077100	3.70254000	2.78048700
C	-2.54938700	2.75898500	-2.31042900
C	-3.75277600	0.57187400	-2.91170500
H	-1.32821900	4.40828000	-1.62856400
C	-3.75856600	-0.81460800	-2.73948600
H	-2.84211600	-2.59898900	-1.85062900
H	5.13763300	0.14398500	-1.99229600
C	-3.16419200	4.17460000	1.40741500
H	-4.47219200	2.57459100	0.74394700
H	-1.64827200	5.52954400	2.16267200
H	-3.22398300	3.38411600	-2.89752300
H	-4.49940900	1.05972800	-3.53805500
H	-4.53041300	-1.40017800	-3.24147800
H	-3.85859000	4.97053200	1.13311200
Cartesian coordinates of step 33			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62658000
C	1.50254800	0.00000000	-0.63192800
C	-0.50689400	0.97879300	2.52405300
C	0.78114800	-1.04153700	2.18507700
N	-0.79954900	1.21700100	-0.75691100
O	-0.81222800	-1.19429900	-0.53116900
C	1.94287600	-0.97597000	-1.54655300
C	2.48637000	0.95618400	-0.31343900
C	-0.18649000	0.91576100	3.90054800
C	-1.46240600	2.04436800	2.10709400
C	1.06645300	-1.12442000	3.55475500

H	1.20030000	-1.79690300	1.51650600
C	-1.79648700	0.64377400	-1.48606400
C	-0.62180700	2.54193200	-0.80720800
C	-1.79175800	-0.76822500	-1.33141100
C	3.25310100	-0.94832200	-2.05857200
H	1.24791200	-1.76225900	-1.84479300
N	3.72481900	1.03517200	-0.76184100
F	2.14317500	1.95634400	0.56761800
C	0.59658300	-0.12244800	4.41943200
H	-0.59181800	1.67957000	4.56713500
C	-2.68892900	1.70081800	1.49747300
C	-1.19532600	3.40615800	2.36283900
H	1.66818800	-1.94993900	3.93941500
C	-2.71357600	1.36087800	-2.29852100
C	-1.48267800	3.34298500	-1.59338500
H	0.18377800	2.95517600	-0.21060300
C	-2.76877100	-1.50573800	-2.00207200
C	4.10754400	0.07699600	-1.63582400
H	3.60181000	-1.70291700	-2.76422500
H	0.82460000	-0.15593200	5.48616600
C	-3.61217700	2.69096700	1.13285600
H	-2.90660400	0.64865700	1.31047300
C	-2.11984000	4.40030900	2.00164200
H	-0.24801000	3.67914200	2.83091500
C	-2.51966900	2.77121300	-2.32749000
C	-3.70065300	0.58550500	-2.97511700
H	-1.32482100	4.41971100	-1.59898900
C	-3.70805000	-0.80202400	-2.81175400
H	-2.81054700	-2.59020800	-1.91146400
H	5.13511700	0.14597000	-2.00006400
C	-3.33075100	4.04609100	1.38254200
H	-4.55236300	2.40500500	0.65816200
H	-1.89321200	5.44939300	2.20070000
H	-3.18522600	3.39933200	-2.92164800
H	-4.43509500	1.07636900	-3.61342500
H	-4.46833300	-1.38550000	-3.33346600
H	-4.05021300	4.81699000	1.10142200
Cartesian coordinates of step 34			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62614000
C	1.50126800	0.00000000	-0.63677600
C	-0.56832400	0.94665300	2.52194400
C	0.82559500	-1.00361500	2.18996900
N	-0.79455900	1.22418600	-0.75017100
O	-0.81467900	-1.18833900	-0.54068100
C	1.93701900	-0.97255200	-1.55718600
C	2.48687600	0.95472700	-0.31932700
C	-0.26223100	0.89154800	3.90230300
C	-1.56665400	1.96987600	2.09906500
C	1.09654200	-1.08048500	3.56286500
H	1.29167000	-1.73267900	1.52331200

C	-1.77698700	0.65733900	-1.50346400
C	-0.62612400	2.55085100	-0.77276300
C	-1.77610000	-0.75565400	-1.35948700
C	3.24485900	-0.94347600	-2.07525500
H	1.24047800	-1.75757800	-1.85499200
N	3.72342000	1.03469300	-0.77297700
F	2.14833300	1.95183600	0.56666200
C	0.56477400	-0.10917700	4.42644500
H	-0.71384200	1.63008100	4.56759300
C	-2.76029200	1.57909600	1.45403200
C	-1.37274000	3.33837200	2.38458100
H	1.73431200	-1.87677100	3.95102600
C	-2.68356100	1.38214300	-2.32035800
C	-1.47873100	3.35986500	-1.56011200
H	0.16683500	2.95854100	-0.15551000
C	-2.74154900	-1.48709600	-2.05320500
C	4.10168200	0.07977400	-1.65242100
H	3.58998300	-1.69555400	-2.78534100
H	0.77958100	-0.13768300	5.49605700
C	-3.72126300	2.53050800	1.08320700
H	-2.92280500	0.52133300	1.24438100
C	-2.33611400	4.29319200	2.01970000
H	-0.45113000	3.64818800	2.88023300
C	-2.49781300	2.79388700	-2.32303600
C	-3.65780900	0.61290600	-3.02195200
H	-1.32887500	4.43768300	-1.54391400
C	-3.66661700	-0.77621100	-2.87284600
H	-2.78628400	-2.57213300	-1.97117300
H	5.12761300	0.14968900	-2.02109400
C	-3.51286300	3.89267700	1.36404900
H	-4.63468900	2.20816600	0.58040600
H	-2.16577700	5.34800000	2.24316300
H	-3.15723900	3.42780900	-2.91784000
H	-4.38295700	1.10976500	-3.66622200
H	-4.41767600	-1.35496900	-3.41285300
H	-4.26218600	4.63296300	1.07872200
Cartesian coordinates of step 35			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62539000
C	1.50012200	0.00000000	-0.64247400
C	-0.62901100	0.91253200	2.51707800
C	0.87441100	-0.95712300	2.19627600
N	-0.78427200	1.23673500	-0.74305700
O	-0.81847200	-1.17761100	-0.55639400
C	1.93065500	-0.96978700	-1.56821600
C	2.48795300	0.95323500	-0.32725100
C	-0.33031000	0.87381000	3.89980800
C	-1.68191500	1.87597700	2.08699600
C	1.13735600	-1.02042800	3.57143900
H	1.38589000	-1.65877000	1.53357400
C	-1.73887400	0.67984100	-1.53823600

C	-0.62843300	2.56468200	-0.72740700
C	-1.74538100	-0.73456800	-1.40944100
C	3.23581800	-0.93996600	-2.09303400
H	1.23220800	-1.75341900	-1.86505400
N	3.72233900	1.03359200	-0.78688300
F	2.15498400	1.94776700	0.56319400
C	0.54623000	-0.08015200	4.43052800
H	-0.82829000	1.58455800	4.56222700
C	-2.82876800	1.42071200	1.40079700
C	-1.58976800	3.24807200	2.40586400
H	1.81446200	-1.78084700	3.96476000
C	-2.62116500	1.41572600	-2.37123600
C	-1.45980000	3.38495500	-1.52637900
H	0.13893700	2.96381600	-0.07309000
C	-2.68714200	-1.45672800	-2.14427000
C	4.09549700	0.08126700	-1.67126800
H	3.57669900	-1.69005100	-2.80726500
H	0.75329900	-0.09744800	5.50191000
C	-3.84217300	2.31293500	1.02235800
H	-2.91457400	0.35923300	1.16669000
C	-2.60559500	4.14337900	2.03329700
H	-0.70568500	3.60910000	2.93425000
C	-2.44515500	2.82844000	-2.33883900
C	-3.56980500	0.65591700	-3.11661400
H	-1.32034200	4.46340100	-1.48034500
C	-3.58282800	-0.73507900	-2.98687500
H	-2.73695000	-2.54244400	-2.07491900
H	5.11958400	0.15171400	-2.04495100
C	-3.73461200	3.67945000	1.33649200
H	-4.71759900	1.94050700	0.48758400
H	-2.51343000	5.20205000	2.28299500
H	-3.08803600	3.47038500	-2.94305000
H	-4.27422700	1.16146300	-3.77693600
H	-4.31498800	-1.30652500	-3.55963900
H	-4.52443000	4.37394800	1.04541900
Cartesian coordinates of step 36			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62501300
C	1.49893100	0.00000000	-0.64802000
C	-0.68828000	0.87532200	2.51149800
C	0.91891500	-0.90906500	2.20410400
N	-0.77594100	1.24601200	-0.73736500
O	-0.82097800	-1.16928400	-0.56963600
C	1.92439200	-0.96691200	-1.57908800
C	2.48800000	0.95338800	-0.33698500
C	-0.40148400	0.85054300	3.89712900
C	-1.78425300	1.78384400	2.07015600
C	1.17083400	-0.96028500	3.58190100
H	1.47402900	-1.58132900	1.54623800
C	-1.70448400	0.69736700	-1.56831300
C	-0.63213800	2.57422000	-0.69095600

C	-1.71676600	-0.71789700	-1.45166000
C	3.22609300	-0.93474000	-2.11233900
H	1.22495100	-1.75058700	-1.87327100
N	3.71947700	1.03571700	-0.80423700
F	2.16028900	1.94535700	0.55774900
C	0.52035400	-0.05516000	4.43567400
H	-0.94437200	1.53127700	4.55572700
C	-2.88397100	1.27774000	1.34381500
C	-1.77886500	3.15346700	2.41329500
H	1.88415400	-1.68337100	3.98145200
C	-2.56496200	1.44200100	-2.41592300
C	-1.44330400	3.40338100	-1.50200200
H	0.11119400	2.96615500	-0.00511700
C	-2.63709500	-1.43241700	-2.22034000
C	4.08767300	0.08605800	-1.69351400
H	3.56288400	-1.68282200	-2.83060200
H	0.71671900	-0.06308300	5.50920200
C	-3.93383500	2.11903000	0.94809700
H	-2.90365600	0.21745400	1.09091900
C	-2.83105600	3.99759500	2.02321100
H	-0.93226900	3.55440900	2.97340900
C	-2.39766000	2.85504600	-2.35590400
C	-3.49062000	0.69001300	-3.19697000
H	-1.31349400	4.48182400	-1.43228300
C	-3.50696700	-0.70227100	-3.08230500
H	-2.69139700	-2.51850500	-2.16062200
H	5.10923200	0.15838800	-2.07371600
C	-3.91093600	3.48419200	1.28448200
H	-4.77076000	1.70768600	0.38119400
H	-2.80518100	5.05540400	2.29146900
H	-3.02521300	3.50340200	-2.96929700
H	-4.17693300	1.20243500	-3.87093500
H	-4.22224900	-1.26762000	-3.68182800
H	-4.72863500	4.13908700	0.97902700
Cartesian coordinates of step 37			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62472200
C	1.49671700	0.00000000	-0.65570600
C	-0.74810500	0.83733900	2.50124100
C	0.97182200	-0.84313800	2.21635500
N	-0.76844900	1.25724000	-0.72971600
O	-0.82605900	-1.15882900	-0.58314700
C	1.91756200	-0.96848900	-1.58731400
C	2.48710200	0.95460900	-0.35269800
C	-0.46944700	0.84023900	3.88865000
C	-1.89592300	1.67047200	2.04415100
C	1.21823300	-0.86768700	3.59604400
H	1.57378300	-1.48258900	1.56730200
C	-1.67296900	0.71884500	-1.59323300
C	-0.63613700	2.58482000	-0.65319400
C	-1.69216200	-0.69722200	-1.48971500

C	3.21594100	-0.93651200	-2.12861600
H	1.21709000	-1.75319400	-1.87597300
N	3.71580200	1.03672500	-0.82742700
F	2.16456300	1.94787800	0.54206500
C	0.50550600	-0.00033200	4.43909900
H	-1.05947600	1.48830400	4.53951900
C	-2.93691100	1.09624700	1.28288200
C	-1.99708200	3.03331100	2.40017200
H	1.97440000	-1.54006300	4.00519100
C	-2.51459200	1.47368300	-2.45033100
C	-1.42976400	3.42428500	-1.47155400
H	0.08572000	2.96811500	0.06018200
C	-2.59456500	-1.40233600	-2.28755400
C	4.07935400	0.08563700	-1.71702200
H	3.54878100	-1.68579900	-2.84745700
H	0.69508800	0.01175600	5.51382400
C	-4.03091000	1.86669600	0.86337700
H	-2.87361300	0.04015200	1.02032700
C	-3.09458500	3.80577900	1.98778800
H	-1.19613400	3.48686800	2.98668900
C	-2.35597000	2.88632900	-2.36218300
C	-3.42076600	0.73141300	-3.26260700
H	-1.30936300	4.50210500	-1.37818700
C	-3.44123200	-0.66198500	-3.16387300
H	-2.65398000	-2.48868200	-2.23808900
H	5.09853100	0.15797700	-2.10357100
C	-4.11378900	3.22620000	1.21243000
H	-4.81959300	1.40440700	0.26734300
H	-3.15048400	4.85993400	2.26567600
H	-2.97037100	3.54226300	-2.98079800
H	-4.09122500	1.25205900	-3.94616600
H	-4.14234700	-1.21985400	-3.78669100
H	-4.96583500	3.82570500	0.88778800
Cartesian coordinates of step 38			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62451200
C	1.49442200	0.00000000	-0.66220200
C	-0.80339700	0.79285000	2.49441900
C	1.00912800	-0.79023700	2.22626300
N	-0.77164900	1.25901400	-0.72352500
O	-0.82540400	-1.15739600	-0.58918000
C	1.91584100	-0.97607000	-1.58571600
C	2.48189100	0.96210400	-0.37372500
C	-0.54320000	0.80534000	3.88525000
C	-1.98139600	1.57486700	2.02365800
C	1.23963500	-0.80568500	3.60893000
H	1.65264200	-1.39458100	1.58372800
C	-1.66028500	0.72256000	-1.60475600
C	-0.65398800	2.58644800	-0.62845300
C	-1.67662600	-0.69393500	-1.50887500
C	3.21160500	-0.94363500	-2.13319400

H	1.21795000	-1.76693900	-1.86328300
N	3.70810900	1.04515600	-0.85475400
F	2.15917000	1.96255100	0.51289100
C	0.46909500	0.01694100	4.44566000
H	-1.17500500	1.41881900	4.53038900
C	-2.98435300	0.95901800	1.24462200
C	-2.14720700	2.93085600	2.38228500
H	2.02689600	-1.43664000	4.02536100
C	-2.49564000	1.47959900	-2.46575500
C	-1.44231200	3.42838900	-1.44978200
H	0.05330900	2.96745800	0.10073100
C	-2.56632800	-1.39745400	-2.32216600
C	4.07211000	0.08672900	-1.73618800
H	3.54463900	-1.69877000	-2.84578900
H	0.64381000	0.03493200	5.52282800
C	-4.10358500	1.68329400	0.80935100
H	-2.87162600	-0.09257700	0.98124100
C	-3.27015100	3.65664600	1.95454100
H	-1.37618500	3.41652400	2.98306800
C	-2.34942800	2.89253500	-2.36095300
C	-3.38781700	0.73910700	-3.29479800
H	-1.33318000	4.50613900	-1.34231400
C	-3.40394600	-0.65497400	-3.20533700
H	-2.62406000	-2.48414300	-2.27822700
H	5.08909600	0.15992800	-2.12831000
C	-4.25072100	3.03660800	1.16068200
H	-4.86174100	1.18960000	0.19903700
H	-3.37596800	4.70642600	2.23454900
H	-2.96005600	3.55005000	-2.98161700
H	-4.05247600	1.26157000	-3.98262000
H	-4.09499900	-1.21154200	-3.84044600
H	-5.12212900	3.60021300	0.82336000
Cartesian coordinates of step 39			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62407400
C	1.49193800	0.00000000	-0.66893700
C	-0.85531900	0.74407900	2.48820200
C	1.04039200	-0.74107800	2.23465300
N	-0.77537900	1.26153000	-0.71572900
O	-0.82550900	-1.15532400	-0.59504400
C	1.91355800	-0.98359100	-1.58448100
C	2.47653500	0.96947600	-0.39568400
C	-0.61423300	0.76083000	3.88228000
C	-2.05845300	1.47902000	2.00473300
C	1.25391800	-0.75301500	3.62020300
H	1.72123900	-1.30925300	1.59782100
C	-1.65141100	0.72818100	-1.61140500
C	-0.66998800	2.58838000	-0.60360300
C	-1.66503500	-0.68879800	-1.52399400
C	3.20639100	-0.95086000	-2.13877500
H	1.21815500	-1.78048100	-1.85053500

N	3.69998000	1.05336100	-0.88366800
F	2.15405900	1.97704500	0.48293300
C	0.43009600	0.02176700	4.45162700
H	-1.28435800	1.33779500	4.52248700
C	-3.02727300	0.82771000	1.21189900
C	-2.27934600	2.82725000	2.36335700
H	2.06775700	-1.34480100	4.04301500
C	-2.48205500	1.48835100	-2.47399900
C	-1.45409400	3.43365100	-1.42588600
H	0.02561200	2.96617900	0.13857600
C	-2.54481100	-1.38961100	-2.35017100
C	4.06402200	0.08770300	-1.75709800
H	3.53931200	-1.71188300	-2.84512100
H	0.58929200	0.04147900	5.53117700
C	-4.16619300	1.51136900	0.76162800
H	-2.87276400	-0.21866500	0.94962200
C	-3.42152400	3.51217600	1.92004600
H	-1.53566500	3.33979400	2.97621000
C	-2.34555900	2.90117100	-2.35423100
C	-3.36316900	0.75062500	-3.31711200
H	-1.35397600	4.51099300	-1.30593400
C	-3.37562400	-0.64406800	-3.23713800
H	-2.60118300	-2.47661900	-2.31237500
H	5.07853600	0.16176200	-2.15541200
C	-4.36693300	2.85815700	1.11109000
H	-4.89711100	0.99105300	0.14029200
H	-3.56991700	4.55687100	2.19980200
H	-2.95289400	3.56092300	-2.97575100
H	-4.02349800	1.27556700	-4.00721400
H	-4.05883900	-1.19856900	-3.88245800
H	-5.25311500	3.39036500	0.76143900
Cartesian coordinates of step 40			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62380800
C	1.48811500	0.00000000	-0.67770800
C	-0.90616900	0.69335600	2.47897700
C	1.07595600	-0.67833500	2.24502000
N	-0.77870400	1.27107600	-0.69812200
O	-0.82952800	-1.14703900	-0.60576200
C	1.90493800	-0.98773100	-1.59126500
C	2.47375300	0.97199700	-0.41682800
C	-0.67841800	0.72686700	3.87489600
C	-2.14635800	1.35532100	1.98297000
C	1.27751000	-0.67532200	3.63251800
H	1.79418100	-1.20736000	1.61576100
C	-1.65220500	0.74861600	-1.60243300
C	-0.67888000	2.59608800	-0.56431700
C	-1.66511700	-0.66922700	-1.53269400
C	3.19338900	-0.95588000	-2.15556300
H	1.20901400	-1.78705200	-1.84818200
N	3.69335300	1.05527900	-0.91464900

F	2.15780800	1.98293300	0.46014100
C	0.40242100	0.05094300	4.45488300
H	-1.38677200	1.26445000	4.50821800
C	-3.06875300	0.64470100	1.18611800
C	-2.45091700	2.68835000	2.33744800
H	2.12079900	-1.21771200	4.06374300
C	-2.48446900	1.51907400	-2.45422900
C	-1.46283300	3.45157300	-1.37657900
H	0.01441000	2.96455000	0.18498900
C	-2.54464500	-1.36001600	-2.36723100
C	4.05224800	0.08590200	-1.78597300
H	3.52199300	-1.72006200	-2.86051400
H	0.55051500	0.08152400	5.53576800
C	-4.24588100	1.25620000	0.72974100
H	-2.84863000	-0.39049400	0.92768200
C	-3.63047000	3.30119000	1.88704500
H	-1.74400500	3.24629200	2.95422200
C	-2.35108700	2.93033900	-2.31433100
C	-3.36480400	0.79159400	-3.30674500
H	-1.36521200	4.52743000	-1.24154500
C	-3.37584800	-0.60403000	-3.24486000
H	-2.60134900	-2.44739400	-2.34205800
H	5.06352500	0.15960700	-2.19251700
C	-4.53045200	2.58857800	1.07532800
H	-4.93986300	0.69106100	0.10528700
H	-3.84397500	4.33537600	2.16369200
H	-2.95847900	3.59754500	-2.92780400
H	-4.02630400	1.32471600	-3.98940000
H	-4.05889500	-1.15077800	-3.89695300
H	-5.44640100	3.06456700	0.72128500
Cartesian coordinates of step 41			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62378700
C	1.48360200	0.00000000	-0.68808900
C	-0.95702400	0.64119000	2.46570900
C	1.11638700	-0.59436000	2.25854500
N	-0.78232200	1.28508800	-0.66979400
O	-0.83537600	-1.13450600	-0.62192300
C	1.89122900	-0.98905700	-1.60481900
C	2.47363200	0.97058400	-0.43772300
C	-0.73765100	0.71146600	3.86142100
C	-2.24448700	1.19777700	1.95880000
C	1.31158100	-0.55618400	3.64664300
H	1.87204200	-1.08170300	1.63977000
C	-1.66488500	0.78104500	-1.57498900
C	-0.67781600	2.60721500	-0.51250900
C	-1.67767500	-0.63806200	-1.53283200
C	3.17417700	-0.95960500	-2.18141000
H	1.19201200	-1.78752800	-1.85494100
N	3.68858400	1.05170600	-0.94737000
F	2.16932600	1.98254500	0.44215800

C	0.38573700	0.12140800	4.45468400
H	-1.48500200	1.20601500	4.48487800
C	-3.10964600	0.40157700	1.17852700
C	-2.65844400	2.50497300	2.29890700
H	2.18831500	-1.03264200	4.08885800
C	-2.50368400	1.56879200	-2.40457700
C	-1.46464300	3.47934900	-1.30408600
H	0.02291700	2.95969300	0.23780700
C	-2.56534400	-1.31169200	-2.37220300
C	4.03795900	0.08131200	-1.82126800
H	3.49474900	-1.72499600	-2.88873800
H	0.52720900	0.17906400	5.53537800
C	-4.34013200	0.90302500	0.72879500
H	-2.80523700	-0.61470200	0.93298600
C	-3.89042700	3.00844600	1.85328600
H	-1.99804500	3.12890900	2.90390500
C	-2.36352900	2.97709800	-2.24236400
C	-3.39325100	0.85844000	-3.26180000
H	-1.36053400	4.55259900	-1.15337000
C	-3.40448000	-0.53806000	-3.22692100
H	-2.62317800	-2.39931900	-2.36757900
H	5.04534100	0.15350700	-2.23765400
C	-4.73488400	2.21003900	1.06154200
H	-4.98944600	0.27191900	0.11985700
H	-4.18904900	4.02426600	2.11901900
H	-2.97340900	3.65668400	-2.83956900
H	-4.06098500	1.40486300	-3.92763000
H	-4.09421900	-1.07167900	-3.88286600
H	-5.69206800	2.60102700	0.71255600
Cartesian coordinates of step 42			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62351600
C	1.47917900	0.00000000	-0.69730700
C	-1.00111600	0.58316400	2.45670100
C	1.14158700	-0.53158700	2.26853700
N	-0.79003800	1.29185000	-0.65172100
O	-0.83888900	-1.12855900	-0.62677000
C	1.88168900	-0.99348100	-1.61183900
C	2.47016200	0.97303700	-0.46015000
C	-0.80168200	0.66104700	3.85471900
C	-2.30789200	1.08194200	1.93680600
C	1.31970900	-0.48558000	3.65884300
H	1.92964600	-0.97448300	1.65701500
C	-1.68425700	0.79529900	-1.54901800
C	-0.68652800	2.61251800	-0.48145100
C	-1.69283000	-0.62425900	-1.52229000
C	3.16003400	-0.96541900	-2.19847700
H	1.18173100	-1.79402900	-1.85280600
N	3.68097200	1.05331100	-0.97978400
F	2.17228000	1.98903800	0.41745900
C	0.34748200	0.13416500	4.45859200

H	-1.58188300	1.11226500	4.47077800
C	-3.14572500	0.24250000	1.17243200
C	-2.76650900	2.37992500	2.25379500
H	2.21784600	-0.91178600	4.10930500
C	-2.53718600	1.58979100	-2.35769100
C	-1.48616900	3.49120400	-1.25252600
H	0.02391700	2.95835400	0.26289200
C	-2.58954900	-1.29102900	-2.35707300
C	4.02505800	0.07876100	-1.85106300
H	3.47609900	-1.73428100	-2.90405800
H	0.47396700	0.19626500	5.54091100
C	-4.39330800	0.69337600	0.71557200
H	-2.80736200	-0.76695600	0.94478900
C	-4.01473800	2.83332300	1.79975200
H	-2.12800500	3.03642800	2.84776200
C	-2.39776400	2.99652600	-2.18275800
C	-3.43724200	0.88630300	-3.20961400
H	-1.38175300	4.56314700	-1.09281000
C	-3.44315600	-0.51044500	-3.19091400
H	-2.64433600	-2.37880700	-2.36384700
H	5.02897000	0.15031200	-2.27585500
C	-4.83209600	1.99204900	1.02407300
H	-5.02137300	0.02924200	0.11970400
H	-4.34760700	3.84309500	2.04732700
H	-3.01770100	3.68084400	-2.76401400
H	-4.11659000	1.43806200	-3.85906900
H	-4.14062000	-1.03881600	-3.84294200
H	-5.80193200	2.34382200	0.66838100

Cartesian coordinates of step 43

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62363800
C	1.47566700	0.00000000	-0.70391900
C	-1.04066900	0.52161600	2.44903800
C	1.16163700	-0.47289900	2.27821400
N	-0.80445500	1.28817000	-0.63974100
O	-0.83678400	-1.13238300	-0.62481600
C	1.87886200	-1.00257000	-1.60843800
C	2.46379200	0.97984000	-0.48312500
C	-0.86299500	0.59939200	3.84959600
C	-2.36110000	0.97025900	1.91587000
C	1.32092500	-0.42656000	3.67097900
H	1.97880200	-0.86996000	1.67368600
C	-1.71017100	0.78954600	-1.52408300
C	-0.70614600	2.60901300	-0.46622400
C	-1.70749000	-0.63020300	-1.50463200
C	3.15439800	-0.97591900	-2.20105800
H	1.18142700	-1.80881800	-1.83715300
N	3.67199000	1.05929800	-1.00904700
F	2.16621300	2.00472700	0.38451700
C	0.30639000	0.13113800	4.46352100
H	-1.67285400	1.00580000	4.45867000

C	-3.17648000	0.09191500	1.17171000
C	-2.85165900	2.26399200	2.19967200
H	2.23613300	-0.80558300	4.12920200
C	-2.58207000	1.58181900	-2.31449200
C	-1.52344000	3.48557000	-1.22070300
H	0.01335800	2.95605400	0.26878800
C	-2.61123300	-1.29931100	-2.32978600
C	4.01640500	0.07607900	-1.87031200
H	3.47050500	-1.75176000	-2.89892900
H	0.41686500	0.19167600	5.54769000
C	-4.43353600	0.50147200	0.70143200
H	-2.81335800	-0.91407300	0.96860700
C	-4.10835400	2.67682800	1.73041200
H	-2.23111700	2.94908800	2.78033100
C	-2.44826300	2.98862700	-2.13670700
C	-3.49086900	0.87591500	-3.15502500
H	-1.42231400	4.55761200	-1.05936300
C	-3.48470600	-0.52088700	-3.14481000
H	-2.65772100	-2.38744000	-2.34188800
H	5.01800800	0.14699200	-2.30062600
C	-4.90314800	1.79713700	0.97425700
H	-5.04418000	-0.19198300	0.12129100
H	-4.46551400	3.68441000	1.95173800
H	-3.08224700	3.67113100	-2.70481000
H	-4.18543600	1.42585500	-3.78973500
H	-4.18834200	-1.05117100	-3.78862000
H	-5.87931300	2.11702300	0.60599300
Cartesian coordinates of step 44			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62392700
C	1.46774300	0.00000000	-0.71664800
C	-1.08466100	0.46089000	2.42779100
C	1.18575700	-0.37257100	2.29802300
N	-0.82133900	1.30053000	-0.60252000
O	-0.84875300	-1.12095300	-0.62523300
C	1.85627900	-1.00198300	-1.62894100
C	2.46428200	0.97333500	-0.50422600
C	-0.93143800	0.58456400	3.82646500
C	-2.43153000	0.78075700	1.86409600
C	1.32450700	-0.28338000	3.69137400
H	2.03584300	-0.72194200	1.70980800
C	-1.78089500	0.81317400	-1.43378200
C	-0.70599400	2.62009300	-0.42500100
C	-1.77163900	-0.60667000	-1.44147600
C	3.12496900	-0.98048300	-2.23583700
H	1.15189400	-1.80341600	-1.85305300
N	3.66701500	1.04779600	-1.04353900
F	2.18422000	1.99740700	0.37065300
C	0.26396300	0.21779000	4.46111100
H	-1.77557900	0.94585300	4.41736200
C	-3.20386700	-0.22414400	1.24484200

C	-2.98413100	2.07341200	1.98843400
H	2.25939400	-0.58415500	4.16761800
C	-2.70101300	1.61575600	-2.15678400
C	-1.56683100	3.50592500	-1.11654200
H	0.05986600	2.95820000	0.26598000
C	-2.71525800	-1.26438300	-2.22961900
C	3.99645100	0.06579700	-1.91176100
H	3.42870600	-1.75580900	-2.93973500
H	0.35939600	0.31217500	5.54432000
C	-4.48151700	0.06055800	0.73933400
H	-2.78786200	-1.22676000	1.15746900
C	-4.25964200	2.36262300	1.47850500
H	-2.39652600	2.85509100	2.47346100
C	-2.55351300	3.01969800	-1.97212000
C	-3.65689800	0.92072800	-2.95316800
H	-1.44982200	4.57633900	-0.95465400
C	-3.64046200	-0.47569600	-2.97390700
H	-2.75534200	-2.35231100	-2.26294900
H	4.99346500	0.13286200	-2.35322200
C	-5.01199400	1.35643900	0.84769500
H	-5.05684700	-0.72806200	0.25262000
H	-4.66450700	3.37217200	1.57129600
H	-3.22203200	3.70900800	-2.49026400
H	-4.39164300	1.47900200	-3.53289500
H	-4.37805200	-0.99761000	-3.58579900
H	-6.00223300	1.57994800	0.44739100
Cartesian coordinates of step 45			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62353000
C	1.46537100	0.00000000	-0.72099800
C	-1.11405100	0.39278700	2.42281800
C	1.19599000	-0.32534600	2.30377900
N	-0.83673000	1.29299500	-0.59755900
O	-0.84291900	-1.12834000	-0.62102400
C	1.86075400	-1.01548000	-1.61533000
C	2.45412000	0.98557000	-0.52935100
C	-0.98308400	0.49525100	3.82508500
C	-2.46312000	0.68126400	1.84563700
C	1.31557900	-0.25455000	3.70006800
H	2.06729800	-0.62524300	1.71968900
C	-1.79383600	0.79728600	-1.42688700
C	-0.73586000	2.61327600	-0.41644300
C	-1.76963300	-0.62235900	-1.43779100
C	3.12808000	-0.99445900	-2.22500300
H	1.16273100	-1.82659800	-1.82371800
N	3.65503000	1.06058700	-1.07259200
F	2.16719800	2.02313600	0.32761200
C	0.22213400	0.17500200	4.46684100
H	-1.84957100	0.80582700	4.41245000
C	-3.21914900	-0.34354900	1.24000700
C	-3.02982800	1.97006000	1.94089800

H	2.25953100	-0.51649600	4.18136700
C	-2.72354800	1.59157800	-2.14687800
C	-1.60847500	3.49131600	-1.10314100
H	0.02806700	2.95781200	0.27345200
C	-2.70398000	-1.28820600	-2.23005300
C	3.99118900	0.06522500	-1.92282500
H	3.43699800	-1.78025800	-2.91488400
H	0.30059100	0.25174100	5.55281400
C	-4.49531900	-0.08189000	0.71826300
H	-2.79053600	-1.34244700	1.17281800
C	-4.30314300	2.23644800	1.41344800
H	-2.45446000	2.76660400	2.41616200
C	-2.59115800	2.99655200	-1.95854300
C	-3.67110100	0.88830000	-2.94601300
H	-1.50278900	4.56256000	-0.93883700
C	-3.63758000	-0.50770300	-2.97251800
H	-2.73164400	-2.37641300	-2.26677800
H	4.98659400	0.13258800	-2.36784700
C	-5.03933000	1.21046800	0.79596500
H	-5.05868500	-0.88540200	0.24212100
H	-4.71891400	3.24346100	1.48244600
H	-3.26765300	3.67993000	-2.47420200
H	-4.41229000	1.44002300	-3.52380400
H	-4.36827500	-1.03599200	-3.58721300
H	-6.02778200	1.41610100	0.38193800
Cartesian coordinates of step 46			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62328400
C	1.46343200	0.00000000	-0.72447900
C	-1.13835900	0.32258300	2.41928000
C	1.20447700	-0.28120600	2.30815700
N	-0.85287300	1.28265100	-0.59547100
O	-0.83538900	-1.13825800	-0.61572500
C	1.86771800	-1.02961500	-1.59847200
C	2.44310200	0.99854300	-0.55434400
C	-1.02592600	0.39903400	3.82451500
C	-2.48936200	0.58435100	1.83213700
C	1.30841000	-0.23267800	3.70673100
H	2.09337800	-0.53102100	1.72737900
C	-1.80571000	0.77621900	-1.42351000
C	-0.76905000	2.60376300	-0.41163400
C	-1.76530500	-0.64293800	-1.43502800
C	3.13439300	-1.00895500	-2.20943200
H	1.17721900	-1.85113400	-1.79031100
N	3.64284500	1.07413700	-1.10003300
F	2.14689200	2.05055800	0.28199200
C	0.18764400	0.12331200	4.47156800
H	-1.91108900	0.65713300	4.40941600
C	-3.23144200	-0.45567400	1.23634400
C	-3.06857100	1.86879800	1.90686700
H	2.26007200	-0.45732800	4.19167700

C	-2.74536900	1.55993800	-2.14229000
C	-1.65473100	3.47168900	-1.09444100
H	-0.00786600	2.95662900	0.27704400
C	-2.68919200	-1.31899500	-2.23089000
C	3.98775000	0.06474900	-1.92998800
H	3.45009000	-1.80568500	-2.88351700
H	0.25218300	0.17943300	5.55972600
C	-4.50734900	-0.21331200	0.70442300
H	-2.79151600	-1.45049900	1.18219200
C	-4.34099400	2.11616400	1.36820700
H	-2.50367400	2.67693000	2.37494400
C	-2.63143400	2.96601300	-1.95044100
C	-3.68270700	0.84629000	-2.94432100
H	-1.56299900	4.54387300	-0.92778900
C	-3.63078200	-0.54904700	-2.97416500
H	-2.70355500	-2.40740600	-2.26896100
H	4.98206400	0.13238100	-2.37739200
C	-5.06385700	1.07476100	0.76105400
H	-5.06073400	-1.02848900	0.23646900
H	-4.76643400	3.12012400	1.42071700
H	-3.31704900	3.64172300	-2.46417600
H	-4.43022600	1.38969400	-3.52183800
H	-4.35338400	-1.08539200	-3.59145000
H	-6.05150100	1.26531900	0.33803500
Cartesian coordinates of step 47			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62291500
C	1.46189900	0.00000000	-0.72721100
C	-1.15883800	0.25100300	2.41462800
C	1.21077600	-0.23885100	2.31270000
N	-0.86762800	1.27177800	-0.59650500
O	-0.82768200	-1.14857900	-0.60941700
C	1.87592000	-1.04371300	-1.57968500
C	2.43250600	1.01062000	-0.57784100
C	-1.06358100	0.29789100	3.82210100
C	-2.51085200	0.48801800	1.81751900
C	1.29999800	-0.21614700	3.71306000
H	2.11478200	-0.43776100	1.73588400
C	-1.81389300	0.75374300	-1.42519900
C	-0.79975900	2.59386400	-0.41309000
C	-1.75815500	-0.66482800	-1.43464700
C	3.14266700	-1.02402700	-2.19046000
H	1.19297200	-1.87507600	-1.75524700
N	3.63160000	1.08637500	-1.12486500
F	2.12629200	2.07664600	0.23730200
C	0.15606400	0.06455000	4.47476300
H	-1.96477900	0.50248900	4.40369700
C	-3.24028400	-0.56537400	1.23091100
C	-3.09972700	1.76901500	1.87046000
H	2.25714200	-0.40567900	4.20219900
C	-2.75986400	1.52614200	-2.14808600

C	-1.69477600	3.45091900	-1.09751500
H	-0.04299600	2.95597000	0.27566300
C	-2.66946800	-1.35183900	-2.23561800
C	3.98607900	0.06307800	-1.93347900
H	3.46589000	-1.83171700	-2.84771500
H	0.20791800	0.09666300	5.56458400
C	-4.51431900	-0.33963600	0.68691200
H	-2.79110500	-1.55677100	1.18988700
C	-4.37005600	1.99981800	1.31972600
H	-2.54429200	2.58746400	2.33177500
C	-2.66304000	2.93348800	-1.95623600
C	-3.68493300	0.80134800	-2.95440400
H	-1.61589500	4.52422300	-0.93137500
C	-3.61593100	-0.59321800	-2.98421800
H	-2.67118400	-2.44035900	-2.27296900
H	4.97981100	0.13053400	-2.38218800
C	-5.08083800	0.94478700	0.72205700
H	-5.05836800	-1.16504800	0.22594400
H	-4.80318700	3.00120800	1.35570000
H	-3.35469800	3.60106600	-2.47252300
H	-4.43609900	1.33579000	-3.53554700
H	-4.32875900	-1.13813900	-3.60534300
H	-6.06656300	1.12212000	0.28899300
Cartesian coordinates of step 48			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62252100
C	1.46061000	0.00000000	-0.72947200
C	-1.17561800	0.17824500	2.40846200
C	1.21576500	-0.19341400	2.31771700
N	-0.87989100	1.26254700	-0.59819800
O	-0.82101700	-1.15705700	-0.60360100
C	1.88302000	-1.05505600	-1.56368900
C	2.42282000	1.02114900	-0.59893700
C	-1.09582200	0.19510100	3.81721800
C	-2.52878900	0.38680300	1.80160200
C	1.29196400	-0.19565400	3.71916100
H	2.13265100	-0.33944000	1.74563700
C	-1.82076700	0.73431800	-1.42694600
C	-0.82633100	2.58530200	-0.41492600
C	-1.75197200	-0.68359900	-1.43395200
C	3.14921100	-1.03523600	-2.17555700
H	1.20709600	-1.89508800	-1.72436200
N	3.62074700	1.09796500	-1.14829800
F	2.10806600	2.09826600	0.19863600
C	0.12855800	0.00704900	4.47605100
H	-2.01061400	0.34442900	4.39442600
C	-3.24705300	-0.68333100	1.23294500
C	-3.12688800	1.66423000	1.82592200
H	2.25336300	-0.34740200	4.21313100
C	-2.77298900	1.49657600	-2.15253300
C	-1.73019800	3.43259800	-1.10006500

H	-0.07294700	2.95580700	0.27310800
C	-2.65272200	-1.38021800	-2.23858700
C	3.98343400	0.06351500	-1.93889100
H	3.47892900	-1.85171000	-2.81857100
H	0.16949000	0.01554900	5.56679000
C	-4.52038200	-0.47752100	0.67893900
H	-2.78900900	-1.67139300	1.20990500
C	-4.39656100	1.87493500	1.26592500
H	-2.57944400	2.49558200	2.27335200
C	-2.69126100	2.90485900	-1.96076500
C	-3.68751500	0.76201000	-2.96205500
H	-1.66272400	4.50675800	-0.93431500
C	-3.60353800	-0.63172200	-2.99162500
H	-2.64349300	-2.46871900	-2.27492600
H	4.97614900	0.13153400	-2.38974300
C	-5.09677700	0.80293700	0.68645000
H	-5.05612200	-1.31560800	0.23117400
H	-4.83716200	2.87359000	1.28041600
H	-3.38872700	3.56517000	-2.47860100
H	-4.44204700	1.28848800	-3.54609900
H	-4.30810000	-1.18415400	-3.61553200
H	-6.08159200	0.96423100	0.24520300
Cartesian coordinates of step 49			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62173400
C	1.45996500	0.00000000	-0.73072600
C	-1.18993200	0.10455400	2.39854500
C	1.21831800	-0.14043000	2.32489000
N	-0.89009200	1.25306500	-0.60293100
O	-0.81407100	-1.16549700	-0.59662000
C	1.89176100	-1.06764400	-1.54393400
C	2.41432200	1.03059000	-0.61872200
C	-1.12582200	0.09547900	3.80765800
C	-2.54346700	0.27053000	1.77764900
C	1.28101200	-0.16264000	3.72702900
H	2.14653200	-0.23212900	1.76003700
C	-1.82313900	0.71408700	-1.43398200
C	-0.84935000	2.57668800	-0.42312600
C	-1.74327400	-0.70306000	-1.43476300
C	3.15895700	-1.05007900	-2.15371000
H	1.22235600	-1.91549900	-1.69004200
N	3.61266900	1.10606800	-1.16730300
F	2.08970900	2.12074200	0.15741400
C	0.10102700	-0.03999700	4.47540400
H	-2.05249300	0.18701700	4.37793600
C	-3.24763100	-0.82946100	1.25074700
C	-3.15284700	1.54211600	1.74345700
H	2.24445600	-0.27143800	4.22833100
C	-2.77551900	1.46593300	-2.17044900
C	-1.75731900	3.41388400	-1.11558300
H	-0.10240300	2.95622000	0.26710000

C	-2.63096300	-1.40970800	-2.24528100
C	3.98466900	0.05917300	-1.93686100
H	3.49594400	-1.87638300	-2.78019000
H	0.13131600	-0.05130200	5.56648100
C	-4.51897500	-0.65875700	0.67997200
H	-2.78014000	-1.81338000	1.27026000
C	-4.42099400	1.71736000	1.16838400
H	-2.61614500	2.39655200	2.15902300
C	-2.70704300	2.87542500	-1.98241000
C	-3.67636600	0.72122200	-2.98587800
H	-1.70031900	4.48912100	-0.95266800
C	-3.58062400	-0.67189800	-3.00974500
H	-2.61218700	-2.49818700	-2.27801100
H	4.97781400	0.12571600	-2.38699200
C	-5.10724300	0.61539800	0.62981500
H	-5.04406600	-1.51972500	0.26379900
H	-4.87088800	2.71150100	1.13875600
H	-3.40574100	3.52846000	-2.50782000
H	-4.42963400	1.23948900	-3.57886300
H	-4.27479600	-1.23222600	-3.63824600
H	-6.09014900	0.74859100	0.17526100
Cartesian coordinates of step 50			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62139300
C	1.46027800	0.00000000	-0.73006500
C	-1.19864200	0.02974300	2.39120400
C	1.22000200	-0.08444800	2.33034900
N	-0.90250800	1.24054200	-0.60895600
O	-0.80531700	-1.17626800	-0.58943700
C	1.90678100	-1.08608700	-1.51034500
C	2.40360100	1.04299800	-0.64385100
C	-1.14424200	-0.00175400	3.79983000
C	-2.55236100	0.14434600	1.75824000
C	1.27426800	-0.12353900	3.73283300
H	2.15531400	-0.12127200	1.77114700
C	-1.82517000	0.68880800	-1.44364100
C	-0.87881500	2.56484600	-0.43120700
C	-1.73219400	-0.72742600	-1.43690300
C	3.17612300	-1.07233200	-2.11576200
H	1.24708300	-1.94496500	-1.63444200
N	3.60303600	1.11594300	-1.19008400
F	2.06542000	2.15003900	0.10266400
C	0.08441700	-0.08078500	4.47416300
H	-2.07808500	0.03146100	4.36474700
C	-3.23345900	-0.99151300	1.27974500
C	-3.18226800	1.40206700	1.65892500
H	2.23901600	-0.18666000	4.23953000
C	-2.77908900	1.42835600	-2.19077500
C	-1.79218300	3.38997300	-1.13126100
H	-0.14059800	2.95471500	0.26266800
C	-2.60647800	-1.44597800	-2.25174400

C	3.98908000	0.05163000	-1.92826100
H	3.52430800	-1.91275700	-2.71683300
H	0.10812600	-0.10923500	5.56510800
C	-4.50214400	-0.87012500	0.69085500
H	-2.74901500	-1.96521000	1.34816200
C	-4.44783600	1.52793800	1.06538700
H	-2.66411400	2.28435000	2.03777900
C	-2.72812200	2.83886300	-2.00534400
C	-3.66457500	0.67168600	-3.01192300
H	-1.74890500	4.46616200	-0.97028900
C	-3.55527100	-0.72053900	-3.02875100
H	-2.57810200	-2.53438100	-2.27847500
H	4.98308100	0.11609800	-2.37678600
C	-5.11080400	0.39036600	0.57436700
H	-5.00928500	-1.75877200	0.31199300
H	-4.91336700	2.51193300	0.98434500
H	-3.42922100	3.48301600	-2.53852600
H	-4.41711200	1.18016000	-3.61427200
H	-4.23820700	-1.29025400	-3.66108600
H	-6.09102300	0.48515500	0.10471600
Cartesian coordinates of step 51			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62144800
C	1.46027400	0.00000000	-0.73028100
C	-1.20062900	-0.04567400	2.38723900
C	1.22062000	-0.03092700	2.33369400
N	-0.91059700	1.23251800	-0.61336600
O	-0.79902800	-1.18331300	-0.58451300
C	1.91687300	-1.10007900	-1.48497500
C	2.39377400	1.05337200	-0.66992200
C	-1.14961200	-0.10345100	3.79485900
C	-2.55483500	0.01574400	1.74779900
C	1.27219400	-0.09042500	3.73562600
H	2.15851900	-0.01273400	1.77824000
C	-1.82715900	0.67198900	-1.44923900
C	-0.90009200	2.55692600	-0.43548000
C	-1.72555500	-0.74342800	-1.43672200
C	3.18530000	-1.08837000	-2.09216400
H	1.26516900	-1.96771100	-1.58843700
N	3.59137700	1.12554400	-1.22014300
F	2.04671900	2.17376700	0.05275000
C	0.07948300	-0.12804500	4.47268600
H	-2.08571200	-0.13063400	4.35631700
C	-3.21068300	-1.15310000	1.31627800
C	-3.20761300	1.25550400	1.59067200
H	2.23724900	-0.11015700	4.24526500
C	-2.78337300	1.40268700	-2.20238500
C	-1.81897600	3.37343600	-1.13885900
H	-0.16740200	2.95403500	0.26023200
C	-2.59227100	-1.47035500	-2.25253900
C	3.98712400	0.04798800	-1.93340300

H	3.54100900	-1.93944700	-2.67350100
H	0.10160800	-0.17633100	5.56295400
C	-4.47720500	-1.08206800	0.71479200
H	-2.70652800	-2.11287900	1.42803800
C	-4.47179300	1.33072800	0.98582900
H	-2.70854400	2.16305400	1.93319400
C	-2.74535200	2.81372000	-2.01779900
C	-3.65955700	0.63786700	-3.02561100
H	-1.78621400	4.45001800	-0.97797600
C	-3.54133800	-0.75383800	-3.03689700
H	-2.55749200	-2.55863600	-2.27424500
H	4.97941500	0.11199900	-2.38572800
C	-5.10914300	0.16036700	0.54050200
H	-4.96469900	-1.99570800	0.37097300
H	-4.95560100	2.30093200	0.85918000
H	-3.44917400	3.45153100	-2.55503500
H	-4.41293000	1.13940200	-3.63271200
H	-4.21808600	-1.33000300	-3.67001100
H	-6.08748900	0.21620500	0.06084400
Cartesian coordinates of step 52			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62189900
C	1.45950900	0.00000000	-0.73248500
C	-1.19693800	-0.12112800	2.38525100
C	1.21982300	0.02466800	2.33592900
N	-0.91495400	1.22714100	-0.61635100
O	-0.79622100	-1.18794800	-0.57852000
C	1.91974600	-1.10805000	-1.47350000
C	2.38752000	1.05898700	-0.69069800
C	-1.14408900	-0.20120600	3.79165400
C	-2.55146100	-0.12110500	1.74399000
C	1.27317700	-0.05164800	3.73704000
H	2.15634000	0.09744100	1.78301500
C	-1.83215300	0.66068800	-1.44793400
C	-0.91055700	2.55204500	-0.44137900
C	-1.72786500	-0.75445000	-1.42821400
C	3.18589700	-1.09819300	-2.08515700
H	1.27268400	-1.98072200	-1.56223700
N	3.58303800	1.12974000	-1.24591600
F	2.03729700	2.18825300	0.01670800
C	0.08381800	-0.16825800	4.47128400
H	-2.07797100	-0.28844500	4.35067400
C	-3.18177700	-1.32494300	1.37445500
C	-3.22938400	1.09438800	1.52084100
H	2.23742200	-0.02576000	4.24793500
C	-2.79138300	1.38556100	-2.20296800
C	-1.83437400	3.36297600	-1.14514500
H	-0.17802300	2.95463400	0.25137700
C	-2.59685300	-1.48726000	-2.23632700
C	3.98223000	0.04452200	-1.94522300
H	3.54421400	-1.95559600	-2.65548500

H	0.10775500	-0.23281800	5.56066800
C	-4.44792400	-1.31247800	0.76854000
H	-2.65781100	-2.26684000	1.53772300
C	-4.49416400	1.11081900	0.91242900
H	-2.75112800	2.02888700	1.81700800
C	-2.75877100	2.79719700	-2.02244800
C	-3.66734500	0.61491800	-3.02079900
H	-1.80571200	4.44007300	-0.98697500
C	-3.54793500	-0.77670300	-3.02341100
H	-2.56126000	-2.57555300	-2.25101200
H	4.97266000	0.10741100	-2.40178200
C	-5.10555900	-0.09427500	0.52888600
H	-4.91599500	-2.25304400	0.47336500
H	-4.99822900	2.06242300	0.73441300
H	-3.46543700	3.43077200	-2.56100900
H	-4.42261800	1.11196800	-3.62924600
H	-4.22583900	-1.35768300	-3.65082000
H	-6.08418500	-0.08422700	0.04661900
Cartesian coordinates of step 53			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62223200
C	1.45870600	0.00000000	-0.73437700
C	-1.18774900	-0.19617400	2.38464000
C	1.21768300	0.07853800	2.33622600
N	-0.91897200	1.22234800	-0.62333500
O	-0.79386700	-1.19222100	-0.57058800
C	1.92312300	-1.11803100	-1.45798000
C	2.38077000	1.06461600	-0.71462500
C	-1.12754200	-0.30585200	3.78873500
C	-2.54272700	-0.24548200	1.74682300
C	1.27718400	-0.01947200	3.73578500
H	2.14877100	0.20830400	1.78488300
C	-1.83640700	0.64803100	-1.44939300
C	-0.91917700	2.54840700	-0.45604100
C	-1.73144200	-0.76669600	-1.41742900
C	3.18653600	-1.11118000	-2.07507400
H	1.28098200	-1.99589500	-1.52928400
N	3.57315700	1.13330300	-1.27678200
F	2.02790300	2.20366600	-0.02394100
C	0.09787200	-0.21931100	4.46809600
H	-2.05437500	-0.45453900	4.34651500
C	-3.16073800	-1.47390500	1.44145100
C	-3.23673800	0.94886300	1.46752500
H	2.23929500	0.05082300	4.24650700
C	-2.79935600	1.36533000	-2.20724700
C	-1.84707900	3.35220200	-1.16278400
H	-0.18721600	2.95804500	0.23316900
C	-2.60561200	-1.50747800	-2.21241800
C	3.97613000	0.03886300	-1.95912100
H	3.54769900	-1.97623300	-2.63189200
H	0.12734400	-0.30566700	5.55583000

C	-4.43061000	-1.50637200	0.84436000
H	-2.62526700	-2.40062200	1.64959800
C	-4.50606600	0.92010400	0.86873700
H	-2.76935700	1.90273900	1.71483500
C	-2.77072100	2.77809400	-2.03569900
C	-3.67811800	0.58676700	-3.01442000
H	-1.82214600	4.43024700	-1.01057400
C	-3.55964400	-0.80487900	-3.00286000
H	-2.57131400	-2.59583000	-2.21458500
H	4.96390700	0.10022200	-2.42158900
C	-5.10503700	-0.30928700	0.54981900
H	-4.88982600	-2.46593400	0.60042400
H	-5.02312000	1.85572800	0.64843400
H	-3.48049700	3.40619200	-2.57663700
H	-4.43575900	1.07785700	-3.62479200
H	-4.24109200	-1.39206500	-3.62054400
H	-6.08703900	-0.33481000	0.07499900
Cartesian coordinates of step 54			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62286300
C	1.45686000	0.00000000	-0.73983500
C	-1.16926100	-0.26948500	2.39217500
C	1.20909200	0.18557900	2.33201900
N	-0.91528500	1.23291500	-0.61330500
O	-0.80202300	-1.18356700	-0.57032000
C	1.91827600	-1.13073200	-1.44654900
C	2.37722900	1.06594700	-0.74879200
C	-1.09459500	-0.35198000	3.79839000
C	-2.51766800	-0.46910600	1.77041600
C	1.27970400	0.11928900	3.73274700
H	2.12682300	0.37328800	1.77553200
C	-1.84849700	0.66589200	-1.42633700
C	-0.90941300	2.55827300	-0.43745200
C	-1.75676700	-0.75018900	-1.39280300
C	3.17602000	-1.13382500	-2.07456400
H	1.27718700	-2.01080000	-1.49659600
N	3.56424500	1.12603100	-1.32330700
F	2.03094500	2.21735700	-0.07492700
C	0.12064200	-0.15643100	4.47255000
H	-2.00523200	-0.56418600	4.36222400
C	-3.06546700	-1.76227900	1.65014300
C	-3.28333100	0.63063800	1.33539900
H	2.23514800	0.27150800	4.23807800
C	-2.82285800	1.39072000	-2.16286500
C	-1.84438600	3.36936700	-1.12644500
H	-0.16859900	2.96194900	0.24556000
C	-2.66007500	-1.48481200	-2.16005300
C	3.96408000	0.01997700	-1.98804600
H	3.53379600	-2.00889300	-2.61773600
H	0.15821900	-0.22006500	5.56159400
C	-4.33828900	-1.95255700	1.09009500

H	-2.47528900	-2.61795600	1.98032400
C	-4.55819500	0.44432000	0.77639900
H	-2.87239100	1.63587800	1.43452500
C	-2.78425400	2.80280700	-1.98727200
C	-3.72852200	0.61832700	-2.94551800
H	-1.81334800	4.44642500	-0.96872100
C	-3.62595900	-0.77480700	-2.92897000
H	-2.64013600	-2.57331800	-2.15446000
H	4.94740000	0.07488900	-2.46071000
C	-5.08838600	-0.84878100	0.64822300
H	-4.74261500	-2.96188200	0.99411500
H	-5.13274500	1.30825400	0.43830400
H	-3.50080300	3.43610900	-2.51303700
H	-4.49646000	1.11481000	-3.53844000
H	-4.33067100	-1.35710400	-3.52474100
H	-6.07445200	-0.99616600	0.20510700
Cartesian coordinates of step 55			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62394800
C	1.45901400	0.00000000	-0.73604000
C	-1.14863400	-0.34195500	2.39621200
C	1.20108300	0.24333700	2.32951300
N	-0.92807000	1.22247500	-0.61410100
O	-0.79028900	-1.19245200	-0.56741700
C	1.93767300	-1.14647100	-1.40527000
C	2.36751800	1.07526300	-0.77254600
C	-1.05890400	-0.44244800	3.80069300
C	-2.49252700	-0.59142600	1.78406100
C	1.28405100	0.16364400	3.72889300
H	2.10432200	0.48630500	1.77103000
C	-1.86279800	0.64399300	-1.41752800
C	-0.93889900	2.54764800	-0.43554500
C	-1.75578900	-0.77103100	-1.38261500
C	3.19879400	-1.15402700	-2.02618000
H	1.30698700	-2.03495400	-1.43242400
N	3.55667000	1.13201700	-1.34293800
F	2.00531000	2.24223700	-0.13410800
C	0.14771100	-0.18941400	4.47089100
H	-1.95305000	-0.71112300	4.36683800
C	-3.01541400	-1.89857200	1.71064300
C	-3.28286200	0.47758300	1.31652300
H	2.23263500	0.36291400	4.23079900
C	-2.85600400	1.35660600	-2.14083500
C	-1.89225900	3.34699700	-1.11289900
H	-0.19595000	2.96069300	0.23952100
C	-2.65895000	-1.51705200	-2.13873300
C	3.97287000	0.01111000	-1.97160500
H	3.56956800	-2.04114700	-2.54031600
H	0.19574000	-0.26717300	5.55860400
C	-4.28711600	-2.13271400	1.16442900
H	-2.40740500	-2.73112100	2.06698400

C	-4.55706200	0.24753600	0.77273700
H	-2.89380000	1.49410100	1.38363800
C	-2.83431900	2.76892300	-1.96371900
C	-3.76205600	0.57285100	-2.91167800
H	-1.87393300	4.42415400	-0.95396500
C	-3.64250200	-0.81901500	-2.89587600
H	-2.62761000	-2.60520200	-2.13040600
H	4.95788300	0.06318000	-2.44105200
C	-5.06209600	-1.05938400	0.69144100
H	-4.67174400	-3.15253400	1.10500500
H	-5.15110700	1.08820800	0.41078900
H	-3.56557100	3.39320900	-2.47994700
H	-4.54356900	1.05965800	-3.49480000
H	-4.34816200	-1.40999700	-3.48188600
H	-6.04812000	-1.24106100	0.26104000
Cartesian coordinates of step 56			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62489400
C	1.46228500	0.00000000	-0.73040700
C	-1.12457900	-0.41328700	2.39816000
C	1.19248800	0.28983800	2.32779600
N	-0.93882300	1.21148300	-0.61811000
O	-0.77709600	-1.20165100	-0.56619700
C	1.95698500	-1.15807100	-1.36738200
C	2.35926600	1.08369000	-0.79081000
C	-1.01766800	-0.54114300	3.79943400
C	-2.46509600	-0.69298500	1.79347900
C	1.28994000	0.18730400	3.72476600
H	2.07896600	0.58676400	1.76874600
C	-1.87137400	0.62141000	-1.41597400
C	-0.96457100	2.53667700	-0.44034800
C	-1.74969700	-0.79238500	-1.37841500
C	3.22093600	-1.16750400	-1.98234300
H	1.33657600	-2.05408000	-1.37450700
N	3.55003100	1.13937300	-1.35781700
F	1.98194200	2.26245500	-0.18272500
C	0.17988700	-0.24218900	4.46658300
H	-1.89335200	-0.86444200	4.36591800
C	-2.97367600	-2.00690300	1.74268000
C	-3.26945000	0.35966400	1.31188000
H	2.23079500	0.42536800	4.22433200
C	-2.87811000	1.32161600	-2.13281400
C	-1.93125100	3.32415500	-1.11270100
H	-0.22300100	2.95922700	0.23037300
C	-2.64882100	-1.54983900	-2.12790200
C	3.98153300	0.00741000	-1.95554300
H	3.60391500	-2.06364000	-2.47127900
H	0.24096100	-0.34172400	5.55186100
C	-4.24409700	-2.26378600	1.20344900
H	-2.35545600	-2.82705800	2.11025300
C	-4.54237700	0.10687800	0.77583100

H	-2.89266300	1.38160800	1.36462900
C	-2.87192600	2.73428600	-1.95695600
C	-3.78094600	0.52642000	-2.89564600
H	-1.92484800	4.40154300	-0.95447300
C	-3.64531000	-0.86408300	-2.87898600
H	-2.60569400	-2.63751900	-2.11710700
H	4.96779400	0.05854000	-2.42245400
C	-5.03274600	-1.20680300	0.71640500
H	-4.61725400	-3.28872200	1.16094900
H	-5.14705300	0.93499900	0.40284800
H	-3.61413200	3.34941700	-2.46852000
H	-4.57229600	1.00342300	-3.47357900
H	-4.34861100	-1.46377700	-3.45895300
H	-6.01802900	-1.40635600	0.29221800
Cartesian coordinates of step 57			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62586000
C	1.46612200	0.00000000	-0.72343800
C	-1.09624100	-0.48301100	2.39985400
C	1.18087300	0.33974600	2.32629600
N	-0.94932200	1.20129300	-0.62050500
O	-0.76398800	-1.20998000	-0.56654200
C	1.97808900	-1.16918200	-1.32566600
C	2.35189500	1.09121400	-0.80647800
C	-0.97065000	-0.63387400	3.79739800
C	-2.43237700	-0.79476700	1.80286600
C	1.29394800	0.21814500	3.72063400
H	2.04728400	0.69074600	1.76721100
C	-1.87826500	0.60086900	-1.41523400
C	-0.98882000	2.52628400	-0.44316900
C	-1.74173100	-0.81159800	-1.37738400
C	3.24654300	-1.18098500	-1.93106600
H	1.36758400	-2.07186400	-1.31386000
N	3.54593300	1.14524100	-1.36665600
F	1.95769300	2.28148300	-0.23155500
C	0.21542700	-0.28663600	4.46147200
H	-1.82492900	-1.01006700	4.36392700
C	-2.92175400	-2.11650200	1.76812100
C	-3.25426700	0.24083400	1.31326100
H	2.22442600	0.49764300	4.21819400
C	-2.89576300	1.28984800	-2.12783900
C	-1.96640300	3.30300200	-1.11228100
H	-0.24977500	2.95726000	0.22503800
C	-2.63369800	-1.57914200	-2.12515900
C	3.99408700	0.00262800	-1.93082800
H	3.64274200	-2.08564800	-2.39300200
H	0.29101100	-0.40470700	5.54397100
C	-4.19035000	-2.39756200	1.23644000
H	-2.29016100	-2.92367500	2.14181200
C	-4.52541600	-0.03597300	0.78550400
H	-2.89239200	1.26859300	1.35553200

C	-2.90418900	2.70265800	-1.95237300
C	-3.79264300	0.48455300	-2.88713200
H	-1.97095100	4.38047200	-0.95461000
C	-3.64076200	-0.90441900	-2.87197000
H	-2.57869600	-2.66625300	-2.11387700
H	4.98300900	0.05217500	-2.39223400
C	-4.99657400	-1.35742600	0.74182800
H	-4.54851900	-3.42826900	1.20602400
H	-5.14386000	0.77921600	0.40671800
H	-3.65499600	3.30957000	-2.46118300
H	-4.59154400	0.95266700	-3.46193500
H	-4.33924700	-1.51175200	-3.44980400
H	-5.98079700	-1.57587200	0.32450200
Cartesian coordinates of step 58			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62638100
C	1.46974700	0.00000000	-0.71644600
C	-1.06291900	-0.55046100	2.40166500
C	1.16525500	0.39634000	2.32370600
N	-0.96104200	1.19171100	-0.61842300
O	-0.75086900	-1.21744000	-0.56951900
C	1.99916000	-1.17875700	-1.28388800
C	2.34318500	1.09887700	-0.82359200
C	-0.91778800	-0.71517800	3.79586400
C	-2.39125000	-0.90518900	1.81265700
C	1.29462300	0.26405500	3.71561500
H	2.00774000	0.80029400	1.76369500
C	-1.88753100	0.58272500	-1.40991100
C	-1.01566600	2.51559800	-0.43622700
C	-1.73496200	-0.82818700	-1.37635900
C	3.27143200	-1.19147300	-1.88107600
H	1.39942400	-2.08810500	-1.25206100
N	3.53974900	1.15255900	-1.37822100
F	1.93129200	2.29938500	-0.28234800
C	0.25261500	-0.31275800	4.45633100
H	-1.74666900	-1.14358000	4.36301000
C	-2.84628700	-2.23922100	1.78567400
C	-3.24371100	0.10728400	1.32628100
H	2.21141400	0.58911500	4.21089600
C	-2.91696900	1.26185600	-2.11495300
C	-2.00613400	3.28269200	-1.09744000
H	-0.27802000	2.95339700	0.22913100
C	-2.61950200	-1.60385100	-2.12468800
C	4.00488200	0.00065200	-1.90872600
H	3.68110900	-2.10345000	-2.31606400
H	0.34352100	-0.44230400	5.53632800
C	-4.11174800	-2.55450600	1.26561500
H	-2.19092500	-3.02874700	2.15623300
C	-4.51221800	-0.20358600	0.81175700
H	-2.90755100	1.14405600	1.36253100
C	-2.94123600	2.67404300	-1.93453600

C	-3.80731900	0.44833600	-2.87320300
H	-2.02260800	4.35952300	-0.93627100
C	-3.63766700	-0.93880500	-2.86465800
H	-2.55140300	-2.69023200	-2.11713000
H	4.99588100	0.04962800	-2.36569700
C	-4.94957400	-1.53701500	0.77644300
H	-4.44321800	-3.59427000	1.24103000
H	-5.15534500	0.59423900	0.43714000
H	-3.70172600	3.27373200	-2.43748000
H	-4.61464000	0.90863800	-3.44251500
H	-4.33066000	-1.55238200	-3.44251700
H	-5.93201700	-1.78206100	0.36979500
Cartesian coordinates of step 59			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62688600
C	1.47300200	0.00000000	-0.70953500
C	-1.02484000	-0.61526400	2.40424100
C	1.14686100	0.45424800	2.31990000
N	-0.97394300	1.18333500	-0.61401000
O	-0.73837600	-1.22348700	-0.57240700
C	2.01889000	-1.18699500	-1.24312400
C	2.33496200	1.10526900	-0.83927900
C	-0.85858700	-0.78799100	3.79521000
C	-2.34305500	-1.01732400	1.82404100
C	1.29476200	0.31487800	3.70921500
H	1.96108300	0.91021500	1.75783900
C	-1.89983300	0.56599700	-1.40012000
C	-1.04213900	2.50611800	-0.42796200
C	-1.73117900	-0.84314400	-1.37224700
C	3.29530400	-1.20060600	-1.83125700
H	1.42903000	-2.10191300	-1.19263400
N	3.53438500	1.15854700	-1.38759100
F	1.90550300	2.31483800	-0.33181300
C	0.29385600	-0.32992000	4.45088500
H	-1.65909600	-1.26509300	4.36418100
C	-2.75449800	-2.36534800	1.80003600
C	-3.23236900	-0.03284600	1.34536000
H	2.19564500	0.68610900	4.20124700
C	-2.94265900	1.23535500	-2.09499000
C	-2.04647100	3.26369500	-1.07918100
H	-0.30420000	2.95059900	0.23269100
C	-2.61077900	-1.62673000	-2.11805200
C	4.01575100	-0.00137700	-1.88509500
H	3.71790600	-2.11878900	-2.24001800
H	0.40142500	-0.46735000	5.52837100
C	-4.01391900	-2.72124700	1.29146200
H	-2.07078400	-3.13340500	2.16453600
C	-4.49513000	-0.38435300	0.84332500
H	-2.92959900	1.01436700	1.37966400
C	-2.98145600	2.64679700	-1.91034800
C	-3.82877600	0.41388600	-2.84974000

H	-2.07380100	4.33983700	-0.91492100
C	-3.64206900	-0.97120200	-2.84821000
H	-2.53016600	-2.71222700	-2.11409700
H	5.00913400	0.04686800	-2.33692700
C	-4.88951100	-1.73139600	0.81183100
H	-4.31170700	-3.77122900	1.26957200
H	-5.16749800	0.39243000	0.47581800
H	-3.75257200	3.23924700	-2.40561400
H	-4.64550600	0.86662200	-3.41165700
H	-4.33163700	-1.59080100	-3.42373400
H	-5.86771100	-2.00814700	0.41539700
Cartesian coordinates of step 60			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62760200
C	1.47693900	0.00000000	-0.70115800
C	-0.98254700	-0.67727200	2.40765200
C	1.12678100	0.50986100	2.31529900
N	-0.98528700	1.17339600	-0.61181400
O	-0.72569100	-1.23063700	-0.57460300
C	2.04036000	-1.19470900	-1.19803000
C	2.32738400	1.11102500	-0.85385800
C	-0.79277300	-0.85664800	3.79485300
C	-2.29017000	-1.12430500	1.83751800
C	1.29504200	0.36539000	3.70169100
H	1.91047900	1.01333200	1.75010100
C	-1.91071000	0.54729600	-1.39199600
C	-1.06581100	2.49536900	-0.42423000
C	-1.72721200	-0.85997300	-1.36742000
C	3.32157600	-1.20928600	-1.77545900
H	1.46060900	-2.11475600	-1.12794300
N	3.53042300	1.16361600	-1.39413800
F	1.87992400	2.32896000	-0.38215300
C	0.33934500	-0.34344900	4.44484400
H	-1.56140800	-1.38108400	4.36612000
C	-2.66120500	-2.48390300	1.81861200
C	-3.21249200	-0.16744800	1.36444900
H	2.17854500	0.78092800	4.18979200
C	-2.96604100	1.20651300	-2.07783800
C	-2.08264100	3.24314400	-1.06731300
H	-0.32750500	2.94710100	0.23107700
C	-2.60303000	-1.65180900	-2.10899300
C	4.02887500	-0.00368800	-1.85623800
H	3.75787800	-2.13322100	-2.15587800
H	0.46514600	-0.48681000	5.51957200
C	-3.91341700	-2.87789100	1.32011900
H	-1.95211400	-3.23089700	2.17849000
C	-4.46784300	-0.55714200	0.87246500
H	-2.94073700	0.88836900	1.39577600
C	-3.01779000	2.61746900	-1.89166500
C	-3.84895900	0.37664900	-2.82713600
H	-2.11950100	4.31885100	-0.90209300

C	-3.64675400	-1.00639600	-2.83003800
H	-2.51068300	-2.73633700	-2.10736400
H	5.02528700	0.04368900	-2.30143000
C	-4.82191700	-1.91552500	0.84573900
H	-4.17988100	-3.93633900	1.30190300
H	-5.16547900	0.19867200	0.50824600
H	-3.79855800	3.20245700	-2.38061200
H	-4.67480500	0.82142600	-3.38203800
H	-4.33382500	-1.63237300	-3.40163600
H	-5.79429900	-2.22222700	0.45710500
Cartesian coordinates of step 61			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62819000
C	1.48139200	0.00000000	-0.69209400
C	-0.93514000	-0.73531600	2.41348900
C	1.10276900	0.56959800	2.30854100
N	-0.99247500	1.16713300	-0.61008700
O	-0.71502300	-1.23472500	-0.57951400
C	2.06098200	-1.20222700	-1.15092000
C	2.32115600	1.11520600	-0.86973000
C	-0.72056300	-0.91263800	3.79763100
C	-2.22879700	-1.23463900	1.85685200
C	1.29259800	0.42779600	3.69229200
H	1.85176900	1.11846500	1.73826400
C	-1.91612200	0.53561100	-1.38849000
C	-1.08260500	2.48810200	-0.41940100
C	-1.72136200	-0.87024200	-1.36850900
C	3.34649500	-1.21916400	-1.71842100
H	1.49050300	-2.12621000	-1.05963600
N	3.52738600	1.16567900	-1.40298800
F	1.85740000	2.34135700	-0.43558700
C	0.38737900	-0.34058000	4.43969300
H	-1.45382200	-1.48086000	4.37350500
C	-2.55706200	-2.60522200	1.86065600
C	-3.18396000	-0.31397900	1.37643300
H	2.15541500	0.89078500	4.17463400
C	-2.98004800	1.18813000	-2.06764700
C	-2.10763800	3.22947900	-1.05690800
H	-0.34508700	2.94439800	0.23363400
C	-2.59284700	-1.66711800	-2.10988000
C	4.04161700	-0.00869000	-1.82825500
H	3.79535000	-2.14867900	-2.06952300
H	0.53227300	-0.48344500	5.51207200
C	-3.79989300	-3.04550500	1.37728200
H	-1.82280400	-3.32451000	2.22663600
C	-4.42948200	-0.74987400	0.89914500
H	-2.94416900	0.74992100	1.39045800
C	-3.04174800	2.59847500	-1.87827100
C	-3.85937200	0.35311800	-2.81546700
H	-2.15180200	4.30454700	-0.88937300
C	-3.64513500	-1.02824500	-2.82409000

H	-2.49161700	-2.75084000	-2.11152600
H	5.04069900	0.03683500	-2.26761000
C	-4.74116700	-2.11903800	0.89518200
H	-4.03340600	-4.11186700	1.37684800
H	-5.15274100	-0.02181000	0.52839000
H	-3.82910200	3.17847900	-2.36253900
H	-4.69136000	0.79263100	-3.36535900
H	-4.32943000	-1.65811400	-3.39475000
H	-5.70629200	-2.46168000	0.51864900
Cartesian coordinates of step 62			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62827200
C	1.48690000	0.00000000	-0.68120300
C	-0.88221300	-0.78819600	2.42272800
C	1.06756900	0.64395900	2.29909400
N	-0.99149500	1.16874600	-0.60569600
O	-0.70870900	-1.23217800	-0.59120400
C	2.08108900	-1.21029100	-1.09867700
C	2.31789500	1.11695200	-0.88567400
C	-0.64564900	-0.94665100	3.80607100
C	-2.15020000	-1.36079700	1.88007300
C	1.27458500	0.52232100	3.68209400
H	1.77658000	1.23625800	1.72073300
C	-1.90726800	0.54103800	-1.39675000
C	-1.08653300	2.48772200	-0.40471400
C	-1.70782800	-0.86419800	-1.38758300
C	3.37158300	-1.23274100	-1.65418100
H	1.51783900	-2.13629800	-0.98505100
N	3.52831500	1.16208300	-1.40989000
F	1.83929000	2.35217400	-0.49471700
C	0.42687600	-0.30145000	4.43832900
H	-1.33772000	-1.55714200	4.38955500
C	-2.41734600	-2.74394400	1.92294500
C	-3.14601400	-0.49629000	1.37777300
H	2.10800500	1.04330500	4.15691200
C	-2.96701700	1.19667800	-2.07958500
C	-2.10794800	3.23194600	-1.04484100
H	-0.35484500	2.94019100	0.25757900
C	-2.56893700	-1.65680900	-2.14575000
C	4.05701500	-0.01976300	-1.79436200
H	3.83166800	-2.16828100	-1.97330500
H	0.58775700	-0.43010900	5.51021100
C	-3.64058000	-3.25168800	1.45575000
H	-1.65183100	-3.41988200	2.30729500
C	-4.37122600	-0.99961000	0.91540400
H	-2.95378500	0.57725700	1.36414300
C	-3.03347300	2.60558800	-1.87923400
C	-3.83621100	0.36591300	-2.84393600
H	-2.15585000	4.30556000	-0.86927300
C	-3.61668500	-1.01474400	-2.86372400
H	-2.46470100	-2.74022300	-2.15566900

H	5.05968700	0.02156200	-2.22588800
C	-4.62221900	-2.38115900	0.95025200
H	-3.82731500	-4.32680600	1.48605400
H	-5.12676400	-0.31460400	0.52718600
H	-3.81755600	3.18784300	-2.36605800
H	-4.66418300	0.80778000	-3.39795700
H	-4.29281100	-1.64142900	-3.44747400
H	-5.57225800	-2.77640100	0.58704200
Cartesian coordinates of step 63			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62842400
C	1.49263600	0.00000000	-0.66938900
C	-0.82733700	-0.83834200	2.43038700
C	1.03095400	0.70954800	2.29072100
N	-0.98820500	1.17304600	-0.60148200
O	-0.70390900	-1.22739900	-0.60397800
C	2.09914100	-1.21681000	-1.04885500
C	2.31725400	1.11706400	-0.89653500
C	-0.57125400	-0.97876500	3.81257400
C	-2.06424800	-1.48363900	1.89934300
C	1.25405600	0.60499900	3.67246600
H	1.70112500	1.33958800	1.70552500
C	-1.89821300	0.55099800	-1.40389100
C	-1.08534300	2.49030400	-0.39090000
C	-1.69736100	-0.85398000	-1.40488100
C	3.39471500	-1.24498100	-1.59174000
H	1.54114000	-2.14351600	-0.91591500
N	3.53213900	1.15658400	-1.41089200
F	1.82644000	2.35950400	-0.54501800
C	0.46391800	-0.26801000	4.43611200
H	-1.22169700	-1.62780500	4.40225000
C	-2.26294900	-2.87719700	1.97048000
C	-3.10056500	-0.67925900	1.37901400
H	2.05733400	1.17710700	4.14037300
C	-2.95310100	1.21169900	-2.08950400
C	-2.10222700	3.23922200	-1.03277900
H	-0.35798000	2.93805200	0.27935700
C	-2.55271600	-1.64104500	-2.17543000
C	4.07295700	-0.03117000	-1.75810300
H	3.86418400	-2.18539300	-1.88154500
H	0.63969900	-0.38412400	5.50706400
C	-3.45816700	-3.45416400	1.51111100
H	-1.46600300	-3.50651200	2.37003400
C	-4.29707700	-1.25178000	0.92328800
H	-2.96190100	0.40211000	1.34465500
C	-3.02116700	2.61924600	-1.87898700
C	-3.81546600	0.38674700	-2.86793000
H	-2.15144000	4.31149500	-0.84960500
C	-3.59506100	-0.99376700	-2.89673800
H	-2.44855300	-2.72439800	-2.19174600
H	5.07938300	0.00584300	-2.18120300

C	-4.47949700	-2.64351900	0.98510600
H	-3.59190900	-4.53631900	1.56307000
H	-5.08406500	-0.61304700	0.51884900
H	-3.80118900	3.20521100	-2.36784300
H	-4.63902400	0.83265500	-3.42525800
H	-4.26612900	-1.61620000	-3.49078200
H	-5.40781600	-3.09236800	0.62794700
Cartesian coordinates of step 64			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62745200
C	1.49993000	0.00000000	-0.65489500
C	-0.76681800	-0.88145600	2.44267200
C	0.97483900	0.79538200	2.27787600
N	-0.97094700	1.19242900	-0.59206300
O	-0.70785800	-1.20983900	-0.62811000
C	2.11680600	-1.22558100	-0.98718500
C	2.32180300	1.11316600	-0.90802400
C	-0.50515000	-0.97468600	3.82848800
C	-1.93938300	-1.64409200	1.92203900
C	1.20076400	0.73436500	3.66141900
H	1.60082900	1.45954400	1.68098200
C	-1.86676500	0.59294000	-1.42689700
C	-1.05949600	2.50683400	-0.36233900
C	-1.67852300	-0.81358600	-1.44657500
C	3.41893500	-1.26559900	-1.51274600
H	1.56076400	-2.15014700	-0.83156300
N	3.54296600	1.14111500	-1.40840400
F	1.82183500	2.36477500	-0.60542900
C	0.47158000	-0.17754900	4.44065900
H	-1.10720000	-1.65933000	4.42913800
C	-2.01855200	-3.04652800	2.04054000
C	-3.03354800	-0.95075400	1.36317800
H	1.95968000	1.37135300	4.11945300
C	-2.89538300	1.27651300	-2.12980700
C	-2.05078700	3.27741000	-1.01836300
H	-0.34432400	2.93527000	0.33322700
C	-2.52371200	-1.57897300	-2.24993300
C	4.09380500	-0.05434400	-1.70968300
H	3.89606400	-2.21267300	-1.76605500
H	0.65047200	-0.25899100	5.51427900
C	-3.15201200	-3.74051700	1.58648400
H	-1.17673500	-3.59076700	2.47189900
C	-4.16809100	-1.63988100	0.91145100
H	-2.98510200	0.13637700	1.28758300
C	-2.95308900	2.68148600	-1.89893500
C	-3.74447500	0.47379700	-2.94549300
H	-2.09296700	4.34716600	-0.81951000
C	-3.53856400	-0.90859100	-2.98967600
H	-2.43038400	-2.66300700	-2.28134500
H	5.10546000	-0.02601600	-2.12083000
C	-4.23075100	-3.03991100	1.01920800

H	-3.19251700	-4.82782800	1.67432800
H	-5.00016000	-1.08551000	0.47399400
H	-3.71253900	3.28412500	-2.39972700
H	-4.54700500	0.93761200	-3.51860200
H	-4.19918300	-1.51409800	-3.61225500
H	-5.11158700	-3.57928300	0.66691600
Cartesian coordinates of step 65			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62700300
C	1.50528100	0.00000000	-0.64289500
C	-0.70349300	-0.91941800	2.45615000
C	0.91424000	0.87533000	2.26352900
N	-0.96151000	1.20547800	-0.58087800
O	-0.71068000	-1.19758100	-0.64365400
C	2.12939600	-1.23195100	-0.93665700
C	2.32596600	1.10879900	-0.91680300
C	-0.43710600	-0.96837900	3.84396300
C	-1.80953800	-1.78386000	1.94898300
C	1.14248000	0.85534300	3.64749000
H	1.49179300	1.57180100	1.65413600
C	-1.85855800	0.62029200	-1.42469700
C	-1.04127400	2.51846100	-0.34024200
C	-1.67884700	-0.78708800	-1.45841600
C	3.43680700	-1.28203100	-1.44752100
H	1.57429500	-2.15396200	-0.76261800
N	3.55243000	1.12685200	-1.40474500
F	1.81951400	2.36698500	-0.65504700
C	0.47805600	-0.09209500	4.44251500
H	-0.98873300	-1.68426100	4.45650300
C	-1.77488900	-3.18524700	2.09836900
C	-2.95321600	-1.19457400	1.37085500
H	1.85373000	1.55244800	4.09430900
C	-2.87799100	1.31824600	-2.12705600
C	-2.02333600	3.30248400	-0.99392500
H	-0.32626000	2.93532900	0.36235900
C	-2.52845700	-1.53920400	-2.26993000
C	4.11027100	-0.07404500	-1.66857300
H	3.91912900	-2.23395800	-1.67101400
H	0.65985700	-0.14122800	5.51759400
C	-2.84502100	-3.97934200	1.65445800
H	-0.89489100	-3.64977500	2.54654200
C	-4.02459200	-1.98338300	0.92882100
H	-2.99235200	-0.10909800	1.26890300
C	-2.92565700	2.72159500	-1.88441200
C	-3.72892200	0.52944500	-2.95447700
H	-2.05786800	4.37076700	-0.78597300
C	-3.53436300	-0.85416500	-3.00902200
H	-2.44194100	-2.62343500	-2.31194300
H	5.12632400	-0.05307800	-2.06918900
C	-3.97334500	-3.38149700	1.06664700
H	-2.79703900	-5.06418600	1.76567800

H	-4.89612000	-1.50797200	0.47556700
H	-3.67734900	3.33466900	-2.38420700
H	-4.52473800	1.00458800	-3.52763200
H	-4.19653100	-1.44899000	-3.64021300
H	-4.80520800	-3.99842200	0.72259900
Cartesian coordinates of step 66			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62675800
C	1.50800400	0.00000000	-0.63441700
C	-0.63864800	-0.95323000	2.46844600
C	0.84950100	0.94739700	2.25052500
N	-0.96083300	1.21545500	-0.56650900
O	-0.71446500	-1.18836200	-0.65158000
C	2.13646800	-1.23633500	-0.89994500
C	2.32842000	1.10486900	-0.92355100
C	-0.37855300	-0.95505300	3.85893500
C	-1.65815900	-1.92554300	1.97349300
C	1.07190000	0.96953900	3.63492000
H	1.38374900	1.66837000	1.62977600
C	-1.87598600	0.63657400	-1.39556100
C	-1.03159500	2.52847800	-0.32226200
C	-1.70057900	-0.77101900	-1.44071700
C	3.44730700	-1.29408800	-1.40072200
H	1.58176600	-2.15599500	-0.71207100
N	3.55837400	1.11530400	-1.40299100
F	1.81855200	2.36729700	-0.69090200
C	0.46730200	-0.00448900	4.44556200
H	-0.87924400	-1.69882300	4.48189800
C	-1.47582000	-3.31462200	2.13009000
C	-2.86196700	-1.46241600	1.40351900
H	1.73284500	1.72102000	4.07077000
C	-2.90549500	1.34041800	-2.07751200
C	-2.02217000	3.31799500	-0.95590100
H	-0.30330500	2.94192600	0.36823400
C	-2.56981600	-1.51786200	-2.23628900
C	4.12026400	-0.08919900	-1.63987100
H	3.93264900	-2.24926200	-1.60273700
H	0.64426500	-0.01967600	5.52242300
C	-2.46171200	-4.21949600	1.70336100
H	-0.54745400	-3.68084400	2.57182600
C	-3.85048900	-2.36190200	0.98012200
H	-3.01340200	-0.38784200	1.29061900
C	-2.94319200	2.74324100	-1.83093800
C	-3.77486900	0.55751200	-2.89139500
H	-2.04791400	4.38593200	-0.74496000
C	-3.58741900	-0.82664600	-2.95378900
H	-2.48595600	-2.60196900	-2.28455700
H	5.13918300	-0.07390500	-2.03339600
C	-3.65277400	-3.74633300	1.12620400
H	-2.29949900	-5.29260500	1.82020400
H	-4.77237600	-1.98312000	0.53545800

H	-3.70127800	3.36051000	-2.31564800
H	-4.57953700	1.03781500	-3.44761200
H	-4.26373200	-1.41687100	-3.57421400
H	-4.42047000	-4.44875500	0.79718600
Cartesian coordinates of step 67			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62733500
C	1.50956100	0.00000000	-0.62889700
C	-0.57684800	-0.99027200	2.47059400
C	0.80011800	0.99141400	2.24816900
N	-0.96523900	1.21662500	-0.56250100
O	-0.71387200	-1.18727900	-0.65116800
C	2.13782800	-1.23720100	-0.89123600
C	2.33352800	1.10381300	-0.91187500
C	-0.31326200	-0.97634000	3.86042900
C	-1.53043500	-2.02942900	1.97843600
C	1.02741600	1.02531400	3.63133800
H	1.29425300	1.73913400	1.62573300
C	-1.89528500	0.63358600	-1.37256200
C	-1.03358300	2.53132900	-0.32490800
C	-1.71828800	-0.77364100	-1.41828300
C	3.45197600	-1.29663500	-1.38307600
H	1.58046300	-2.15620800	-0.70792600
N	3.56677900	1.11252700	-1.38254400
F	1.82343400	2.36714900	-0.68422200
C	0.47930900	0.02041700	4.44452000
H	-0.76728600	-1.74860000	4.48446900
C	-1.23794500	-3.40215000	2.10914300
C	-2.77589700	-1.65286700	1.43502200
H	1.64912600	1.81114900	4.06436800
C	-2.93853300	1.33303500	-2.03837300
C	-2.03679900	3.31657200	-0.94362300
H	-0.29407000	2.95103300	0.34918700
C	-2.60214700	-1.52509000	-2.19327200
C	4.12862500	-0.09265300	-1.61619600
H	3.93706800	-2.25245300	-1.58264200
H	0.66042900	0.01546400	5.52076400
C	-2.15680900	-4.37485300	1.68155700
H	-0.27710800	-3.70138400	2.53162900
C	-3.69766600	-2.62035800	1.01094900
H	-3.01300300	-0.59196100	1.34214400
C	-2.97385400	2.73680800	-1.79787000
C	-3.82230100	0.54590500	-2.83251600
H	-2.05915200	4.38555500	-0.73763500
C	-3.63472600	-0.83820100	-2.89332500
H	-2.51635100	-2.60908300	-2.23927700
H	5.15039500	-0.07860300	-2.00229000
C	-3.39001200	-3.98726900	1.12987300
H	-1.90953800	-5.43365300	1.77810700
H	-4.65386400	-2.30788600	0.58762500
H	-3.74183400	3.35073400	-2.27110000

H	-4.63813600	1.02338400	-3.37470400
H	-4.32224500	-1.43163100	-3.49818900
H	-4.10586900	-4.74221200	0.80025400
Cartesian coordinates of step 68			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62776000
C	1.51153800	0.00000000	-0.62256200
C	-0.51412700	-1.02572800	2.46919000
C	0.75413400	1.02708000	2.24817500
N	-0.96959700	1.21568900	-0.56233200
O	-0.71135300	-1.18806400	-0.65010600
C	2.13996400	-1.23744900	-0.88349100
C	2.33881300	1.10347100	-0.89704200
C	-0.24124900	-1.00526300	3.85711300
C	-1.41268200	-2.11340800	1.97762000
C	0.99148100	1.06467100	3.62945900
H	1.20688300	1.80130300	1.62656900
C	-1.90900800	0.62699600	-1.35805400
C	-1.03754800	2.53225200	-0.33353500
C	-1.72901300	-0.77984700	-1.40197700
C	3.45740600	-1.29729300	-1.36645900
H	1.58029700	-2.15621400	-0.70604300
N	3.57521800	1.11169400	-1.35911400
F	1.82838900	2.36696400	-0.67083600
C	0.50233000	0.02846700	4.44114100
H	-0.64843600	-1.80428200	4.47978000
C	-1.03713900	-3.46782600	2.08350500
C	-2.68684000	-1.80391100	1.45874600
H	1.57623600	1.87861700	4.06203100
C	-2.96187700	1.32081300	-2.01492900
C	-2.04985500	3.31204700	-0.94420200
H	-0.29109900	2.95912600	0.32783600
C	-2.62109300	-1.53706200	-2.16201100
C	4.13723300	-0.09364700	-1.59177500
H	3.94259600	-2.25325100	-1.56512900
H	0.69210800	0.02710500	5.51589000
C	-1.90312400	-4.48759600	1.65457900
H	-0.05408900	-3.71538800	2.48806500
C	-3.55576700	-2.81854300	1.03361300
H	-2.98769900	-0.75772900	1.38472600
C	-2.99703800	2.72583200	-1.78247800
C	-3.85419400	0.52815900	-2.79386200
H	-2.07072800	4.38228200	-0.74463800
C	-3.66470200	-0.85577500	-2.85104500
H	-2.53125700	-2.62076700	-2.20637800
H	5.16174900	-0.07992700	-1.97052000
C	-3.16529800	-4.16629200	1.12659800
H	-1.59212600	-5.53106400	1.73182200
H	-4.53563200	-2.55777100	0.62978600
H	-3.77207300	3.33549900	-2.24966200
H	-4.67791100	1.00171500	-3.32750400

H	-4.35867000	-1.45328300	-3.44442500
H	-3.84005400	-4.95781500	0.79605600
Cartesian coordinates of step 69			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63873200
C	1.44027800	0.00000000	-0.75607700
C	-0.46541100	-1.09530000	2.42556600
C	0.32768000	1.18968300	2.32936500
N	-0.97706700	1.29817600	-0.46902800
O	-0.85756800	-1.11742200	-0.56616200
C	1.84434000	-1.14321500	-1.48259000
C	2.42221000	1.00919200	-0.74083800
C	-0.63670600	-0.94495200	3.82104300
C	-0.70714300	-2.45518300	1.85966900
C	0.18283000	1.32696500	3.71791000
H	0.70072800	2.04398900	1.76875600
C	-2.14889900	0.74145700	-0.89141100
C	-0.88182600	2.63196300	-0.40394000
C	-2.05954600	-0.67412200	-0.92429500
C	3.10571300	-1.21207700	-2.09771600
H	1.15454000	-1.98386600	-1.55509500
N	3.61578700	1.00560900	-1.30291400
F	2.13969300	2.18449600	-0.07366700
C	-0.32378100	0.25622600	4.47035900
H	-0.99210000	-1.80128500	4.39748000
C	0.33763300	-3.14786700	1.21174900
C	-1.95611500	-3.09249500	2.00235000
H	0.45609300	2.26543100	4.20402800
C	-3.31113100	1.47258200	-1.26106200
C	-1.98470100	3.45049200	-0.75474800
H	0.06629000	3.04811800	-0.08331500
C	-3.17784000	-1.40562600	-1.32323000
C	3.96126100	-0.11070800	-1.97979100
H	3.41416700	-2.09704800	-2.65491000
H	-0.45528400	0.34701800	5.55000600
C	0.13220500	-4.43470100	0.69609400
H	1.30717200	-2.65936700	1.10714800
C	-2.16681000	-4.38035000	1.48189900
H	-2.76863200	-2.56182100	2.50189500
C	-3.18912200	2.88870100	-1.17243800
C	-4.44174400	0.70674100	-1.66978300
H	-1.86751900	4.53127400	-0.69033600
C	-4.35272200	-0.68771900	-1.68942400
H	-3.14909900	-2.49370700	-1.34616200
H	4.95379900	-0.10683100	-2.43593600
C	-1.12424300	-5.05501500	0.82402900
H	0.95110200	-4.95641500	0.19708000
H	-3.14386800	-4.85548700	1.58935400
H	-4.03482600	3.52623300	-1.43514000
H	-5.36297000	1.21145300	-1.96015400
H	-5.22660300	-1.26260100	-1.99991700

H	-1.28588700	-6.05669500	0.42211200
Cartesian coordinates of step 70			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63947000
C	1.43165600	0.00000000	-0.76992000
C	-0.39885200	-1.13125200	2.41327700
C	0.23750200	1.20253400	2.34326800
N	-0.94937000	1.31129300	-0.48065500
O	-0.88066500	-1.10662900	-0.55493600
C	1.79446100	-1.09021600	-1.59175200
C	2.44174100	0.97733100	-0.68150200
C	-0.58829100	-1.00662000	3.80876300
C	-0.54524700	-2.49689900	1.83057000
C	0.07433700	1.31652500	3.73207500
H	0.55023200	2.08795900	1.79443700
C	-2.13410900	0.77695100	-0.89337200
C	-0.81475300	2.64277900	-0.44895300
C	-2.07462000	-0.64072900	-0.91273100
C	3.04779800	-1.14274900	-2.22510900
H	1.08053900	-1.90350100	-1.72128300
N	3.62995300	0.98676400	-1.25500500
F	2.19529100	2.09860500	0.08374300
C	-0.36156300	0.20655700	4.47137100
H	-0.88814400	-1.89049700	4.37501900
C	0.53037800	-3.09168300	1.13757900
C	-1.73383700	-3.23644100	1.99799200
H	0.27682400	2.26777700	4.22779500
C	-3.27750100	1.53086600	-1.27513000
C	-1.89674500	3.48324500	-0.81299900
H	0.14835500	3.03800100	-0.14473100
C	-3.20928300	-1.35052100	-1.30505600
C	3.93577900	-0.07923800	-2.02615200
H	3.32624300	-1.98688700	-2.85654900
H	-0.50575400	0.27784400	5.55087000
C	0.41340000	-4.38253500	0.60415700
H	1.45395500	-2.52554400	1.01270500
C	-1.85601500	-4.52831500	1.46026500
H	-2.57097400	-2.78212300	2.53109300
C	-3.11802600	2.94492200	-1.21296300
C	-4.42594100	0.78639600	-1.67342700
H	-1.75045500	4.56166700	-0.77325300
C	-4.36825900	-0.60990800	-1.67731400
H	-3.20386200	-2.43912500	-1.32344500
H	4.92400200	-0.06608700	-2.49142200
C	-0.78342900	-5.10558300	0.75885400
H	1.25607500	-4.82715100	0.07115400
H	-2.78769900	-5.08301000	1.58794700
H	-3.94746100	3.59945300	-1.48556500
H	-5.33522900	1.30827000	-1.97094400
H	-5.25476100	-1.16826700	-1.98211200
H	-0.87624700	-6.11041200	0.34329300

Cartesian coordinates of step 71

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63922900
C	1.42681500	0.00000000	-0.77712200
C	-0.32858000	-1.15952000	2.40502800
C	0.16144600	1.20958700	2.35157300
N	-0.92575700	1.31939000	-0.49658900
O	-0.89550100	-1.10037000	-0.54832900
C	1.76449900	-1.04632000	-1.66305800
C	2.45208500	0.95534200	-0.63938500
C	-0.52303300	-1.05739800	3.80150400
C	-0.39575300	-2.52554000	1.80933300
C	-0.00732600	1.30314300	3.74136000
H	0.41787400	2.11802600	1.81079900
C	-2.11204200	0.80155000	-0.92387500
C	-0.76248100	2.64797400	-0.48703700
C	-2.07538100	-0.61729300	-0.92988400
C	3.01191500	-1.08035700	-2.30943300
H	1.03753700	-1.84117600	-1.82991900
N	3.63621200	0.98014100	-1.22131100
F	2.22622900	2.03019400	0.19406800
C	-0.37142300	0.16266800	4.47287100
H	-0.76582400	-1.96230200	4.36177700
C	0.69701700	-3.03656800	1.07773800
C	-1.52554500	-3.34770600	1.99939600
H	0.13518400	2.26174700	4.24369100
C	-3.23299300	1.57182600	-1.33813200
C	-1.82087900	3.50398500	-0.88298100
H	0.20465500	3.02759000	-0.17427000
C	-3.21466100	-1.31054100	-1.33895100
C	3.91789100	-0.04353600	-2.05664700
H	3.27295100	-1.89038600	-2.99104500
H	-0.51783700	0.21689200	5.55306400
C	0.65261700	-4.32559700	0.52868200
H	1.57729200	-2.40919400	0.93690100
C	-1.57468500	-4.63826600	1.44769000
H	-2.37587300	-2.95876600	2.56248900
C	-3.04621500	2.98333600	-1.29427200
C	-4.38680900	0.84371000	-1.75054900
H	-1.65339200	4.57978300	-0.85913900
C	-4.35341600	-0.55341900	-1.73959400
H	-3.22756600	-2.39925100	-1.35136600
H	4.90231000	-0.01858000	-2.52946200
C	-0.48647500	-5.13131400	0.70681100
H	1.50811900	-4.70407300	-0.03416300
H	-2.46207500	-5.25720000	1.59413300
H	-3.85732600	3.64979000	-1.59196900
H	-5.28046000	1.37813900	-2.07212800
H	-5.24321500	-1.09938000	-2.05698700
H	-0.52259000	-6.13473800	0.27919600

Cartesian coordinates of step 72

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63841100
C	1.42667300	0.00000000	-0.77671900
C	-0.25579700	-1.18097100	2.39912500
C	0.09517300	1.21299700	2.35608200
N	-0.91066100	1.31669500	-0.51635500
O	-0.89842000	-1.10413400	-0.54226300
C	1.75635500	-1.01811300	-1.69698000
C	2.45691900	0.94421500	-0.60620400
C	-0.44696500	-1.09802200	3.79714800
C	-0.25376600	-2.54399000	1.79308200
C	-0.07104300	1.28919700	3.74737900
H	0.29733600	2.13818800	1.82000600
C	-2.08807900	0.80401500	-0.97263800
C	-0.73417800	2.64377000	-0.51855900
C	-2.06165100	-0.61524300	-0.96512900
C	3.00395000	-1.03793200	-2.34370500
H	1.02481500	-1.80329700	-1.88801600
N	3.64220700	0.98064100	-1.18548800
F	2.23377100	1.99078900	0.26250700
C	-0.36297900	0.12549800	4.47440300
H	-0.63296900	-2.01843800	4.35380500
C	0.85402100	-2.98616900	1.03983800
C	-1.33106600	-3.43152300	1.99515400
H	0.01800900	2.25178700	4.25438600
C	-3.18912300	1.57955500	-1.42851200
C	-1.77298500	3.50453100	-0.95384900
H	0.22837700	3.01729900	-0.18431800
C	-3.19347600	-1.30271400	-1.40460800
C	3.91686800	-0.01640200	-2.05485700
H	3.26075900	-1.82602400	-3.05213300
H	-0.50565000	0.16541300	5.55571500
C	0.87477700	-4.27186100	0.48122700
H	1.69503200	-2.30948100	0.89026900
C	-1.31452700	-4.71908400	1.43504300
H	-2.19296000	-3.09593600	2.57468500
C	-2.99083100	2.98984800	-1.39414200
C	-4.33569400	0.85697600	-1.86947400
H	-1.59639800	4.57900500	-0.93759700
C	-4.31343300	-0.54027600	-1.84582000
H	-3.21465400	-2.39138500	-1.41124700
H	4.90188700	0.01726800	-2.52590400
C	-0.21242100	-5.14330200	0.67224000
H	1.74127900	-4.59613000	-0.09831900
H	-2.16200200	-5.38935300	1.59139000
H	-3.78675300	3.65999600	-1.72288500
H	-5.21459100	1.39531700	-2.22350500
H	-5.19705200	-1.08222500	-2.18651400
H	-0.19783400	-6.14428500	0.23764500
Cartesian coordinates of step 73			
B	0.00000000	0.00000000	0.00000000

C	0.00000000	0.00000000	1.63746500
C	1.42695800	0.00000000	-0.77522700
C	-0.18146600	-1.19686300	2.39413700
C	0.03564200	1.21296400	2.36001200
N	-0.90343200	1.31068400	-0.53157200
O	-0.89699100	-1.11065100	-0.53680400
C	1.75474800	-0.99929000	-1.71583900
C	2.45791800	0.93889100	-0.58290800
C	-0.35868900	-1.13181600	3.79476600
C	-0.12767900	-2.55400600	1.77713600
C	-0.11749500	1.27305700	3.75367400
H	0.17921200	2.15120400	1.82704500
C	-2.07389800	0.79726800	-1.00410500
C	-0.72083500	2.63697400	-0.54399600
C	-2.05087300	-0.62213700	-0.98487500
C	3.00391300	-1.00832500	-2.35981700
H	1.02214700	-1.77942200	-1.92270900
N	3.64536100	0.98408800	-1.15744600
F	2.23164900	1.96791700	0.30537000
C	-0.33317600	0.09120400	4.47790500
H	-0.48857500	-2.06383400	4.34805200
C	0.99274500	-2.94822000	1.01672300
C	-1.17152600	-3.48206500	1.97355900
H	-0.07716100	2.23670500	4.26488600
C	-3.16358000	1.57247700	-1.48716100
C	-1.74863600	3.49715400	-1.00564300
H	0.23785000	3.00901700	-0.19654100
C	-3.17675300	-1.30949800	-1.44027500
C	3.91908100	0.00427000	-2.04660200
H	3.26089300	-1.78184500	-3.08408400
H	-0.46375700	0.11794700	5.56114200
C	1.05807000	-4.22690600	0.44492900
H	1.80961700	-2.24177900	0.87327900
C	-1.11034900	-4.76237300	1.40055200
H	-2.04302900	-3.18349400	2.55894100
C	-2.96046800	2.98237200	-1.46235000
C	-4.30401500	0.84971500	-1.94312900
H	-1.56855000	4.57112400	-0.99665900
C	-4.28610800	-0.54745000	-1.90778200
H	-3.20101200	-2.39814000	-1.44047500
H	4.90559200	0.04441900	-2.51403100
C	0.00373900	-5.13872200	0.62990200
H	1.93424400	-4.51385400	-0.13967900
H	-1.93241900	-5.46447100	1.55271800
H	-3.74782300	3.65219800	-1.81171400
H	-5.17446600	1.38750200	-2.31822600
H	-5.16470700	-1.08969000	-2.26079400
H	0.05289000	-6.13402600	0.18492600
Cartesian coordinates of step 74			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63654100

C	1.42753800	0.00000000	-0.77403500
C	-0.10612400	-1.20779900	2.38961400
C	-0.02166300	1.21022800	2.36368100
N	-0.89891000	1.30283700	-0.54532800
O	-0.89336600	-1.11867300	-0.53179700
C	1.75416500	-0.98537500	-1.72905000
C	2.45826100	0.93573000	-0.56686100
C	-0.26556600	-1.15832300	3.79280200
C	-0.00600700	-2.55809200	1.76283200
C	-0.15810500	1.25639000	3.75973300
H	0.06250000	2.15754200	1.83351600
C	-2.06053600	0.78631500	-1.03562600
C	-0.71434800	2.62890800	-0.56375200
C	-2.03799800	-0.63313800	-1.00587000
C	3.00431600	-0.98628900	-2.37111400
H	1.02122800	-1.76218300	-1.94666300
N	3.64718200	0.98751500	-1.13816500
F	2.22937300	1.95226600	0.33469800
C	-0.29576000	0.06162400	4.48154000
H	-0.33918800	-2.09830300	4.34298600
C	1.12578100	-2.91168900	1.00010700
C	-1.02076400	-3.51937400	1.95226800
H	-0.16479400	2.21885000	4.27473100
C	-3.14045500	1.55891700	-1.54414000
C	-1.73295700	3.48633500	-1.05006400
H	0.23873500	3.00162800	-0.20140300
C	-3.15589400	-1.32280200	-1.47778100
C	3.92063200	0.02009200	-2.04092700
H	3.26171300	-1.74927500	-3.10633300
H	-0.41117200	0.07682100	5.56671600
C	1.23008100	-4.18361200	0.41824300
H	1.92119200	-2.18028600	0.86326000
C	-0.92062700	-4.79261700	1.36944200
H	-1.90092700	-3.25203900	2.53979100
C	-2.93653600	2.96885600	-1.52538600
C	-4.27251500	0.83356200	-2.01633300
H	-1.55252200	4.56026500	-1.04526800
C	-4.25583600	-0.56340400	-1.97100100
H	-3.18086700	-2.41142700	-1.47176000
H	4.90814400	0.06509000	-2.50582400
C	0.20434300	-5.12860300	0.59585000
H	2.11478900	-4.43890700	-0.16817700
H	-1.72073300	-5.52074000	1.51617100
H	-3.71676400	3.63671000	-1.89396800
H	-5.13545400	1.36896100	-2.41163700
H	-5.12786200	-1.10774100	-2.33687000
H	0.28390600	-6.11836500	0.14299400
Cartesian coordinates of step 75			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63541300
C	1.42636300	0.00000000	-0.77623900

C	-0.03014900	-1.21500300	2.38338000
C	-0.08648100	1.20376600	2.36800800
N	-0.89181300	1.29694500	-0.55811000
O	-0.89241400	-1.12484200	-0.52663400
C	1.74764800	-0.97155400	-1.74655300
C	2.45931800	0.93010600	-0.55645000
C	-0.17877900	-1.18122200	3.78789000
C	0.12760400	-2.55536500	1.74637700
C	-0.21206700	1.23591400	3.76566100
H	-0.06591600	2.15726100	1.84196500
C	-2.04271900	0.77962600	-1.07179700
C	-0.70246300	2.62240300	-0.58047000
C	-2.02363700	-0.63982100	-1.03230300
C	2.99698100	-0.96653200	-2.39002800
H	1.01247800	-1.74367200	-1.97295100
N	3.64820800	0.98644600	-1.12776800
F	2.23294600	1.93362600	0.35981900
C	-0.27158000	0.03218300	4.48301400
H	-0.19580000	-2.12649800	4.33373900
C	1.27794600	-2.86088700	0.99146700
C	-0.85350200	-3.55428700	1.91835000
H	-0.27141400	2.19412800	4.28515600
C	-3.10816900	1.55185100	-1.61061700
C	-1.70706600	3.47911500	-1.09610000
H	0.24317600	2.99379100	-0.19732900
C	-3.13225400	-1.32935300	-1.52653600
C	3.91714900	0.03161300	-2.04521800
H	3.25142700	-1.71924100	-3.13677800
H	-0.37710100	0.03591400	5.56929000
C	1.43330500	-4.12322900	0.39944300
H	2.04890700	-2.10141400	0.87043900
C	-0.70226900	-4.81772200	1.32578200
H	-1.74772600	-3.32389200	2.50025400
C	-2.90041500	2.96137800	-1.59647000
C	-4.23062500	0.82632000	-2.10464800
H	-1.52423600	4.55263900	-1.09383900
C	-4.21830900	-0.57044900	-2.05003300
H	-3.16050400	-2.41786400	-1.51526800
H	4.90443100	0.07992200	-2.51029700
C	0.44102300	-5.10595100	0.55952900
H	2.33200600	-4.34100000	-0.18076500
H	-1.47668700	-5.57558600	1.45892800
H	-3.66970700	3.62882000	-1.98804400
H	-5.08258400	1.36107200	-2.52388000
H	-5.08267200	-1.11507500	-2.43326300
H	0.56026000	-6.08811700	0.09891600
Cartesian coordinates of step 76			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63417700
C	1.42485100	0.00000000	-0.77785100
C	0.04633800	-1.21809000	2.37550000

C	-0.15509300	1.19290900	2.37281600
N	-0.88806300	1.29157600	-0.56671100
O	-0.89170300	-1.13053600	-0.52088500
C	1.74407600	-0.96175600	-1.75803400
C	2.45778600	0.92746800	-0.54860400
C	-0.09905000	-1.20140500	3.78016100
C	0.27570200	-2.54303900	1.72683900
C	-0.27625200	1.20993400	3.77132500
H	-0.19399700	2.14901700	1.85168500
C	-2.03091400	0.77244000	-1.09586500
C	-0.69730600	2.61688200	-0.58974500
C	-2.01354500	-0.64706100	-1.04853400
C	2.99340800	-0.95101500	-2.40131400
H	1.00897100	-1.73211400	-1.99049300
N	3.64730300	0.98817200	-1.11839800
F	2.23072000	1.92101100	0.37819200
C	-0.26098300	0.00111200	4.48215800
H	-0.05960300	-2.14920800	4.32055300
C	1.45810900	-2.79137900	1.00160900
C	-0.66931000	-3.58203600	1.85815000
H	-0.39048300	2.16004700	4.29650300
C	-3.08704700	1.54337600	-1.65461300
C	-1.69299500	3.47206000	-1.12478200
H	0.24210600	2.98817300	-0.19110500
C	-3.11546300	-1.33743000	-1.55696900
C	3.91484300	0.04228400	-2.04562600
H	3.24755000	-1.69635700	-3.15552100
H	-0.36259900	-0.00708400	5.56878000
C	1.68035600	-4.03842900	0.39774000
H	2.20176300	-2.00078300	0.91465800
C	-0.45115900	-4.82994900	1.25397600
H	-1.58758200	-3.39455200	2.41747600
C	-2.87815200	2.95282800	-1.64290000
C	-4.20222000	0.81668800	-2.16296000
H	-1.51005900	4.54556400	-1.12317900
C	-4.19209100	-0.57988500	-2.10131600
H	-3.14572300	-2.42584100	-1.54119100
H	4.90238700	0.09377900	-2.50983900
C	0.72401300	-5.06143900	0.51685600
H	2.60265000	-4.21198300	-0.15979600
H	-1.19784700	-5.61991300	1.35494700
H	-3.64042500	3.61919500	-2.04972300
H	-5.04689000	1.35014200	-2.59825900
H	-5.05080000	-1.12551800	-2.49567200
H	0.89520600	-6.03150800	0.04701300
Cartesian coordinates of step 77			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63262200
C	1.42383100	0.00000000	-0.77906200
C	0.12305700	-1.21599300	2.36781600
C	-0.22817900	1.17772500	2.37633300

N	-0.88464300	1.28595700	-0.57540700
O	-0.88998800	-1.13632500	-0.51622900
C	1.74131100	-0.95409800	-1.76677100
C	2.45742100	0.92436700	-0.54150200
C	-0.01881300	-1.21546100	3.77243000
C	0.42337200	-2.52228000	1.70880900
C	-0.34610000	1.18051900	3.77542300
H	-0.32934500	2.13187700	1.85938500
C	-2.01731100	0.76434900	-1.12320600
C	-0.69356900	2.61130400	-0.59759900
C	-2.00093400	-0.65516200	-1.06853300
C	2.99091600	-0.93967900	-2.40934800
H	1.00596300	-1.72260100	-2.00447100
N	3.64785600	0.98744300	-1.10921700
F	2.23033000	1.90983700	0.39380200
C	-0.25287300	-0.02803100	4.48044400
H	0.07848500	-2.16190200	4.30791800
C	1.63598900	-2.71464500	1.01769000
C	-0.48510800	-3.59768000	1.79633100
H	-0.51850700	2.11906500	4.30552300
C	-3.06300500	1.53336100	-1.70386600
C	-1.67926300	3.46434300	-1.15402600
H	0.23780200	2.98315700	-0.18072200
C	-3.09426000	-1.34708600	-1.59357000
C	3.91401600	0.04869800	-2.04426300
H	3.24464900	-1.67945700	-3.16914200
H	-0.35101700	-0.04742200	5.56724400
C	1.92508800	-3.94421700	0.40551600
H	2.35157400	-1.89559400	0.96512000
C	-0.20053300	-4.82767300	1.18338900
H	-1.42641800	-3.45247400	2.32917800
C	-2.85407400	2.94287500	-1.69324100
C	-4.16894700	0.80477900	-2.22920200
H	-1.49722800	4.53799500	-1.15182100
C	-4.16035700	-0.59155000	-2.16091200
H	-3.12593500	-2.43539700	-1.57331000
H	4.90212900	0.10194200	-2.50709700
C	1.00534800	-5.00391000	0.48111000
H	2.87005500	-4.07441400	-0.12506000
H	-0.91906100	-5.64681900	1.25041500
H	-3.60852400	3.60776100	-2.11672100
H	-5.00543700	1.33639300	-2.68215600
H	-5.01195400	-1.13873100	-2.56833700
H	1.22811400	-5.96017000	0.00455300
Cartesian coordinates of step 78			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.63104500
C	1.42337200	0.00000000	-0.77956600
C	0.19947700	-1.20774100	2.36220800
C	-0.30023800	1.15944100	2.37783700
N	-0.87932800	1.28288700	-0.58212600

O	-0.88956000	-1.13957200	-0.51395500
C	1.73700800	-0.94294700	-1.77870600
C	2.45932400	0.91869000	-0.53124500
C	0.06568100	-1.21893100	3.76735400
C	0.56513600	-2.49545700	1.69814600
C	-0.41104800	1.15200000	3.77756600
H	-0.46559800	2.10597200	1.86296100
C	-2.00309100	0.76123700	-1.14737800
C	-0.68648800	2.60805100	-0.60081300
C	-1.98973500	-0.65832200	-1.08765900
C	2.98652900	-0.92485900	-2.42120500
H	0.99957000	-1.70679700	-2.02479600
N	3.65044900	0.98398100	-1.09737300
F	2.23473300	1.89317200	0.41576900
C	-0.23709100	-0.04935900	4.47938800
H	0.22175300	-2.15908600	4.29998800
C	1.79916900	-2.63730900	1.03341600
C	-0.30307200	-3.60541700	1.75945000
H	-0.64052700	2.07648000	4.31075100
C	-3.03803100	1.53070900	-1.74642500
C	-1.66170700	3.46127100	-1.17509900
H	0.23726400	2.97861100	-0.16588400
C	-3.07623600	-1.34944400	-1.62805800
C	3.91327000	0.05539700	-2.04357900
H	3.23803000	-1.65662100	-3.18944100
H	-0.32773800	-0.07685600	5.56666200
C	2.14998100	-3.85254100	0.42422300
H	2.48403100	-1.79133600	0.99944700
C	0.04296000	-4.82085200	1.14915600
H	-1.26088300	-3.49966000	2.27171800
C	-2.82725000	2.94001400	-1.73446300
C	-4.13647000	0.80259400	-2.28771700
H	-1.47940300	4.53486500	-1.17018800
C	-4.13137300	-0.59360400	-2.21505700
H	-3.11108500	-2.43760500	-1.60475400
H	4.90180200	0.11034700	-2.50534900
C	1.27094100	-4.94746300	0.47509800
H	3.11088900	-3.94308800	-0.08539900
H	-0.64472200	-5.66735800	1.19688800
H	-3.57353000	3.60515000	-2.17179100
H	-4.96468400	1.33420700	-2.75560000
H	-4.97722700	-1.14050800	-2.63463000
H	1.54196400	-5.89243500	0.00101300
Cartesian coordinates of step 79			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62922800
C	1.42377500	0.00000000	-0.77780300
C	0.27565400	-1.19602800	2.35394800
C	-0.37338100	1.13475100	2.38085800
N	-0.87202000	1.28341900	-0.58619100
O	-0.89139700	-1.13932900	-0.51423100

C	1.73446000	-0.93129700	-1.78817400
C	2.46365100	0.90974600	-0.51414000
C	0.14916700	-1.22154900	3.75926400
C	0.71237200	-2.45855900	1.68233700
C	-0.47845900	1.11423000	3.78105100
H	-0.60271800	2.07035900	1.87009300
C	-1.98734300	0.76488700	-1.16997800
C	-0.67630700	2.60822000	-0.59634500
C	-1.97949300	-0.65487500	-1.10847300
C	2.98606900	-0.91211800	-2.42650100
H	0.99366200	-1.68797400	-2.04619200
N	3.65746200	0.97455200	-1.07450000
F	2.24090100	1.87223400	0.44514400
C	-0.22386500	-0.07582700	4.47724800
H	0.36492700	-2.15243400	4.28729300
C	1.97460100	-2.54688300	1.06281800
C	-0.11608400	-3.59999700	1.69797500
H	-0.76619100	2.01945100	4.31905500
C	-3.01038200	1.53787900	-1.78472300
C	-1.63966100	3.46459600	-1.18575500
H	0.23969100	2.97512800	-0.14198700
C	-3.05997400	-1.34221600	-1.66574200
C	3.91765200	0.05673900	-2.03216300
H	3.23603200	-1.63559500	-3.20301700
H	-0.30817600	-0.11320500	5.56474200
C	2.39350100	-3.74182800	0.45609600
H	2.62856400	-1.67588800	1.06210900
C	0.29807900	-4.79519400	1.09006500
H	-1.09571000	-3.53583500	2.17453900
C	-2.79608800	2.94668300	-1.76697200
C	-4.10215300	0.81321800	-2.34372000
H	-1.45597300	4.53790900	-1.17469500
C	-4.10267300	-0.58299600	-2.27038600
H	-3.09991000	-2.43019400	-1.64200100
H	4.90842900	0.11110100	-2.48919600
C	1.55496000	-4.86911600	0.46328800
H	3.37528600	-3.79069500	-0.01807100
H	-0.35888800	-5.66693400	1.10336400
H	-3.53317000	3.61434800	-2.21588800
H	-4.92116700	1.34723700	-2.82484600
H	-4.94345700	-1.12732600	-2.70327700
H	1.87927700	-5.79827900	-0.00858200
Cartesian coordinates of step 80			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62720800
C	1.42615200	0.00000000	-0.77257100
C	0.35147400	-1.18061000	2.34308900
C	-0.44850100	1.10281000	2.38519600
N	-0.86460800	1.28566400	-0.58822300
O	-0.89299000	-1.13726700	-0.51845400
C	1.73858300	-0.92571500	-1.78701900

C	2.46857700	0.90263200	-0.49526200
C	0.23258600	-1.22356900	3.74806900
C	0.86752500	-2.40751600	1.65865600
C	-0.54820700	1.06613900	3.78561700
H	-0.74304500	2.02328400	1.87984500
C	-1.97114400	0.77167600	-1.19165900
C	-0.66719500	2.61020300	-0.58556100
C	-1.96872800	-0.64838900	-1.13190000
C	2.99422800	-0.90812800	-2.41731100
H	0.99637700	-1.67790800	-2.05428200
N	3.66647500	0.96495300	-1.04670400
F	2.24488600	1.85754000	0.47133000
C	-0.21239500	-0.10837600	4.47382100
H	0.50863800	-2.14209700	4.26964600
C	2.16840200	-2.43647800	1.11813000
C	0.07510300	-3.57132700	1.58286000
H	-0.89532400	1.94622800	4.33031000
C	-2.98253100	1.54950700	-1.81933000
C	-1.61915600	3.47108300	-1.18681500
H	0.24051900	2.97260400	-0.11119800
C	-3.04277300	-1.33081800	-1.70740500
C	3.92809200	0.05270700	-2.00960600
H	3.24615600	-1.62824200	-3.19627500
H	-0.29097400	-0.15749800	5.56128400
C	2.66288900	-3.59756600	0.50275200
H	2.79109200	-1.54470700	1.18244900
C	0.56493000	-4.73281300	0.96541700
H	-0.93435200	-3.55146700	1.99653900
C	-2.76580800	2.95779500	-1.79127800
C	-4.06733100	0.82947800	-2.39758400
H	-1.43495900	4.54416500	-1.16597700
C	-4.07312100	-0.56684300	-2.32739800
H	-3.08767900	-2.41864500	-1.68596700
H	4.92232500	0.10499100	-2.45935000
C	1.86140700	-4.74854500	0.42065800
H	3.67266800	-3.60089400	0.08892800
H	-0.06361400	-5.62350000	0.90792500
H	-3.49404300	3.62900200	-2.24926300
H	-4.87726100	1.36698900	-2.89005100
H	-4.90855300	-1.10772800	-2.77471800
H	2.24434500	-5.65142800	-0.05833700
Cartesian coordinates of step 81			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62424400
C	1.44641900	0.00000000	-0.73218900
C	0.42904100	-1.16744600	2.31675500
C	-0.53748600	1.04994300	2.39861100
N	-0.83556900	1.31071900	-0.58186000
O	-0.90458700	-1.11047800	-0.54925200
C	1.78551700	-0.93963400	-1.72524000
C	2.49307400	0.88438200	-0.41510700

C	0.32632900	-1.24491400	3.71991600
C	1.10414900	-2.29454400	1.59368900
C	-0.63360800	0.97692700	3.79820600
H	-0.89756600	1.95595000	1.90879100
C	-1.93277000	0.82569900	-1.22399900
C	-0.62324700	2.63216800	-0.54120300
C	-1.95426100	-0.59445500	-1.18752400
C	3.06442400	-0.94515300	-2.30688800
H	1.04419700	-1.68508000	-2.01343200
N	3.71010600	0.92731600	-0.92342700
F	2.25235000	1.84191300	0.54564800
C	-0.20711100	-0.18110300	4.46454500
H	0.67652200	-2.14725000	4.22507200
C	2.50819000	-2.28592300	1.46074400
C	0.37560000	-3.36566800	1.04277500
H	-1.04787700	1.81617200	4.36027900
C	-2.91621800	1.62980300	-1.86230200
C	-1.54720300	3.51858600	-1.14941400
H	0.27400100	2.97174900	-0.03156200
C	-3.02187400	-1.25051100	-1.80341200
C	3.99449800	0.00633100	-1.87162600
H	3.33692600	-1.67730100	-3.06742300
H	-0.28222800	-0.25587400	5.55080400
C	3.17022400	-3.31945200	0.78029800
H	3.07521500	-1.45371800	1.88040700
C	1.03522600	-4.40209200	0.36183400
H	-0.71020100	-3.36954800	1.13341700
C	-2.68213300	3.03411400	-1.79815800
C	-3.99527400	0.93641300	-2.48282500
H	-1.35093100	4.58852100	-1.09814600
C	-4.02340900	-0.46048100	-2.43817300
H	-3.08517500	-2.33766900	-1.80185200
H	5.00541700	0.04262700	-2.28429300
C	2.43408200	-4.38050100	0.22571600
H	4.25619700	-3.29115200	0.67667200
H	0.45725100	-5.22469400	-0.06378700
H	-3.38852500	3.72479200	-2.26137200
H	-4.78405300	1.49466300	-2.98646000
H	-4.85415800	-0.98086600	-2.91731000
H	2.94586500	-5.18420600	-0.30664600
Cartesian coordinates of step 82			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62340600
C	1.45214600	0.00000000	-0.72207400
C	0.50058300	-1.13612200	2.31966200
C	-0.58494100	1.02604300	2.39570800
N	-0.82627200	1.31501600	-0.58223800
O	-0.90503000	-1.10551000	-0.56039700
C	1.79573100	-0.93284300	-1.71975500
C	2.49970500	0.87777700	-0.38947900
C	0.42911600	-1.20114300	3.72558200

C	1.21663600	-2.23662500	1.59587500
C	-0.65502200	0.96303600	3.79724100
H	-1.00103500	1.90586800	1.90229800
C	-1.91601600	0.83745600	-1.24200900
C	-0.61120700	2.63546300	-0.52784900
C	-1.94359000	-0.58276700	-1.21190400
C	3.07955900	-0.93946900	-2.29047500
H	1.05343300	-1.67190200	-2.02113100
N	3.72092400	0.91966400	-0.88750700
F	2.25522500	1.82911300	0.57641400
C	-0.14984600	-0.16014400	4.46821300
H	0.83627800	-2.07729000	4.23411600
C	2.62583500	-2.21902100	1.53344200
C	0.52167600	-3.28951400	0.97129600
H	-1.10786600	1.78324300	4.35764700
C	-2.88795400	1.64866300	-1.88873100
C	-1.52375700	3.52861500	-1.14338600
H	0.27886500	2.96842600	-0.00143600
C	-3.00552000	-1.23161900	-1.84494200
C	4.00974800	0.00461600	-1.84002100
H	3.35546400	-1.66712600	-3.05406200
H	-0.20117800	-0.22608900	5.55642600
C	3.32541700	-3.22411500	0.84826700
H	3.16732200	-1.39916600	2.00772200
C	1.21957800	-4.29890600	0.28780500
H	-0.56688000	-3.30012800	1.00768600
C	-2.65038500	3.05178400	-1.81212500
C	-3.96101000	0.96240600	-2.52741300
H	-1.32572400	4.59766000	-1.08148300
C	-3.99504800	-0.43456700	-2.48983100
H	-3.07395800	-2.31846800	-1.84861900
H	5.02440100	0.03953300	-2.24353700
C	2.62301800	-4.26751700	0.22094400
H	4.41492700	-3.18751200	0.79752500
H	0.66727200	-5.10833200	-0.19350800
H	-3.34802500	3.74771300	-2.28071700
H	-4.74095200	1.52604200	-3.03875500
H	-4.82125000	-0.94942500	-2.98258400
H	3.16458000	-5.04942100	-0.31441200
Cartesian coordinates of step 83			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62292100
C	1.45689500	0.00000000	-0.71420800
C	0.56957000	-1.09981800	2.32483400
C	-0.63577700	0.99870600	2.39126300
N	-0.82194400	1.31650000	-0.58351600
O	-0.90320700	-1.10384200	-0.56940500
C	1.81019500	-0.93720600	-1.70416800
C	2.50073300	0.88066700	-0.37725800
C	0.51974900	-1.15072100	3.73255600
C	1.33260700	-2.17061600	1.60598600

C	-0.68784100	0.94718800	3.79400300
H	-1.10470700	1.84875300	1.89293700
C	-1.90159500	0.84183000	-1.26165100
C	-0.61015300	2.63686100	-0.51612000
C	-1.93082900	-0.57842500	-1.23633400
C	3.09818700	-0.94379100	-2.26537600
H	1.07205800	-1.68006100	-2.00596600
N	3.72497400	0.92376300	-0.86735700
F	2.24889100	1.83374400	0.58532400
C	-0.10912100	-0.13617300	4.47085200
H	0.98083800	-1.99688800	4.24575900
C	2.74311400	-2.13593400	1.61347800
C	0.68224600	-3.21024000	0.91424200
H	-1.18181400	1.74571600	4.35093500
C	-2.86427600	1.65596100	-1.91837900
C	-1.51391800	3.53272300	-1.14057300
H	0.27019700	2.96741700	0.02775500
C	-2.98391700	-1.22433600	-1.88682900
C	4.02256800	0.00528800	-1.81374700
H	3.38157700	-1.67533400	-3.02245200
H	-0.14352000	-0.19234600	5.56028300
C	3.48768100	-3.10851100	0.92913200
H	3.25020500	-1.32465300	2.13781200
C	1.42553500	-4.18814400	0.23311500
H	-0.40622600	-3.23497300	0.89793900
C	-2.62905800	3.05876800	-1.83031000
C	-3.92805500	0.97263200	-2.57553900
H	-1.31853600	4.60160700	-1.06841500
C	-3.96327300	-0.42440300	-2.54370900
H	-3.05369000	-2.31108600	-1.89440100
H	5.03982100	0.04088300	-2.21060100
C	2.82982500	-4.13829700	0.23439800
H	4.57777000	-3.05691300	0.93101400
H	0.90741900	-4.98784000	-0.29975700
H	-3.32003700	3.75679000	-2.30562200
H	-4.70036500	1.53862100	-3.09578900
H	-4.78243500	-0.93704800	-3.05031100
H	3.40661200	-4.89487500	-0.30054400
Cartesian coordinates of step 84			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62262200
C	1.45851300	0.00000000	-0.71255800
C	0.63580600	-1.05905500	2.33056000
C	-0.67845200	0.97391000	2.38676600
N	-0.81932300	1.31674900	-0.58354700
O	-0.90156800	-1.10354900	-0.57661400
C	1.81484600	-0.93524000	-1.70311100
C	2.49984200	0.88366900	-0.37520400
C	0.61105700	-1.09001100	3.73978600
C	1.42755100	-2.11014400	1.61594800
C	-0.70883100	0.93951900	3.79062100

H	-1.19770400	1.79114200	1.88326400
C	-1.88895200	0.84422600	-1.27873800
C	-0.61152400	2.63696300	-0.50337500
C	-1.91881600	-0.57617300	-1.25790300
C	3.10279500	-0.93710600	-2.26448300
H	1.07957300	-1.68096500	-2.00459300
N	3.72345800	0.93198900	-0.86616600
F	2.24595100	1.83412300	0.58956900
C	-0.05964800	-0.09946800	4.47346900
H	1.12222300	-1.90394800	4.25760700
C	2.83719700	-2.06400200	1.65592300
C	0.80165300	-3.14482900	0.89420200
H	-1.23838900	1.71743400	4.34402600
C	-2.84328800	1.66079000	-1.94445400
C	-1.50749500	3.53506200	-1.13572300
H	0.25917400	2.96511900	0.05717300
C	-2.96312200	-1.21969100	-1.92480900
C	4.02381700	0.01527700	-1.81328300
H	3.38869000	-1.66777900	-3.02144700
H	-0.07392900	-0.14079800	5.56402100
C	3.60490600	-3.01910100	0.97255100
H	3.32537300	-1.25566000	2.20227200
C	1.56837900	-4.10576300	0.21535700
H	-0.28577800	-3.17851800	0.85345100
C	-2.61115200	3.06336400	-1.84527700
C	-3.89772100	0.97979200	-2.61890800
H	-1.31556600	4.60384800	-1.05363700
C	-3.93316700	-0.41734200	-2.59262600
H	-3.03349800	-2.30637400	-1.93624500
H	5.04061100	0.05482600	-2.21093700
C	2.97171000	-4.04372300	0.24808100
H	4.69418100	-2.95757000	0.99808600
H	1.06927100	-4.90180200	-0.34067400
H	-3.29615200	3.76313000	-2.32665100
H	-4.66312500	1.54762600	-3.14729000
H	-4.74527700	-0.92821500	-3.11220900
H	3.56698100	-4.78637800	-0.28609800
Cartesian coordinates of step 85			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62249100
C	1.45851700	0.00000000	-0.71421400
C	0.69880600	-1.01378900	2.33730900
C	-0.71896300	0.94907600	2.38136900
N	-0.81837500	1.31628500	-0.58278600
O	-0.89987600	-1.10408600	-0.58201000
C	1.81394100	-0.92886300	-1.71085800
C	2.49848000	0.88555100	-0.37701800
C	0.69874100	-1.01970100	3.74736800
C	1.51182400	-2.05108000	1.62901100
C	-0.72825500	0.93625900	3.78583400
H	-1.28721200	1.72955100	1.87222400

C	-1.87934100	0.84494900	-1.29180900
C	-0.61502200	2.63634200	-0.49135800
C	-1.90881100	-0.57560500	-1.27475400
C	3.10036900	-0.92505500	-2.27579600
H	1.07907400	-1.67363400	-2.01546600
N	3.72028600	0.93976700	-0.87174800
F	2.24503500	1.83142300	0.59237600
C	-0.01125600	-0.05275300	4.47520300
H	1.25749900	-1.79830500	4.27033500
C	2.92040700	-1.99504000	1.68687500
C	0.90212800	-3.08769600	0.89553300
H	-1.29209600	1.69295800	4.33480400
C	-2.82743400	1.66312400	-1.96436100
C	-1.50524100	3.53591200	-1.12967200
H	0.24732500	2.96272000	0.08298100
C	-2.94558100	-1.21752500	-1.95494400
C	4.02028300	0.02770600	-1.82334000
H	3.38575700	-1.65155600	-3.03695600
H	-0.00569400	-0.07514900	5.56639100
C	3.70308400	-2.94168200	1.00862500
H	3.39603500	-1.18504100	2.24179800
C	1.68387900	-4.04078900	0.22329600
H	-0.18448900	-3.12938500	0.84168600
C	-2.59892400	3.06559900	-1.85550900
C	-3.87373200	0.98358500	-2.65282100
H	-1.31717100	4.60468300	-1.03899000
C	-3.90838900	-0.41366600	-2.63136800
H	-3.01589700	-2.30417900	-1.96961500
H	5.03570800	0.07155300	-2.22402400
C	3.08621200	-3.96848900	0.27308700
H	4.79149500	-2.87197700	1.04696000
H	1.19739200	-4.83863500	-0.34128100
H	-3.27955800	3.76653100	-2.34137000
H	-4.63389100	1.55255600	-3.18751400
H	-4.71437200	-0.92342500	-3.16148900
H	3.69347000	-4.70455100	-0.25668200

Cartesian coordinates of step 86

B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62250800
C	1.45723400	0.00000000	-0.71780300
C	0.75852900	-0.96466100	2.34441800
C	-0.76184000	0.92017600	2.37560400
N	-0.82299000	1.31184600	-0.58161200
O	-0.89635400	-1.10897200	-0.58325900
C	1.81366900	-0.92769100	-1.71498500
C	2.49358900	0.89229900	-0.38695600
C	0.77712700	-0.94557300	3.75443900
C	1.59543600	-1.98619000	1.64344000
C	-0.75564500	0.92881000	3.78009200
H	-1.37717900	1.66059800	1.86113300
C	-1.87832100	0.83736800	-1.29696900

C	-0.62800300	2.63251100	-0.48210300
C	-1.90285900	-0.58343400	-1.28154000
C	3.09801300	-0.91781300	-2.28460900
H	1.08128800	-1.67583700	-2.01715600
N	3.71297800	0.95297500	-0.88664900
F	2.23878900	1.83837600	0.58210600
C	0.02545700	-0.00582800	4.47580700
H	1.38117100	-1.68598900	4.28252400
C	3.00255700	-1.91018200	1.70961400
C	1.00443500	-3.03244800	0.90774400
H	-1.35553900	1.66096400	4.32414300
C	-2.82716700	1.65322200	-1.97126700
C	-1.51951600	3.52975600	-1.12180700
H	0.22861700	2.96093100	0.09955700
C	-2.93440900	-1.22785000	-1.96746600
C	4.01441500	0.04073100	-1.83752400
H	3.38436900	-1.64408400	-3.04561600
H	0.04626600	-0.00901600	5.56702900
C	3.80216600	-2.84637100	1.03652600
H	3.46353600	-1.09233500	2.26542500
C	1.80320000	-3.97564200	0.24210300
H	-0.08124200	-3.08943200	0.84760000
C	-2.60625200	3.05641100	-1.85613400
C	-3.86755400	0.97099200	-2.66598000
H	-1.33822400	4.59917800	-1.02526700
C	-3.89681900	-0.42643900	-2.64729900
H	-3.00130000	-2.31470700	-1.98346700
H	5.02796000	0.08943400	-2.24237500
C	3.20406300	-3.88329100	0.29965200
H	4.88923500	-2.76061500	1.07988900
H	1.33132500	-4.78115600	-0.32398800
H	-3.28795200	3.75565600	-2.34293800
H	-4.62773000	1.53804900	-3.20267300
H	-4.69845700	-0.93831600	-3.18196100
H	3.82479100	-4.61114600	-0.22580300
Cartesian coordinates of step 87			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62269900
C	1.45608400	0.00000000	-0.72116100
C	0.81484200	-0.91203800	2.35188500
C	-0.79721000	0.89514300	2.36969300
N	-0.82792200	1.30726500	-0.58103900
O	-0.89259300	-1.11392000	-0.58431300
C	1.81469700	-0.92948900	-1.71575300
C	2.48805700	0.90023700	-0.39826200
C	0.85350700	-0.86203500	3.76099200
C	1.67230600	-1.92168600	1.66096100
C	-0.77329700	0.93122900	3.77351200
H	-1.45463300	1.59485800	1.85011300
C	-1.87662100	0.82914000	-1.30381800
C	-0.64175500	2.62854600	-0.47417800

C	-1.89588700	-0.59185500	-1.28955200
C	3.09693000	-0.91394700	-2.28995500
H	1.08574300	-1.68311300	-2.01250000
N	3.70507200	0.96703000	-0.90289400
F	2.23102600	1.84831300	0.56837900
C	0.06656400	0.05371400	4.47523100
H	1.49970200	-1.56208600	4.29420100
C	3.07790600	-1.83224900	1.73895700
C	1.09728500	-2.97630900	0.92382400
H	-1.40321100	1.64182800	4.31219300
C	-2.82545300	1.64214300	-1.98153400
C	-1.53390900	3.52299700	-1.11682500
H	0.20834000	2.95943800	0.11552700
C	-2.92101600	-1.23932700	-1.98237600
C	4.00877800	0.05262400	-1.85082700
H	3.38513300	-1.64186400	-3.04867800
H	0.10401400	0.07448500	5.56580200
C	3.89168300	-2.76352600	1.07595500
H	3.52657100	-1.00762900	2.29487300
C	1.91016600	-3.91481800	0.26940300
H	0.01264900	-3.04290700	0.85422900
C	-2.61267100	3.04611500	-1.86059500
C	-3.85877800	0.95674700	-2.68361400
H	-1.35960900	4.59307400	-1.01490000
C	-3.88232900	-0.44085000	-2.66718600
H	-2.98402200	-2.32640600	-1.99947000
H	5.02033400	0.10607800	-2.26002400
C	3.30962100	-3.80921900	0.33874200
H	4.97750300	-2.66709200	1.12749200
H	1.45071300	-4.72681800	-0.29763000
H	-3.29493900	3.74324100	-2.34964200
H	-4.61828700	1.52151000	-3.22365200
H	-4.67869400	-0.95520900	-3.20732700
H	3.94166600	-4.53318200	-0.17850900
Cartesian coordinates of step 88			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62290200
C	1.45410900	0.00000000	-0.72588200
C	0.86790900	-0.85651500	2.35856500
C	-0.82799100	0.87225900	2.36382100
N	-0.83224600	1.30335900	-0.58047100
O	-0.88990900	-1.11810600	-0.58516000
C	1.81277900	-0.92976600	-1.72002500
C	2.48273200	0.90680500	-0.41073900
C	0.92451900	-0.77377400	3.76572000
C	1.74425000	-1.85591900	1.67870800
C	-0.78710100	0.93860900	3.76610600
H	-1.52231100	1.53180200	1.83951700
C	-1.87529500	0.82237500	-1.30955300
C	-0.65340000	2.62501200	-0.46716000
C	-1.89029100	-0.59879900	-1.29626100

C	3.09211100	-0.90855200	-2.30052900
H	1.08611500	-1.68742000	-2.01206200
N	3.69668700	0.97957900	-0.92181500
F	2.22543300	1.85523700	0.55552000
C	0.10576400	0.11912100	4.47272600
H	1.60885700	-1.43283100	4.30354400
C	3.14828800	-1.75213600	1.76488900
C	1.18411200	-2.92147500	0.94510600
H	-1.44317800	1.62924500	4.29948700
C	-2.82404100	1.63320700	-1.98994600
C	-1.54594400	3.51733800	-1.11213700
H	0.19107000	2.95755700	0.12961100
C	-2.91016900	-1.24857100	-1.99484800
C	4.00067800	0.06441500	-1.86881300
H	3.38055800	-1.63687000	-3.05877200
H	0.15848700	0.16562200	5.56186300
C	3.97500900	-2.68008700	1.11315700
H	3.58549000	-0.91880000	2.31694600
C	2.00977000	-3.85678900	0.30289400
H	0.10048200	-2.99882400	0.86947200
C	-2.61794800	3.03775000	-1.86394800
C	-3.85154900	0.94538000	-2.69815000
H	-1.37751500	4.58788700	-1.00546200
C	-3.87045200	-0.45233400	-2.68370400
H	-2.97014100	-2.33581300	-2.01289900
H	5.00969000	0.12252900	-2.28361300
C	3.40773400	-3.73697600	0.38023700
H	5.05950900	-2.57236200	1.17008300
H	1.56176000	-4.67719000	-0.26118000
H	-3.30063800	3.73324800	-2.35472700
H	-4.61048200	1.50835900	-3.24085000
H	-4.66248600	-0.96860300	-3.22839000
H	4.05009300	-4.45835200	-0.12782400
Cartesian coordinates of step 89			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62296000
C	1.45011800	0.00000000	-0.73385900
C	0.91722700	-0.79793600	2.36503200
C	-0.86039000	0.84665500	2.35708200
N	-0.83668100	1.30099800	-0.57843700
O	-0.88917600	-1.12096900	-0.58457300
C	1.80455900	-0.92698500	-1.73191600
C	2.47580000	0.91399100	-0.43001300
C	0.98607000	-0.68331100	3.76948700
C	1.81605100	-1.78379500	1.69675900
C	-0.80802900	0.94252700	3.75723900
H	-1.58853900	1.46429800	1.82744600
C	-1.87663400	0.81789700	-1.31051100
C	-0.66359300	2.62277300	-0.45953700
C	-1.88849300	-0.60343800	-1.29818300
C	3.07747700	-0.89668300	-2.32612200

H	1.07984600	-1.68921000	-2.01685800
N	3.68352100	0.99578400	-0.95409600
F	2.22233800	1.85977700	0.53997600
C	0.13332200	0.18341700	4.46858900
H	1.70595500	-1.29912200	4.31210200
C	3.21787900	-1.65702700	1.78603700
C	1.27504700	-2.86435400	0.97016200
H	-1.49114600	1.61085400	4.28504900
C	-2.82644900	1.62722200	-1.99128200
C	-1.55749800	3.51365000	-1.10459400
H	0.17731900	2.95635000	0.14165900
C	-2.90539900	-1.25469200	-1.99989300
C	3.98357900	0.08307800	-1.90465000
H	3.36282800	-1.62285300	-3.08759100
H	0.19654900	0.25496000	5.55580700
C	4.06083400	-2.57736400	1.14416500
H	3.64034700	-0.81122800	2.33054500
C	2.11693300	-3.79205500	0.33866400
H	0.19281700	-2.95903000	0.89205900
C	-2.62529000	3.03222000	-1.86124700
C	-3.85045500	0.93781700	-2.70292600
H	-1.39354300	4.58451000	-0.99424000
C	-3.86591100	-0.45997700	-2.69024100
H	-2.96351600	-2.34202300	-2.01826800
H	4.98726300	0.14882700	-2.33103600
C	3.51262000	-3.64938200	0.41907100
H	5.14332700	-2.45155400	1.20211100
H	1.68360800	-4.62393300	-0.22001500
H	-3.30890100	3.72663100	-2.35227400
H	-4.60974800	1.49966000	-3.24629200
H	-4.65550500	-0.97755400	-3.23721800
H	4.16795000	-4.36466000	-0.08094400
Cartesian coordinates of step 90			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62291500
C	1.44448200	0.00000000	-0.74504600
C	0.96137700	-0.73559800	2.37364500
C	-0.89766100	0.81639600	2.34733800
N	-0.83948700	1.30024700	-0.57589400
O	-0.89101200	-1.12207800	-0.58313700
C	1.79033400	-0.92180300	-1.75068200
C	2.46933400	0.91872600	-0.45262600
C	1.03383400	-0.58862800	3.77514600
C	1.88611500	-1.70671800	1.72150700
C	-0.84226400	0.94197600	3.74491100
H	-1.65780300	1.38709800	1.80991400
C	-1.87711100	0.81686200	-1.31093600
C	-0.67034800	2.62183900	-0.45076500
C	-1.88808900	-0.60465600	-1.29977800
C	3.05499900	-0.88283800	-2.36196700
H	1.06535100	-1.68614600	-2.02942500

N	3.66922300	1.00912500	-0.99294200
F	2.22352100	1.86020800	0.52346600
C	0.14335100	0.24815400	4.46331000
H	1.78539200	-1.15853800	4.32485100
C	3.28484300	-1.56285000	1.83011500
C	1.36865300	-2.79773600	0.99256600
H	-1.55587300	1.58399100	4.26497700
C	-2.82766900	1.62633700	-1.99044700
C	-1.56489400	3.51281600	-1.09468900
H	0.16793500	2.95501200	0.15437100
C	-2.90374000	-1.25563000	-2.00361700
C	3.96131500	0.10087400	-1.95018900
H	3.33374600	-1.60489900	-3.12979700
H	0.21073000	0.34515800	5.54832700
C	4.14759600	-2.47718700	1.20591300
H	3.68975200	-0.70887500	2.37523500
C	2.23003300	-3.71919900	0.37920000
H	0.28861300	-2.90529600	0.89929000
C	-2.62975000	3.03134000	-1.85552900
C	-3.85010800	0.93702400	-2.70450600
H	-1.40419400	4.58369800	-0.97985800
C	-3.86392600	-0.46076600	-2.69428300
H	-2.96104900	-2.34297900	-2.02361100
H	4.95864700	0.17348200	-2.39013500
C	3.62267800	-3.55980400	0.47938600
H	5.22763000	-2.33854600	1.27882100
H	1.81456700	-4.55911800	-0.18099200
H	-3.31425700	3.72582200	-2.34522500
H	-4.60957000	1.49895500	-3.24755200
H	-4.65224400	-0.97835700	-3.24310400
H	4.29369900	-4.27032100	-0.00637800
Cartesian coordinates of step 91			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62265800
C	1.43144900	0.00000000	-0.76960500
C	0.99707300	-0.66802300	2.38941400
C	-0.95071100	0.77019200	2.33118000
N	-0.83734500	1.30523900	-0.56942500
O	-0.90189100	-1.11729700	-0.57806900
C	1.74555000	-0.89447400	-1.80965300
C	2.46446400	0.91262900	-0.48677000
C	1.05004900	-0.49692100	3.78972400
C	1.97161600	-1.60489000	1.76283000
C	-0.91523300	0.91610700	3.72710200
H	-1.73867700	1.28764800	1.77994700
C	-1.87861000	0.82799700	-1.30282400
C	-0.66033200	2.62523500	-0.44196400
C	-1.89764600	-0.59367500	-1.29215700
C	2.99039400	-0.83867200	-2.45944000
H	1.01103900	-1.65011000	-2.08804200
N	3.64751100	1.01693700	-1.06086300

F	2.24615600	1.83233800	0.51574800
C	0.10637500	0.29367800	4.46080600
H	1.82791500	-1.01616200	4.35273300
C	3.36128600	-1.42925200	1.92822400
C	1.51001800	-2.70405300	1.00830700
H	-1.67161200	1.51855500	4.23386000
C	-2.82596300	1.64361800	-1.97941200
C	-1.55071200	3.52208000	-1.08349600
H	0.18030800	2.95218100	0.16363200
C	-2.91889000	-1.23803000	-1.99405500
C	3.90965800	0.13406700	-2.04987500
H	3.24388300	-1.53843800	-3.25617200
H	0.15957700	0.40764300	5.54498000
C	4.26955000	-2.32135100	1.33703000
H	3.72412400	-0.56841300	2.49180500
C	2.41636800	-3.60211500	0.42652400
H	0.43708100	-2.83741600	0.87285700
C	-2.61944300	3.04733300	-1.84332500
C	-3.85389500	0.96072100	-2.69177900
H	-1.38418500	4.59194400	-0.96752000
C	-3.87585400	-0.43698000	-2.68212900
H	-2.98321700	-2.32498200	-2.01405000
H	4.89262000	0.21915200	-2.51893000
C	3.79986100	-3.41217700	0.58538600
H	5.34227600	-2.15837400	1.45414400
H	2.04351300	-4.44782200	-0.15446400
H	-3.30077600	3.74631500	-2.33103700
H	-4.61120100	1.52724200	-3.23306800
H	-4.66853200	-0.94958600	-3.22935700
H	4.50628900	-4.10494000	0.12491300
Cartesian coordinates of step 92			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62260000
C	1.42348100	0.00000000	-0.78424700
C	1.03163500	-0.60094300	2.39864800
C	-0.99189400	0.72710500	2.32103000
N	-0.84362900	1.30360500	-0.56566900
O	-0.90354900	-1.11952800	-0.57278200
C	1.72818100	-0.89623000	-1.82564700
C	2.45392800	0.92169600	-0.52204700
C	1.07497300	-0.40622900	3.79645200
C	2.04478600	-1.50669700	1.78888400
C	-0.96574700	0.89438800	3.71459500
H	-1.80543500	1.19442500	1.76187400
C	-1.88357900	0.82355700	-1.29924400
C	-0.67259100	2.62385900	-0.43437500
C	-1.89953400	-0.59830100	-1.28800900
C	2.96239200	-0.83399400	-2.49492100
H	0.99481700	-1.65781800	-2.09074000
N	3.62653600	1.03328700	-1.11567600
F	2.24429000	1.84412400	0.47985900

C	0.08962700	0.34144400	4.45645600
H	1.87904900	-0.87529100	4.36660800
C	3.42621600	-1.28013600	1.95978600
C	1.62677700	-2.63227200	1.04769200
H	-1.75436200	1.46151200	4.21285700
C	-2.83398900	1.63686400	-1.97438900
C	-1.56627700	3.51850000	-1.07440900
H	0.16599300	2.95292600	0.17287600
C	-2.91973900	-1.24496000	-1.98945700
C	3.88021600	0.14792700	-2.10458700
H	3.20869100	-1.53525000	-3.29260900
H	0.13686200	0.47470800	5.53870800
C	4.36856800	-2.14929300	1.38820500
H	3.75525300	-0.39896900	2.51245800
C	2.56714100	-3.50745900	0.48573800
H	0.55962700	-2.80560000	0.90969900
C	-2.63251400	3.04109400	-1.83605200
C	-3.86044000	0.95158800	-2.68660500
H	-1.40417200	4.58875800	-0.95586600
C	-3.87885300	-0.44617200	-2.67722000
H	-2.98190300	-2.33204600	-2.00868700
H	4.85493300	0.23863100	-2.58950600
C	3.94217400	-3.26735100	0.65080600
H	5.43421600	-1.94780300	1.50986300
H	2.22752700	-4.37440400	-0.08411300
H	-3.31619700	3.73839300	-2.32288200
H	-4.61978400	1.51635900	-3.22685800
H	-4.67072400	-0.96066600	-3.22385400
H	4.67537500	-3.94263300	0.20654800
Cartesian coordinates of step 93			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62235200
C	1.40970000	0.00000000	-0.80787400
C	1.05725600	-0.52992800	2.41503300
C	-1.04661500	0.66427100	2.30463400
N	-0.84647100	1.30560000	-0.55901000
O	-0.91188700	-1.11799900	-0.56338300
C	1.68637300	-0.88261400	-1.86859800
C	2.44681800	0.91876500	-0.56185700
C	1.06543900	-0.32844300	3.81338400
C	2.13748300	-1.37296000	1.83224400
C	-1.05309100	0.83706800	3.69730500
H	-1.88001400	1.07700700	1.73159700
C	-1.89121000	0.82722100	-1.28635700
C	-0.67306400	2.62520200	-0.42642200
C	-1.91029300	-0.59479400	-1.27386200
C	2.90342400	-0.81360800	-2.56785500
H	0.94456200	-1.63875500	-2.12638400
N	3.60501800	1.03509300	-1.18219400
F	2.26005700	1.83339800	0.45134200
C	0.02469400	0.35503500	4.45648900

H	1.88886900	-0.74400600	4.39714500
C	3.49717200	-1.08022900	2.06674400
C	1.81036600	-2.51239100	1.06679300
H	-1.88444300	1.35289800	4.18158100
C	-2.84482000	1.64243600	-1.95457500
C	-1.56930600	3.52169300	-1.06021400
H	0.16981900	2.95203900	0.17625800
C	-2.93619600	-1.23935400	-1.96892200
C	3.83288300	0.16134000	-2.18751500
H	3.12774100	-1.50355000	-3.38176600
H	0.04692300	0.49272800	5.53899600
C	4.50674600	-1.89790900	1.53624900
H	3.75654200	-0.18808800	2.63840000
C	2.81772000	-3.33594000	0.54456700
H	0.76027500	-2.73871900	0.88071700
C	-2.64054700	3.04616900	-1.81611700
C	-3.87713100	0.95904400	-2.66019900
H	-1.40554800	4.59168500	-0.94153000
C	-3.89788900	-0.43869400	-2.65076400
H	-3.00116200	-2.32631500	-1.98701800
H	4.79560800	0.25641900	-2.69500700
C	4.17032700	-3.03064200	0.77507300
H	5.55437100	-1.64477200	1.70764600
H	2.54794900	-4.21377800	-0.04548600
H	-3.32647600	3.74480600	-2.29785600
H	-4.63908800	1.52513000	-3.19538700
H	-4.69416600	-0.95167100	-3.19241300
H	4.95519800	-3.66641800	0.36187800
Cartesian coordinates of step 94			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62225400
C	1.39682900	0.00000000	-0.82936300
C	1.07740400	-0.45780600	2.43241400
C	-1.09861000	0.59535700	2.28737700
N	-0.84559100	1.31273600	-0.55187000
O	-0.92267700	-1.11109100	-0.55623800
C	1.64827800	-0.87272800	-1.90458900
C	2.44074600	0.91487600	-0.59791700
C	1.04926200	-0.25236700	3.83064700
C	2.22053200	-1.23108900	1.87487500
C	-1.13896800	0.77104400	3.67865300
H	-1.94865400	0.94961700	1.69954700
C	-1.89299600	0.83945800	-1.27846300
C	-0.66701100	2.63104500	-0.41661300
C	-1.91872600	-0.58259100	-1.26645800
C	2.85129500	-0.80190200	-2.62744000
H	0.89821000	-1.62315700	-2.15558800
N	3.58708600	1.03185400	-1.23967900
F	2.27409800	1.82491200	0.42241000
C	-0.04341700	0.36238200	4.45578400
H	1.88785400	-0.61334200	4.42884500

C	3.55345200	-0.86509200	2.15668200
C	1.98385700	-2.37922300	1.08932700
H	-2.01025600	1.23164500	4.14817700
C	-2.84431800	1.65941900	-1.94397000
C	-1.56028300	3.53230100	-1.04797300
H	0.17791800	2.95334800	0.18583700
C	-2.94849600	-1.22203600	-1.96038200
C	3.79219400	0.16571600	-2.25635900
H	3.05592800	-1.48388400	-3.45320000
H	-0.04722800	0.50227500	5.53824200
C	4.62443200	-1.61955700	1.65410100
H	3.74321100	0.03446800	2.74372500
C	3.05264700	-3.13931200	0.59357300
H	0.95468900	-2.66402900	0.86869800
C	-2.63411500	3.06223900	-1.80363400
C	-3.88066200	0.98114700	-2.64874000
H	-1.39236800	4.60145600	-0.92752500
C	-3.90767200	-0.41644800	-2.64032600
H	-3.01886700	-2.30865300	-1.97840100
H	4.74525000	0.26169900	-2.78161500
C	4.37748800	-2.76126200	0.87233200
H	5.64994400	-1.30981500	1.86211400
H	2.85251300	-4.02442400	-0.01305000
H	-3.31772000	3.76441000	-2.28353600
H	-4.64109700	1.55098100	-3.18212800
H	-4.70727800	-0.92546700	-3.18080300
H	5.20994400	-3.34767600	0.47980000
Cartesian coordinates of step 95			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62250700
C	1.38748000	0.00000000	-0.84460600
C	1.09532000	-0.38618300	2.44600200
C	-1.13907000	0.53311800	2.27304900
N	-0.84866100	1.31656200	-0.54608000
O	-0.92899200	-1.10766000	-0.55091700
C	1.62650100	-0.87819600	-1.91841100
C	2.43174700	0.91967200	-0.63366500
C	1.04054300	-0.17083700	3.84250200
C	2.28629900	-1.09968500	1.90947500
C	-1.20387200	0.71749300	3.66187200
H	-2.00273700	0.82999600	1.67323900
C	-1.89565700	0.84455900	-1.27415800
C	-0.67231700	2.63455900	-0.40607800
C	-1.92255900	-0.57745600	-1.26339000
C	2.82055200	-0.81041500	-2.65625200
H	0.87429300	-1.63078400	-2.15636800
N	3.57003000	1.03370800	-1.28982500
F	2.27400300	1.83901900	0.37946600
C	-0.09272300	0.38239700	4.45222100
H	1.89263000	-0.47696500	4.45201300
C	3.59411000	-0.66648200	2.21316100

C	2.12229600	-2.26014800	1.12365200
H	-2.10592900	1.12815800	4.11946100
C	-2.84744000	1.66556100	-1.93775800
C	-1.56611700	3.53690400	-1.03528400
H	0.17183900	2.95636200	0.19759600
C	-2.95212100	-1.21565900	-1.95877300
C	3.76469500	0.16047200	-2.30250900
H	3.01574800	-1.49668400	-3.48075900
H	-0.11524800	0.53054700	5.53336000
C	4.71039600	-1.36683700	1.73139100
H	3.72837500	0.24328500	2.79971700
C	3.23654800	-2.96630600	0.64840900
H	1.11281200	-2.59917300	0.88903100
C	-2.63860100	3.06808800	-1.79350900
C	-3.88355000	0.98857300	-2.64416200
H	-1.39945600	4.60585300	-0.91130300
C	-3.91064700	-0.40902200	-2.63818000
H	-3.02305400	-2.30223900	-1.97768800
H	4.71151100	0.25398000	-2.83935500
C	4.53537000	-2.52137300	0.94917500
H	5.71509700	-1.00476900	1.95572300
H	3.09173100	-3.86141400	0.04079600
H	-3.32260900	3.77092200	-2.27186600
H	-4.64374800	1.55944100	-3.17679400
H	-4.70995700	-0.91705900	-3.18002100
H	5.40307800	-3.06576800	0.57285200
Cartesian coordinates of step 96			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62292100
C	1.37932900	0.00000000	-0.85749500
C	1.10968900	-0.31445900	2.45787800
C	-1.17375600	0.47073800	2.26046300
N	-0.85808400	1.31515500	-0.54234200
O	-0.92994300	-1.10986000	-0.54379800
C	1.61630400	-0.89594800	-1.91715200
C	2.41703600	0.93309900	-0.67429000
C	1.02958000	-0.09244900	3.85258800
C	2.34423500	-0.96425900	1.93896000
C	-1.26149600	0.66151100	3.64684700
H	-2.04768000	0.71180500	1.65039000
C	-1.90272300	0.83791500	-1.27078400
C	-0.69113700	2.63404100	-0.39990600
C	-1.92393600	-0.58413500	-1.25890100
C	2.80378500	-0.83290500	-2.66581500
H	0.86831300	-1.65869700	-2.13506400
N	3.54872700	1.04376400	-1.34205000
F	2.25939500	1.87073200	0.32171700
C	-0.13916200	0.39786900	4.44870500
H	1.89212200	-0.34476600	4.47193800
C	3.62326800	-0.46122100	2.25709600
C	2.25272000	-2.13388300	1.15514800

H	-2.18999800	1.02173600	4.09389300
C	-2.85928100	1.65391200	-1.93366100
C	-1.59016700	3.53179600	-1.02836600
H	0.14991800	2.96113700	0.20499700
C	-2.95048100	-1.22745600	-1.95395800
C	3.74273200	0.15230100	-2.33886100
H	2.99759800	-1.53300600	-3.47896100
H	-0.17965000	0.55177700	5.52852700
C	4.78108000	-1.10101100	1.78951100
H	3.70192800	0.45580900	2.84235200
C	3.40859900	-2.77928800	0.69307500
H	1.26564700	-2.52786800	0.91119200
C	-2.65896400	3.05752300	-1.78817400
C	-3.89213500	0.97190800	-2.64008100
H	-1.43022100	4.60154200	-0.90240300
C	-3.91269100	-0.42572600	-2.63394100
H	-3.01674600	-2.31435500	-1.97147000
H	4.68439400	0.24305200	-2.88515000
C	4.67782700	-2.26413600	1.00729900
H	5.76210400	-0.68468900	2.02420700
H	3.31885300	-3.68121900	0.08507800
H	-3.34702200	3.75663500	-2.26617600
H	-4.65518600	1.53921600	-3.17244100
H	-4.70966100	-0.93771400	-3.17550900
H	5.57797800	-2.76070200	0.64121200
Cartesian coordinates of step 97			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62353500
C	1.37158800	0.00000000	-0.86976300
C	1.11569200	-0.24165800	2.47436100
C	-1.21241200	0.38890000	2.24492500
N	-0.87066900	1.31120700	-0.53840700
O	-0.92883300	-1.11444200	-0.53491400
C	1.61175100	-0.92195400	-1.90637900
C	2.40162600	0.94739400	-0.71760400
C	0.99753900	-0.03262900	3.86906100
C	2.40686000	-0.79103700	1.97661400
C	-1.33494800	0.56816700	3.62972300
H	-2.09112000	0.57100000	1.62130100
C	-1.91059500	0.82612700	-1.26893500
C	-0.71794600	2.63130600	-0.39181000
C	-1.92261500	-0.59589100	-1.25552000
C	2.79717600	-0.87147400	-2.65921700
H	0.86887000	-1.69563300	-2.10184500
N	3.53158900	1.04616900	-1.38964600
F	2.23725000	1.91414400	0.24872300
C	-0.21043000	0.37465300	4.44862700
H	1.86545200	-0.22852300	4.50122400
C	3.63346000	-0.18037800	2.31237200
C	2.42749700	-1.96552300	1.19559100
H	-2.29234600	0.86393800	4.06292000

C	-2.87327300	1.63459900	-1.93210700
C	-1.62397200	3.52211100	-1.02023900
H	0.11796000	2.96572500	0.21586200
C	-2.94319700	-1.24701100	-1.95201100
C	3.73091400	0.12729500	-2.36017100
H	2.99366000	-1.59172500	-3.45393300
H	-0.27804600	0.51919200	5.52840000
C	4.84821000	-0.71543500	1.85881600
H	3.62461900	0.73909300	2.89890000
C	3.64084900	-2.50617200	0.74628500
H	1.48174800	-2.44504500	0.94111000
C	-2.68609800	3.03971300	-1.78404400
C	-3.89975200	0.94488600	-2.64042700
H	-1.47448300	4.59297900	-0.89097800
C	-3.90996800	-0.45279800	-2.63431900
H	-3.00204600	-2.33436800	-1.96810400
H	4.67204700	0.20783900	-2.90894500
C	4.85607800	-1.88116000	1.07391900
H	5.78614700	-0.21511000	2.10505700
H	3.63744700	-3.41148400	0.13691700
H	-3.37952800	3.73332100	-2.26230400
H	-4.66637000	1.50660700	-3.17359200
H	-4.70224500	-0.97081900	-3.17703600
H	5.80018700	-2.29517600	0.71606600
Cartesian coordinates of step 98			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62396800
C	1.36687400	0.00000000	-0.87711800
C	1.11846600	-0.16958000	2.48815700
C	-1.24344500	0.30613200	2.23139900
N	-0.88461700	1.30616800	-0.53367400
O	-0.92482200	-1.12008200	-0.52861800
C	1.61848300	-0.95131000	-1.88427000
C	2.38566800	0.96429500	-0.75568100
C	0.96740100	0.02592900	3.88229300
C	2.45538900	-0.62026900	2.01136300
C	-1.39592200	0.47298700	3.61431100
H	-2.12421900	0.42950900	1.59634400
C	-1.92085400	0.81249000	-1.26413200
C	-0.74728400	2.62735800	-0.38240200
C	-1.92147500	-0.60946300	-1.25089900
C	2.80518000	-0.91274500	-2.63581800
H	0.88407200	-1.73833300	-2.05689800
N	3.51628800	1.05243900	-1.42755700
F	2.20840500	1.96134000	0.17669200
C	-0.27180900	0.34988800	4.44744500
H	1.83828900	-0.11403700	4.52511800
C	3.62435800	0.08530500	2.36718200
C	2.58313500	-1.79074600	1.23469600
H	-2.37628500	0.70363800	4.03554200
C	-2.89236400	1.61268600	-1.92441900

C	-1.66300600	3.51048800	-1.00768400
H	0.08423100	2.96927900	0.22674200
C	-2.93696400	-1.26908500	-1.94671200
C	3.72843300	0.10384600	-2.36620600
H	3.01066400	-1.65579600	-3.40693400
H	-0.36261500	0.48467700	5.52678800
C	4.88554900	-0.35286800	1.93744100
H	3.53256700	1.00116700	2.95238200
C	3.84325800	-2.23366600	0.80724600
H	1.68392100	-2.34578100	0.96603800
C	-2.71973800	3.01928500	-1.77314800
C	-3.91335100	0.91459200	-2.63255000
H	-1.52506300	4.58242800	-0.87456000
C	-3.91123200	-0.48306200	-2.62786400
H	-2.98688000	-2.35690000	-1.96230600
H	4.67079500	0.17557000	-2.91408100
C	4.99916400	-1.51434100	1.15466900
H	5.77654300	0.21975800	2.19974700
H	3.92216300	-3.13740000	0.20073700
H	-3.42062200	3.70680900	-2.24931300
H	-4.68574600	1.47013100	-3.16384900
H	-4.69953900	-1.00764900	-3.17004200
H	5.97903200	-1.85227600	0.81346800
Cartesian coordinates of step 99			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62402500
C	1.36355900	0.00000000	-0.88213000
C	1.12370000	-0.09873400	2.49260600
C	-1.26000900	0.24596500	2.22508600
N	-0.89608900	1.30244400	-0.52783900
O	-0.92125000	-1.12413400	-0.52618100
C	1.62762900	-0.97664300	-1.86162000
C	2.36904700	0.98177600	-0.79082400
C	0.95824000	0.10648900	3.88394900
C	2.48319900	-0.49108500	2.02743600
C	-1.42517700	0.42162000	3.60525800
H	-2.14384500	0.31344700	1.58588300
C	-1.92926300	0.80300500	-1.25908200
C	-0.77298300	2.62395700	-0.36804000
C	-1.92017300	-0.61888600	-1.24904400
C	2.81276800	-0.94339400	-2.61582200
H	0.90373000	-1.77800400	-2.01084500
N	3.49668900	1.06686800	-1.46788000
F	2.18066300	2.00206000	0.11383900
C	-0.29803700	0.37077300	4.44212900
H	1.83336600	0.02049200	4.53047200
C	3.61641200	0.27206200	2.37988900
C	2.66996700	-1.66607600	1.26971700
H	-2.41768700	0.60392100	4.02168900
C	-2.90873700	1.59748800	-1.91443000
C	-1.69748000	3.50179300	-0.98784600

H	0.05453300	2.97064700	0.24355400
C	-2.93116400	-1.28423900	-1.94583700
C	3.72133800	0.09412400	-2.37849600
H	3.02769300	-1.70581400	-3.36516100
H	-0.39897300	0.51434100	5.51944900
C	4.89936900	-0.11504700	1.96582500
H	3.47909100	1.19163600	2.95026000
C	3.95200000	-2.05805200	0.85783400
H	1.79891600	-2.26560600	1.00428700
C	-2.74924700	3.00485000	-1.75626900
C	-3.92482300	0.89381600	-2.62416600
H	-1.56997700	4.57418800	-0.84813400
C	-3.91185600	-0.50369700	-2.62425600
H	-2.97328000	-2.37235400	-1.96363000
H	4.66142300	0.16376700	-2.93053900
C	5.07148800	-1.28183900	1.20205900
H	5.76152800	0.50126900	2.22545900
H	4.07613600	-2.96640200	0.26600400
H	-3.45685900	3.68812900	-2.22857800
H	-4.70228100	1.44521000	-3.15239600
H	-4.69660000	-1.03271000	-3.16730700
H	6.06828800	-1.58005300	0.87313500
Cartesian coordinates of step 100			
B	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.62431100
C	1.36156400	0.00000000	-0.88534200
C	1.12624400	-0.02794600	2.49518700
C	-1.27179900	0.19102800	2.22062200
N	-0.90728500	1.29781200	-0.52233000
O	-0.91652100	-1.12888600	-0.52502400
C	1.63983700	-0.99978500	-1.83732100
C	2.35366500	0.99775900	-0.82159500
C	0.94855700	0.19121700	3.88300000
C	2.50249800	-0.36996600	2.03914900
C	-1.44760300	0.37942700	3.59772900
H	-2.15626600	0.20491800	1.57900100
C	-1.93722000	0.79260300	-1.25451100
C	-0.79853100	2.61940900	-0.35353600
C	-1.91793800	-0.62910800	-1.24814700
C	2.82512300	-0.97144400	-2.59146600
H	0.92655500	-1.81421200	-1.96509500
N	3.47985100	1.08006600	-1.50121000
F	2.15220600	2.03964800	0.05531700
C	-0.32039300	0.40041700	4.43586000
H	1.82578400	0.15857800	4.53154700
C	3.60366800	0.44265900	2.38184700
C	2.73791100	-1.54923000	1.30162700
H	-2.44866900	0.51710700	4.01081700
C	-2.92481200	1.58130100	-1.90459400
C	-1.73200500	3.49181800	-0.96745800
H	0.02497900	2.97070100	0.26057100

C	-2.92425300	-1.30013900	-1.94619900
C	3.71881300	0.08511400	-2.38371300
H	3.05096900	-1.75154900	-3.31909200
H	-0.43011600	0.55598800	5.51066100
C	4.90216300	0.09931800	1.97749000
H	3.42878200	1.36562600	2.93628000
C	4.03562500	-1.89780000	0.90001100
H	1.89158100	-2.18643300	1.04446800
C	-2.77875500	2.98923200	-1.73894100
C	-3.93579200	0.87205400	-2.61614100
H	-1.61524100	4.56450200	-0.82077400
C	-3.91156900	-0.52522800	-2.62148800
H	-2.95831100	-2.38849400	-1.96662800
H	4.65793900	0.15255100	-2.93766500
C	5.12250700	-1.07233000	1.23389500
H	5.73865800	0.75327200	2.22892700
H	4.19694100	-2.81025200	0.32373100
H	-3.49327700	3.66822900	-2.20700000
H	-4.71849500	1.41916600	-3.14106700
H	-4.69261000	-1.05863800	-3.16557700
H	6.13131500	-1.33625200	0.91241600