

The parameter of a1 as mol2 format

@<TRIPOS>MOLECULE

MOL

47 47 1 0 0

SMALL

No Charge or Current Charge

@<TRIPOS>ATOM

1	C1	-1.1760	2.6740	-0.4360	c3	1	MOL	0.1542651013
2	O1	-4.4000	-0.7390	2.5090	oh	1	MOL	-0.5747834023
3	S1	3.4790	1.2250	1.0580	ss	1	MOL	-0.2451808072
4	C2	-1.3050	3.0520	1.0420	c3	1	MOL	-0.4046101224
5	O2	2.5130	0.4960	-1.2910	o	1	MOL	-0.3466038190
6	C3	-2.4850	2.0710	-0.9930	c3	1	MOL	-0.2313153959
7	O3	2.9390	-2.7090	-0.9300	o	1	MOL	-0.5313287596
8	C4	-2.8390	0.7100	-0.4350	ca	1	MOL	0.1748942915
9	O4	-0.0220	1.3350	-2.0330	oh	1	MOL	-0.6157229704
10	C5	-3.4800	0.5910	0.7990	ca	1	MOL	-0.4050235523
11	C6	-3.7800	-0.6770	1.2960	ca	1	MOL	0.4385748955
12	C7	-3.4620	-1.8240	0.5750	ca	1	MOL	-0.5933428999
13	C8	-2.8370	-1.7070	-0.6720	ca	1	MOL	0.5987693177
14	C9	-2.5150	-0.4360	-1.1610	ca	1	MOL	-0.4490955506
15	C10	-0.0030	1.7210	-0.6740	c3	1	MOL	0.2995085533
16	C11	1.3590	2.3590	-0.3320	c3	1	MOL	-0.4259626704
17	C12	2.4230	1.2840	-0.3720	c	1	MOL	0.4221875514
18	C13	4.3610	-0.3330	0.7350	c3	1	MOL	0.1599477130
19	C14	3.6770	-1.5160	1.4280	c3	1	MOL	-0.1605158450
20	C15	2.0560	-2.2260	-0.2460	c	1	MOL	0.7579168675
21	C16	0.6100	-2.1560	-0.6910	c3	1	MOL	-0.5509772926
22	H1	-0.9780	3.5840	-1.0200	hc	1	MOL	0.0326773126
23	H2	-4.5990	-1.6630	2.7150	ho	1	MOL	0.4196717417
24	H3	-0.4690	3.6650	1.3880	hc	1	MOL	0.1008172707
25	H4	-2.2190	3.6310	1.2060	hc	1	MOL	0.1008172707
26	H5	-1.3600	2.1590	1.6730	hc	1	MOL	0.1008172707
27	H6	-2.3930	1.9980	-2.0790	hc	1	MOL	0.0913620356
28	H7	-3.2970	2.7760	-0.7780	hc	1	MOL	0.0913620356
29	H8	0.8100	0.8610	-2.2070	ho	1	MOL	0.3961663395
30	H9	-3.7690	1.4620	1.3780	ha	1	MOL	0.2010004635
31	H10	-3.7260	-2.8070	0.9610	ha	1	MOL	0.2034781341
32	H11	-2.0100	-0.3340	-2.1180	ha	1	MOL	0.1935842318
33	H12	-0.1480	0.8360	-0.0260	h1	1	MOL	-0.0121290214
34	H13	1.3510	2.8460	0.6460	hc	1	MOL	0.1526598853
35	H14	1.5870	3.1090	-1.0990	hc	1	MOL	0.1526598853
36	H15	5.3870	-0.2060	1.0880	h1	1	MOL	0.0421878326
37	H16	4.3650	-0.4880	-0.3470	h1	1	MOL	0.0421878326
38	H17	4.2310	-2.4260	1.1820	h1	1	MOL	0.1310434180
39	H18	3.6840	-1.3860	2.5130	h1	1	MOL	0.1310434180
40	H19	0.4130	-3.0100	-1.3400	hc	1	MOL	0.1281005478
41	H20	-0.0950	-2.1540	0.1450	hc	1	MOL	0.1281005478
42	H21	0.4520	-1.2360	-1.2680	hc	1	MOL	0.1281005478
43	N1	2.3100	-1.7020	0.9950	n	1	MOL	-0.6003845793
44	H22	1.5820	-1.1810	1.4630	hn	1	MOL	0.3366965235
45	N2	-2.5930	-2.8430	-1.4440	nh	1	MOL	-0.9436903096
46	H23	-1.8940	-2.7150	-2.1640	hn	1	MOL	0.3894909219
47	H24	-2.4330	-3.6930	-0.9180	hn	1	MOL	0.3905772393

@<TRIPOS>BOND

1	1	4	1
2	1	6	1
3	1	15	1

```

4 1 22 1
5 2 11 1
6 2 23 1
7 3 17 1
8 3 18 1
9 4 24 1
10 4 25 1
11 4 26 1
12 5 17 2
13 6 8 1
14 6 27 1
15 6 28 1
16 7 20 2
17 8 10 ar
18 8 14 ar
19 9 15 1
20 9 29 1
21 10 11 ar
22 10 30 1
23 11 12 ar
24 12 13 ar
25 12 31 1
26 13 14 ar
27 13 45 1
28 14 32 1
29 15 16 1
30 15 33 1
31 16 17 1
32 16 34 1
33 16 35 1
34 18 19 1
35 18 36 1
36 18 37 1
37 19 38 1
38 19 39 1
39 19 43 1
40 20 21 1
41 20 43 1
42 21 40 1
43 21 41 1
44 21 42 1
45 43 44 1
46 45 46 1
47 45 47 1

```

@<TRIPOS>SUBSTRUCTURE

1 MOL 1 TEMP

0 **** * 0 ROOT

The parameter of b1 as mol2 format

@<TRIPOS>MOLECULE

MOL

52 52 1 0 0

SMALL

No Charge or Current Charge

@<TRIPOS>ATOM

1 N1	4.9800	1.9240	-0.7710 n	1 MOL	-0.7735593149
2 N2	-8.4180	-0.1710	-0.1660 nh	1 MOL	-0.8245462145
3 C1	-5.4510	1.9620	0.3360 ca	1 MOL	0.4240504678
4 C2	-4.4400	1.1600	-0.1860 ca	1 MOL	-0.4748541556

5 C3	-4.7590	-0.1020	-0.6930 ca	1 MOL	0.3098471496
6 C4	-6.0740	-0.5500	-0.6630 ca	1 MOL	-0.4583089583
7 C5	-7.0920	0.2620	-0.1370 ca	1 MOL	0.4131347603
8 C6	-6.7730	1.5230	0.3640 ca	1 MOL	-0.4582201004
9 C7	-3.6570	-0.9710	-1.2680 c3	1 MOL	-0.3342329353
10 C8	-2.5240	-1.1980	-0.2900 c2	1 MOL	0.1865661294
11 C9	-2.9290	-1.9070	0.9740 c3	1 MOL	-0.3150890094
12 C10	-1.2930	-0.7580	-0.5740 c2	1 MOL	-0.3877957619
13 C11	-0.0540	-0.8930	0.2650 c3	1 MOL	0.1179132449
14 C12	1.0980	-1.4620	-0.5560 c3	1 MOL	0.0718817552
15 C13	2.3280	-1.8470	0.2880 c3	1 MOL	0.0139369642
16 C14	2.6280	-0.8230	1.3930 c	1 MOL	0.3936465632
17 C15	4.2020	0.7370	-0.6170 c3	1 MOL	0.1717168258
18 C16	6.3300	2.0510	-0.5050 c	1 MOL	0.8256762289
19 C17	7.0850	0.7640	-0.2420 c3	1 MOL	-0.4409533963
20 C18	4.4970	-2.7130	-0.0530 c3	1 MOL	0.0528953273
21 O1	-5.2050	3.2000	0.8470 oh	1 MOL	-0.5734320775
22 O2	2.1120	-0.9590	2.4750 o	1 MOL	-0.4012333335
23 O3	6.8630	3.1400	-0.5170 o	1 MOL	-0.5732858731
24 O4	3.3810	-2.0520	-0.6180 os	1 MOL	-0.3345545018
25 O5	1.4580	-0.5000	-1.5280 oh	1 MOL	-0.5256553983
26 S1	3.7110	0.5860	1.1730 ss	1 MOL	-0.2052868019
27 H1	-3.2640	-0.5080	-2.1800 hc	1 MOL	0.1113475856
28 H2	-2.0950	-2.0950	1.6520 hc	1 MOL	0.0938292492
29 H3	-0.2130	-1.5200	1.1470 hc	1 MOL	0.0461526398
30 H4	4.7750	-0.1360	-0.9200 h2	1 MOL	0.0908941565
31 H5	8.1170	1.0260	-0.0180 hc	1 MOL	0.1191193354
32 H6	5.2270	-2.8450	-0.8530 h1	1 MOL	0.0503741824
33 H7	-4.0870	-1.9390	-1.5580 hc	1 MOL	0.1113475856
34 H8	-3.4010	-2.8680	0.7350 hc	1 MOL	0.0938292492
35 H9	0.2610	0.0930	0.6330 hc	1 MOL	0.0461526398
36 H10	3.2910	0.7970	-1.2090 h2	1 MOL	0.0908941565
37 H11	6.6520	0.2170	0.6030 hc	1 MOL	0.1191193354
38 H12	4.9450	-2.1200	0.7550 h1	1 MOL	0.0503741824
39 H13	-3.6780	-1.3140	1.5110 hc	1 MOL	0.0938292492
40 H14	7.0620	0.1110	-1.1210 hc	1 MOL	0.1191193354
41 H15	4.2100	-3.6960	0.3410 h1	1 MOL	0.0503741824
42 H16	-4.2590	3.3850	0.7730 ho	1 MOL	0.4230820401
43 H17	4.4950	2.8110	-0.8410 hn	1 MOL	0.4089088594
44 H18	2.1400	-0.9140	-2.0800 ho	1 MOL	0.3690755339
45 H19	-8.5300	-1.1760	-0.1730 hn	1 MOL	0.3587229380
46 H20	-9.0170	0.2650	0.5230 hn	1 MOL	0.3499171536
47 H21	-3.4070	1.5020	-0.1910 ha	1 MOL	0.1717147507
48 H22	-6.3220	-1.5310	-1.0600 ha	1 MOL	0.1867626483
49 H23	-7.5360	2.1770	0.7750 ha	1 MOL	0.2252209055
50 H24	-1.1370	-0.2470	-1.5240 ha	1 MOL	0.1624804221
51 H25	0.7680	-2.3860	-1.0550 h1	1 MOL	0.0678088023
52 H26	2.0990	-2.7700	0.8410 h1	1 MOL	0.0892912976

@<TRIPOS>BOND

1	1	17 1
2	1	18 1
3	1	43 1
4	2	7 1
5	2	45 1
6	2	46 1
7	3	4 ar
8	3	8 ar
9	3	21 1

10	4	5 ar
11	4	47 1
12	5	6 ar
13	5	9 1
14	6	7 ar
15	6	48 1
16	7	8 ar
17	8	49 1
18	9	10 1
19	9	27 1
20	9	33 1
21	10	11 1
22	10	12 2
23	11	28 1
24	11	34 1
25	11	39 1
26	12	13 1
27	12	50 1
28	13	14 1
29	13	29 1
30	13	35 1
31	14	15 1
32	14	25 1
33	14	51 1
34	15	16 1
35	15	24 1
36	15	52 1
37	16	22 2
38	16	26 1
39	17	26 1
40	17	30 1
41	17	36 1
42	18	19 1
43	18	23 2
44	19	31 1
45	19	37 1
46	19	40 1
47	20	24 1
48	20	32 1
49	20	38 1
50	20	41 1
51	21	42 1
52	25	44 1

@<TRIPOS>SUBSTRUCTURE

1 MOL

1 TEMP

0 **** *

0 ROOT

Coordinates of DH2-R(a1) system

C	47.27575000	37.90674400	50.31336200	H	49.97766000	45.74559300	45.11828700
C	46.10958000	38.57428200	49.57384700	H	49.40199700	45.11967300	46.66145800
C	46.22977800	38.37796400	48.10256800	N	46.36202400	41.62507700	45.49322600
C	45.50718100	37.63829500	47.19647200	C	45.44604000	40.77464300	44.76106600
N	47.29606900	38.88020200	47.37879500	C	45.09719200	41.39846000	43.40352400
C	47.17868800	38.43877900	46.10015300	O	45.02489000	42.61414800	43.23770200
N	46.10030700	37.68689000	45.95114900	C	44.21830700	40.70343500	45.67873300
H	47.29836600	36.83359300	50.09940600	C	44.28216100	42.01741100	46.45743800
H	45.15888900	38.14185100	49.90250400	C	45.77986100	42.23613200	46.68394400
H	46.07464200	39.64416700	49.82401800	H	45.89282600	39.79118200	44.59989100
H	48.01968100	39.51029600	47.72145400	H	43.29463100	40.59267800	45.11541200
H	44.61641400	37.05181200	47.37370100	H	44.32234800	39.84897500	46.34751600
H	47.88726100	38.68385600	45.32251300	H	43.89218000	42.82468100	45.83723100
C	50.85389700	34.04405200	49.09585900	H	43.72171200	41.98071100	47.38923000
C	50.33820300	34.04410200	47.66153900	H	46.02908200	43.29254300	46.75364200
C	49.15456100	34.99150700	47.43234100	H	46.13549000	41.70973900	47.57662500
C	48.89569200	35.14563900	45.93454200	C	44.41493700	40.80832500	41.09467700
C	47.88664600	34.49765500	48.12603100	H	45.11980600	40.41819800	40.35272500
H	50.10098400	33.66357100	49.78104500	H	43.42094500	40.39578500	40.88418400
H	51.15538200	34.34239300	46.99946900	C	44.40099200	45.64273000	40.59104500
H	50.04040700	33.03039200	47.38407400	C	45.32879600	44.78758500	39.73216600
H	49.41510300	35.97551900	47.83966500	C	46.49402200	44.17602300	40.52002300
H	48.65001500	34.17926400	45.49831800	C	47.19823000	43.10230500	39.69013000
H	48.06884500	35.82975300	45.76208100	C	47.50711500	45.23791600	40.94029700
H	49.77349300	35.53931400	45.42625300	H	44.90698100	46.53751200	40.94392300
H	47.62325000	33.50159700	47.77715300	H	44.74251500	43.97613300	39.29254100
H	48.01831100	34.45556500	49.20398400	H	45.72381700	45.38873600	38.90863000
H	47.05257600	35.16351200	47.91324500	H	46.08956200	43.70882700	41.42313100
C	51.33507100	40.09303700	46.60608600	H	47.68584700	43.54796700	38.82428200
C	50.05800400	40.93929400	46.74167400	H	47.95202900	42.59690100	40.28958100
O	49.29231000	40.76087100	47.68279300	H	46.48977300	42.35734500	39.33570400
C	51.06459500	38.78448100	45.84880500	H	47.04653100	45.98256100	41.58309100
C	50.77500300	39.04924300	44.37466700	H	48.32619200	44.77612400	41.48723600
C	52.26782100	37.85421600	45.99229100	H	47.91823700	45.74173300	40.06630800
H	52.11149700	40.66292400	46.09351900	C	50.44689000	39.75820300	34.05388800
H	50.19522100	38.29456500	46.30100700	C	51.89854900	39.81425200	33.48307300
H	49.89368500	39.67165200	44.24355100	O	52.17384000	39.21245400	32.46548900
H	51.61526800	39.54880700	43.89638700	C	50.41092100	38.56023300	35.05780900
H	50.60013500	38.10690100	43.85962300	C	49.23651300	38.61662500	36.00056000
H	53.16086300	38.32062600	45.58119500	N	48.05701200	38.21340900	35.53144400
H	52.45312000	37.61663900	47.03711100	O	49.34188100	38.99958500	37.16807500
H	52.09044700	36.92381500	45.45800400	H	50.21019400	40.68069800	34.58352700
N	49.82275900	41.89671600	45.81896200	H	50.43632000	37.62249700	34.50716400
C	48.55088400	42.65301800	45.72596900	H	51.31174000	38.62569800	35.67082600
C	47.58555100	41.75220900	44.98442900	H	47.27055700	38.26797100	36.16849100
O	47.93820500	41.13252300	43.98839300	C	54.23495500	40.65097200	33.86067300
C	48.79022100	43.95390900	44.94914300	C	55.16413800	40.27079300	35.04508800
C	47.48106600	44.70782100	44.72513700	O	56.01990400	39.42160100	34.90572100
C	49.79343700	44.83688600	45.68642800	C	54.56288400	42.04462600	33.33513300
H	50.36369200	41.88325400	44.96569900	H	54.42524700	39.91048700	33.07608800
H	48.22916100	42.84543900	46.74957600	H	53.93978100	42.26451000	32.47106000
H	49.19917700	43.67358200	43.97136200	H	54.39314000	42.80399400	34.09320500
H	46.74972600	44.09167100	44.20714600	N	55.00892400	40.96642000	36.19278000
H	47.06184200	45.03783600	45.67384700	C	55.86004000	40.78808900	37.37808800
H	47.66798000	45.59051100	44.11889900	C	54.90436100	40.89327900	38.57192100
H	50.73829400	44.31995000	45.83563000	O	54.11802900	41.83894100	38.63174600
				C	56.92502900	41.90103800	37.47361900

C	57.77312100	41.72796100	38.73142300	N	51.93856500	44.47786800	34.61355100
C	57.80723500	41.90765600	36.22928200	C	50.73096500	44.07797300	33.80906500
H	54.20714100	41.57276400	36.32450000	C	49.45940600	44.74383700	34.33528100
H	56.33670100	39.81130800	37.28505700	C	48.31092900	44.47509800	33.36576700
H	56.40202700	42.86124200	37.54147100	C	49.11791200	44.23355100	35.73270600
H	58.47756200	42.55248500	38.81168400	H	52.23990100	45.42705600	34.44987400
H	57.15843300	41.72418500	39.62875100	H	50.65629600	42.99277800	33.87769500
H	58.34324200	40.80188300	38.68310100	H	49.63082800	45.82554000	34.38610800
H	58.56932300	42.67801200	36.32010500	H	48.13344300	43.40572800	33.27602000
H	58.29589400	40.94434600	36.10486800	H	47.39876300	44.94527900	33.72376100
H	57.22267900	42.10601200	35.33446500	H	48.53607200	44.87067500	32.37816800
N	54.89692600	39.94926400	39.51042400	H	49.94771900	44.39289100	36.41707900
C	54.06315600	40.11996700	40.69710200	H	48.24511800	44.75159700	36.12266800
C	54.47196700	41.42356800	41.38776000	H	48.90103600	43.16789600	35.70395300
O	55.60634200	41.86174100	41.29579000	C	47.78503100	30.31789800	51.18505300
C	54.38924100	38.91015700	41.57366400	C	47.08972800	29.50998000	50.08774800
C	55.82569000	38.59335700	41.17181800	C	47.49981700	29.96882000	48.72900300
C	55.80183500	38.83882500	39.66361200	C	48.68730100	29.76949000	48.07338900
H	53.00986700	40.16173200	40.41362000	N	46.67721600	30.71509900	47.93569100
H	54.28358600	39.13999600	42.63203300	C	47.35169300	30.95540300	46.83703800
H	53.72748600	38.07851100	41.32758300	N	48.57694000	30.40517000	46.87212900
H	56.50493100	39.29943700	41.64967500	H	47.55816600	31.37679000	51.08048300
H	56.12749900	37.57913400	41.42330600	H	47.34222800	28.45341400	50.20470500
H	56.79347700	39.06965100	39.27808700	H	46.00735300	29.61464900	50.17978300
H	55.40581000	37.96483700	39.14395600	H	49.56967600	29.23789000	48.36227200
N	53.50138200	41.96924600	42.12201500	H	46.98106000	31.52020600	46.00641800
C	53.69895800	43.24114000	42.76982700	H	49.25191800	30.43931300	46.11024800
C	52.84419700	44.33161100	42.11698300	C	44.59753800	36.04161000	52.89443300
C	53.31958700	45.75321000	42.43102800	C	43.65299500	36.07215200	51.69901100
C	52.47309500	46.75806000	41.65182900	C	43.95025900	35.05704800	50.62329400
C	53.25703800	46.05637800	43.92541700	C	43.43161200	35.25092900	49.34675600
H	52.53977900	41.63849100	42.02237200	C	44.68449300	33.90228500	50.85440800
H	54.75877300	43.49004600	42.67386800	C	43.60339700	34.31834300	48.34289500
H	52.88690600	44.18857000	41.03527600	C	44.87101400	32.96394800	49.85706000
H	51.80347900	44.21298700	42.42877300	C	44.31479200	33.14744800	48.59670300
H	54.35803600	45.85148600	42.09792500	O	44.42800500	32.21882600	47.62175300
H	52.55241700	46.57394400	40.58298500	H	45.63188700	36.11394100	52.56593300
H	51.42628100	46.68362400	41.94158400	H	42.62942500	35.91033900	52.05653900
H	52.81411400	47.77151500	41.84617600	H	43.67370300	37.07050900	51.25242500
H	53.92420400	45.40630900	44.48496000	H	42.86782900	36.15163100	49.14093800
H	53.55605400	47.08520800	44.11051700	H	45.11449300	33.71598200	51.82603700
H	52.24457300	45.92162700	44.29884800	H	43.19189100	34.47947100	47.35779400
C	53.83084400	44.39212600	36.32308800	H	45.44385900	32.06992100	50.05046900
C	52.60160900	43.77215800	35.57182000	H	45.13808900	31.56831100	47.85911400
O	52.24868200	42.64153700	35.88133300	C	40.57810100	38.99770000	46.50977500
C	53.33301400	44.83802700	37.72102100	C	41.58432300	37.91256300	46.92840900
C	54.45470600	45.28509300	38.58888200	C	41.97464800	36.97171300	45.80212500
C	55.04952600	46.50176500	38.79513700	O	41.69253700	35.78462800	45.78527100
N	55.13573000	44.41206500	39.39189000	O	42.66902500	37.58943400	44.83948300
C	56.08576600	45.12264600	40.03333900	H	40.98132900	39.61312600	45.70056800
N	56.05967800	46.38431600	39.69637100	H	42.50029000	38.38904200	47.29819100
H	54.57758200	43.61293600	36.44125000	H	41.16716700	37.29704100	47.72986400
H	52.60943600	45.64856600	37.60493200	H	42.93927200	36.93750700	44.13469300
H	52.84192000	43.98214800	38.18499000	C	38.54603100	33.27302800	42.34804200
H	54.93582300	43.42403800	39.47045600	C	38.81998100	31.93062300	43.08548700
H	54.80919900	47.45114600	38.35896500	O	38.21263300	30.93022000	42.74477800
H	56.76935100	44.68364000	40.73154600	C	39.62065000	34.34113400	42.49230100

C	39.29213100	35.65144600	41.76333800	C	48.97838400	34.46064200	39.99926600
C	40.28410000	36.73042100	42.19801400	H	46.15969100	32.57944100	40.73146700
C	39.33124800	35.48560700	40.24650000	H	47.23571800	34.67545300	41.22302400
H	38.38973300	33.00497200	41.30622500	H	47.80902700	32.75850200	42.76304800
H	39.75461800	34.58467500	43.54964400	H	49.30333100	32.53723100	41.85243500
H	40.56271100	33.95083200	42.10333900	H	49.03044100	34.04194800	42.74259100
H	38.28388400	35.96943900	42.05302000	H	49.60479600	35.14949100	40.56332800
H	41.30260200	36.42053800	41.97527000	H	49.60591400	33.67289900	39.58983900
H	40.08562200	37.66697100	41.68164900	H	48.53523900	35.00143200	39.16570500
H	40.20947200	36.90957700	43.26822300	N	45.83848700	34.18887800	38.45170900
H	40.29577900	35.09361300	39.93143900	C	45.51397200	34.62196600	37.09600100
H	38.55461400	34.80571300	39.90821100	C	44.79125500	35.95206300	37.21637000
H	39.17297100	36.44441200	39.75730000	C	44.09010000	35.79856000	38.55722200
N	39.71464800	31.90017000	44.10356800	C	45.16023400	35.06781300	39.35506500
C	40.01595000	30.72396300	44.93999600	H	44.86762900	33.86684600	36.62964100
C	39.73196000	30.99499900	46.41315800	H	45.49918600	36.77881400	37.26580400
C	40.75827300	31.92577800	47.05319000	H	44.10682300	36.11722600	36.38754000
C	40.39320400	32.18483700	48.52518800	H	43.82463900	36.74818600	39.01645800
N	40.59553900	33.45400000	48.95626700	H	43.18679800	35.19603900	38.45546200
O	39.93016400	31.31781600	49.23805100	H	45.86163000	35.80980100	39.76381300
H	40.20804900	32.74312700	44.34807700	H	44.74367500	34.51160700	40.19843600
H	41.06498000	30.45382400	44.78895900	C	40.54998600	33.82397000	32.70503600
H	38.73587200	31.43127100	46.50831300	C	40.25116800	34.08718800	34.17670500
H	39.72991600	30.05256600	46.96196800	C	41.34049000	33.58845000	35.13373300
H	41.75026800	31.46824400	47.04180300	C	41.08502600	34.14405600	36.53399700
H	40.81264100	32.87961700	46.52605500	C	41.40097800	32.06319700	35.19221900
H	41.07790600	34.10047100	48.35067000	H	41.50436800	34.26493000	32.42398000
C	39.22705300	28.08700800	40.23201100	H	40.13381400	35.16448300	34.31969500
C	40.02958400	26.78338200	40.42025300	H	39.30243700	33.61607400	34.44346300
O	40.40958300	26.12616900	39.46774000	H	42.30945500	33.95981600	34.77863800
C	40.11384500	29.27669800	39.82707900	H	41.17049700	35.22888400	36.54454200
C	39.20407800	30.48926500	39.59973700	H	40.08436400	33.87845300	36.86649000
C	40.93522800	28.96556000	38.57881300	H	41.79505300	33.72608500	37.24301700
C	39.97343500	31.77436900	39.32590000	H	40.44858600	31.66568000	35.53854400
H	38.51094200	27.89240500	39.43237000	H	41.62107700	31.64277100	34.21452000
H	40.79839500	29.50247800	40.65242400	H	42.18137800	31.74857600	35.88246100
H	38.53886200	30.27784100	38.75799700	C	45.94599300	30.63600200	35.28699700
H	38.58396500	30.62471000	40.48730200	C	45.98839500	30.06215700	36.69832200
H	40.27274200	28.87203800	37.71925500	O	44.73284300	30.10606100	37.34935500
H	41.65788700	29.75649600	38.39936900	H	45.65250000	31.68196900	35.32082500
H	41.46789900	28.02708800	38.70353100	H	46.34945800	29.02477100	36.66739600
H	40.60705800	32.02152400	40.17334000	H	46.66879900	30.65864900	37.30806700
H	40.60442900	31.68030100	38.44775100	H	44.09645800	29.60943500	36.79959700
H	39.28094500	32.59534900	39.15468500	C	55.42102900	35.46311000	36.33819400
N	40.29078700	26.38930900	41.69437900	C	54.69065800	36.43089800	37.25619400
C	41.06010700	25.19097000	42.06391700	C	53.17242700	36.50314600	37.05924700
C	42.29213800	25.57162800	42.87280200	C	52.48921300	35.17435200	37.37254200
H	39.97828700	26.97236300	42.45526600	C	52.59832800	37.60357500	37.95468800
H	41.33883600	24.71128400	41.12450900	H	55.11917900	34.43483700	36.52159200
H	42.90623300	26.27377700	42.31402700	H	54.89417500	36.14609500	38.29316600
H	42.00117200	26.03286900	43.81506800	H	55.09927200	37.42737000	37.07228400
H	42.88196500	24.68522400	43.09001200	H	52.97745700	36.76060500	36.01243100
C	47.07606200	32.79494200	40.17998900	H	51.40909600	35.27313700	37.28668600
C	46.74912900	33.21653700	38.72242500	H	52.81219200	34.39791700	36.68537700
O	47.32008300	32.66018100	37.79818000	H	52.72227300	34.85728200	38.38744600
C	47.90280900	33.86714700	40.90800800	H	51.52184800	37.69045400	37.82786400
C	48.55074300	33.26369500	42.15135800	H	52.79312100	37.37419400	39.00126600

H	53.04951500	38.56744200	37.72464500	O	49.73272500	30.76555600	44.35897700
C	44.27976100	34.25492800	44.21441100	H	48.86567300	30.66606600	43.91665600
N	49.80347400	39.94540600	39.85597600	H	50.10095700	31.59054300	44.03951800
O	44.05473900	28.82159400	42.47894400	O	46.59820000	29.17560700	41.06080000
S	48.13537300	37.45547300	42.63407800	H	46.46425800	29.55444100	40.18822900
C	45.38868600	33.33289000	44.72517000	H	45.74145600	28.82688000	41.34089400
N	43.30222900	32.06636000	39.06642700	H	46.93117000	30.56639700	34.83699700
O	45.66060100	37.56836700	41.65523600	H	45.23240100	30.08566700	34.67543500
C	43.00244600	33.45954000	43.83843900	H	40.41368900	24.51888200	42.63593800
O	50.92038000	41.00187200	41.52364800	H	38.68511100	28.33905600	41.14364100
C	43.19989400	32.40572000	42.77073200	H	40.34842800	39.64975900	47.35805000
O	43.65564600	36.05826800	42.75183400	H	39.64036500	38.54997900	46.16362200
C	43.49673500	31.08881300	43.14559000	H	46.42979700	34.67408600	36.49900300
C	43.72643400	30.12654000	42.16178800	H	44.38586900	36.88007500	53.55494400
C	43.67371600	30.44622900	40.80938000	H	44.47508400	35.12579400	53.46684700
C	43.38527600	31.76172600	40.41929300	H	51.73611700	33.41331300	49.17916300
C	43.13100500	32.73141500	41.41214100	H	51.12280600	35.05210400	49.40485800
C	44.74188300	35.15773600	43.06647800	H	48.23431500	38.33432100	49.99909400
C	46.00483100	35.94251400	43.42329600	H	47.18789100	38.04570300	51.39671600
C	46.42251900	37.00708300	42.44624700	H	44.06588600	45.07438800	41.45569000
C	48.31064000	38.93437600	41.56226000	H	43.52975300	45.95068600	40.01692200
C	49.53608200	38.76114600	40.65405100	H	55.22012700	35.70546200	35.29733000
C	50.53555900	40.97413600	40.34452100	H	56.49340500	35.53735800	36.50114400
C	50.88506700	42.06634200	39.35938000	H	40.59011600	32.75816100	32.49605600
H	43.98722300	34.91751600	45.03673600	H	39.77412700	34.26084900	32.08066400
H	43.94649800	28.70722400	43.43554400	H	47.45355400	29.98699100	52.16645700
H	44.98286500	32.69612400	45.51784400	H	48.86359600	30.19268100	51.12156500
H	45.77799700	32.68370900	43.93306800	H	37.59389200	33.63748300	42.74291500
H	46.21530600	33.90110200	45.16021700	H	49.76825100	39.60597200	33.22046800
H	42.23855500	34.17936700	43.53985600	H	50.93331700	44.36829000	32.77835400
H	42.65419700	32.97942700	44.75938200	H	39.37664100	29.92264100	44.56545200
H	44.03482200	36.71598000	42.13464100	H	51.66545000	39.86544600	47.61982300
H	43.57033100	30.82814500	44.19904700	H	53.45279900	43.14295700	43.83191900
H	43.83888800	29.67981400	40.05855600	H	47.66410500	31.88303900	40.08883100
H	42.86502100	33.74603700	41.12264900	H	44.37681200	41.89529100	41.02050700
H	44.93696300	34.53174500	42.18820600	H	55.60568300	42.07940200	33.02928600
H	46.84357900	35.26216700	43.59256200	N	44.84090500	40.47224700	42.44096000
H	45.85744400	36.48638000	44.37485400	H	44.96477400	39.49419900	42.66557100
H	48.43039100	39.80788800	42.20704200	N	52.80966700	40.50809100	34.21064300
H	47.38065000	39.04088500	40.99989100	H	52.47853200	41.09654200	34.96863500
H	50.41717800	38.55392300	41.26902200	H	54.25159400	45.23576900	35.77585200
H	49.39177100	37.91900600	39.97108700	C	47.80890600	37.74860800	34.19929900
H	50.32396700	41.99422400	38.42379300	H	46.85451600	37.22422200	34.18287200
H	50.69881300	43.04121900	39.81854600	H	47.75286900	38.57471500	33.48609500
H	51.95472400	42.00438200	39.11935500	H	48.58011100	37.05500100	33.86640800
H	49.62842700	39.89749300	38.85892900	C	40.38708700	33.88855300	50.33041600
H	43.48911100	33.03265100	38.83754200	H	41.34324200	34.09486900	50.81281700
H	43.82198600	31.43454000	38.46013300	H	39.76456000	34.78330300	50.34468000
O	47.19295400	30.50760600	43.35666600	H	39.88187200	33.07909500	50.85344000
H	47.10135400	30.09859400	42.47221300				
H	46.76448400	29.90447600	43.96701600				
O	46.79822500	38.48325600	38.18798600				
H	47.73109900	38.74333200	38.08199700				
H	46.67382600	38.20702900	39.09827900				
O	42.78827100	28.67038900	35.91566700				
H	42.00280000	29.21415900	35.81587100				
H	42.52971200	27.90610600	36.43799200				

Coordinates of DH2-TS_{1a} system

C	47.27575000	37.90673000	50.31333800
C	46.06890100	38.24991700	49.42283200
C	46.30106200	38.00472900	47.96605000
C	45.65655300	37.19160500	47.06765800
N	47.31189500	38.62473500	47.24074600

C 47.27136500 38.19688000 45.96838600
N 46.27184700 37.32910800 45.83985000
H 47.54268900 36.85034400 50.21120600
H 45.20717900 37.64372000 49.71916400
H 45.78575800 39.30002500 49.57920900
H 47.98410200 39.32510300 47.57783400
H 44.82347400 36.52112500 47.21556800
H 47.93962500 38.49746000 45.17468200
C 50.85399000 34.04400000 49.09599600
C 50.50400200 33.95660300 47.61719200
C 49.35149500 34.87924900 47.20752500
C 49.21257800 34.87179100 45.68714700
C 48.03596800 34.45952600 47.86096100
H 50.04028300 33.67338800 49.71382400
H 51.38775700 34.22420300 47.03280600
H 50.24112100 32.92676400 47.36693900
H 49.59507000 35.89937900 47.52982600
H 48.92154300 33.88100000 45.34585800
H 48.46362700 35.58772300 45.35900100
H 50.15511300 35.13614900 45.21290300
H 47.81525700 33.41860600 47.63728000
H 48.07881100 34.57228800 48.94095200
H 47.21142600 35.06665900 47.49450200
C 51.33507200 40.09306100 46.60609100
C 50.01588100 40.87799100 46.69089400
O 49.16103500 40.57575000 47.52391900
C 51.13732500 38.78764700 45.81973200
C 50.83828100 39.07253900 44.35177900
C 52.38304800 37.91412800 45.94894600
H 52.10684800 40.69932500 46.13146000
H 50.29126900 38.24652800 46.25887000
H 49.95087900 39.68883800 44.23285500
H 51.67060200 39.58911600 43.87855600
H 50.66949700 38.13883000 43.82083100
H 53.25337600 38.43048300 45.54972500
H 52.57825700 37.66346100 46.98916800
H 52.24896700 36.98925500 45.39364800
N 49.83305200 41.91651200 45.85350100
C 48.55090000 42.65303800 45.72594700
C 47.59950400 41.71983900 45.00995500
O 47.97058700 41.05206500 44.05571400
C 48.77769100 43.93158100 44.91002700
C 47.46128300 44.66784300 44.66914400
C 49.77118900 44.84888500 45.61895000
H 50.45330000 42.00345700 45.06100000
H 48.21659000 42.87746200 46.73975700
H 49.18709700 43.62656100 43.94003500
H 46.73242400 44.03589300 44.16722700
H 47.04084900 45.01810600 45.61007700
H 47.64097200 45.53673100 44.04161900
H 50.72426300 44.35268200 45.78508500
H 49.94295100 45.74058500 45.02097400
H 49.37586800 45.15919100 46.58411500
N 46.36082500 41.62696700 45.49270900
C 45.44602200 40.77464000 44.76108200
C 45.05844900 41.39764200 43.40850500
O 44.90524100 42.61179900 43.27573900

C 44.23759600 40.66961900 45.69957500
C 44.28403900 41.98673300 46.47433600
C 45.77986300 42.23612600 46.68395400
H 45.91330400 39.80340700 44.57596900
H 43.30826700 40.53558300 45.15209900
H 44.36873400 39.81969000 46.37059500
H 43.87424800 42.78205500 45.85224400
H 43.73194100 41.94550300 47.41096900
H 46.00531800 43.29883500 46.74203400
H 46.15885800 41.72720400 47.57784200
C 44.41494300 40.80832300 41.09466800
H 45.21028300 40.62891500 40.36269100
H 43.54626100 40.20019900 40.82028900
C 44.40098600 45.64273700 40.59103800
C 45.29724600 44.78447600 39.70246100
C 46.46055500 44.13316900 40.46014900
C 47.14567000 43.08171300 39.58725800
C 47.49021400 45.16757900 40.90801200
H 44.92773500 46.52512500 40.94501900
H 44.68795600 43.99306100 39.25823600
H 45.69256900 45.39228700 38.88400000
H 46.05514900 43.64034200 41.34935600
H 47.63756900 43.55359500 38.73797300
H 47.89402300 42.54120000 40.16253900
H 46.42419500 42.36355400 39.20495300
H 47.04431000 45.89497600 41.58024900
H 48.30896000 44.67703900 41.43008000
H 47.89915800 45.69637200 40.04796500
C 50.44689000 39.75820200 34.05388700
C 51.89711700 39.81781300 33.48119300
O 52.17141900 39.22591400 32.45740600
C 50.41092100 38.56023300 35.05781000
C 49.23481200 38.62487200 35.99925400
N 48.05566100 38.21821300 35.53070200
O 49.34006300 39.02179800 37.16080100
H 50.20965400 40.68017400 34.58434100
H 50.43338800 37.62184900 34.50840300
H 51.31134700 38.62452700 35.67128100
H 47.27080300 38.27001700 36.17019600
C 54.23495400 40.65097200 33.86067300
C 55.16749900 40.27460600 35.04341300
O 56.03025700 39.43296500 34.90084100
C 54.55955800 42.04500500 33.33348800
H 54.42547900 39.91057400 33.07607700
H 53.93431900 42.26300600 32.47048800
H 54.38968400 42.80447400 34.09145400
N 55.00829800 40.96598600 36.19328000
C 55.86004500 40.78809000 37.37809000
C 54.90627400 40.89457800 38.57335900
O 54.12347800 41.84319200 38.63526200
C 56.92493100 41.90126200 37.47352000
C 57.77140300 41.72965700 38.73271300
C 57.80885600 41.90722900 36.23043800
H 54.20292400 41.56721500 36.32675300
H 56.33695300 39.81135100 37.28552000
H 56.40161000 42.86143700 37.53974100
H 58.47486500 42.55500100 38.81378800

H	57.15566100	41.72508800	39.62940600	H	50.65390900	42.99325000	33.88222100
H	58.34255200	40.80415400	38.68542800	H	49.63294300	45.83038600	34.37569500
H	58.57096900	42.67757300	36.32181100	H	48.13258100	43.40582200	33.28005000
H	58.29735700	40.94373200	36.10700000	H	47.40011400	44.94938500	33.71712300
H	57.22536900	42.10513800	35.33485200	H	48.53807000	44.86406300	32.37256500
N	54.89927600	39.95131400	39.51206900	H	49.94667600	44.40989100	36.41535900
C	54.06315000	40.11997100	40.69708600	H	48.24424500	44.76699100	36.11705400
C	54.47358900	41.41988500	41.39364300	H	48.90060400	43.18078800	35.70852300
O	55.61241700	41.85001600	41.31580300	C	47.78503000	30.31789900	51.18505900
C	54.38308100	38.90572800	41.56949900	C	47.11166800	29.50306700	50.07962700
C	55.81984500	38.58652800	41.17074200	C	47.53043300	29.96919300	48.72612500
C	55.80183200	38.83882100	39.66361900	C	48.72739000	29.78876800	48.08234600
H	53.01047500	40.16646600	40.41131800	N	46.70450300	30.70341200	47.92504100
H	54.27474800	39.13142100	42.62853000	C	47.38563300	30.95350600	46.83199600
H	53.71918100	38.07757000	41.31816900	N	48.61872400	30.42251700	46.88003500
H	56.49968700	39.28848500	41.65396100	H	47.55024600	31.37492500	51.07844500
H	56.11778500	37.57018600	41.41843000	H	47.37631200	28.44975900	50.19812300
H	56.79518200	39.07016900	39.28252900	H	46.02702300	29.59345300	50.15995000
H	55.40647300	37.96773100	39.13862900	H	49.61494100	29.27084000	48.38004400
N	53.49867400	41.97180300	42.11801400	H	47.01302200	31.50740000	45.99504400
C	53.69895500	43.24114000	42.76982500	H	49.30176300	30.47169100	46.12555100
C	52.84890900	44.33698900	42.12000100	C	44.59753900	36.04161000	52.89443300
C	53.33153800	45.75579800	42.43565800	C	43.63280700	36.03718600	51.71500400
C	52.48970900	46.76621100	41.65868100	C	43.95075200	35.02993200	50.63750300
C	53.27305700	46.05819400	43.93049500	C	43.43168900	35.21380100	49.35962100
H	52.53379300	41.65142800	42.00136800	C	44.69848600	33.88406100	50.87238200
H	54.75980800	43.48727100	42.67640800	C	43.61043600	34.27609800	48.36165800
H	52.89043500	44.19547900	41.03822000	C	44.89699100	32.94436600	49.87897500
H	51.80752100	44.22247700	42.43124900	C	44.33399000	33.11285200	48.61877200
H	54.37006000	45.84912200	42.10159300	O	44.45089000	32.18423000	47.64898500
H	52.56855700	46.58380500	40.58959900	H	45.62506600	36.13678200	52.55000700
H	51.44236100	46.69585500	41.94774700	H	42.62349300	35.83518500	52.09132800
H	52.83528700	47.77775400	41.85508300	H	43.60433300	37.03617100	51.26921700
H	53.93390600	45.40060800	44.48885600	H	42.85666200	36.10622900	49.14699700
H	53.58314600	47.08365500	44.11616500	H	45.12743000	33.70504500	51.84576300
H	52.25936300	45.93440700	44.30469600	H	43.18312000	34.42186600	47.38118900
C	53.83084400	44.39212600	36.32308800	H	45.47766900	32.05670200	50.07698900
C	52.60127800	43.77223300	35.57188000	H	45.17039800	31.53705400	47.87649200
O	52.24863200	42.64203200	35.88155300	C	40.57809100	38.99771100	46.50978300
C	53.33301400	44.83802800	37.72102100	C	41.62760800	38.01187500	47.04879800
C	54.45410200	45.28308100	38.59067600	C	42.09913200	37.03768700	45.98455300
C	55.04895200	46.49889200	38.80195900	O	41.79696600	35.85519400	45.97761000
N	55.13305300	44.40737900	39.39230000	O	42.86500700	37.63055300	45.06562100
C	56.08236600	45.11517000	40.03754800	H	40.98100900	39.57700900	45.67426500
N	56.05747800	46.37814600	39.70478300	H	42.49635500	38.56766900	47.42174600
H	54.57701400	43.61233400	36.44106100	H	41.20960100	37.42499100	47.87111000
H	52.61042200	45.64951000	37.60478600	H	43.12101700	36.99234100	44.32807700
H	52.84050900	43.98263300	38.18400700	C	38.54600700	33.27302200	42.34803200
H	54.93145700	43.41900000	39.46523500	C	38.78130300	31.94118900	43.11785400
H	54.81000000	47.44978600	38.36826400	O	38.11795700	30.96031000	42.82771100
H	56.76464200	44.67347600	40.73539800	C	39.57095000	34.36505800	42.62472600
N	51.93837100	44.47826700	34.61345700	C	39.32218600	35.67324600	41.86209800
C	50.73096500	44.07797300	33.80906500	C	40.24804100	36.75845000	42.41324200
C	49.46019200	44.74851900	34.33102300	C	39.55154000	35.50748400	40.36236500
C	48.31174500	44.47543700	33.36268800	H	38.53157400	33.00155200	41.29561900
C	49.11747200	44.24654400	35.73113300	H	39.56524800	34.60387900	43.69205500
H	52.24006700	45.42724600	34.44930700	H	40.56157000	33.99417000	42.35565500

H 38.28359700 35.98373500 42.02564500
H 41.28940200 36.46801400 42.29170600
H 40.08996500 37.70025500 41.89239900
H 40.06266000 36.91995900 43.47322900
H 40.55599500 35.13577200 40.17266700
H 38.83976100 34.81027700 39.93096000
H 39.43761600 36.46287900 39.85462800
N 39.71667700 31.89579800 44.09893200
C 40.01596200 30.72397300 44.93999900
C 39.73115100 30.99512900 46.41468900
C 40.75827000 31.92576800 47.05318900
C 40.41730700 32.17721000 48.53118500
N 40.57688200 33.45663000 48.95258400
O 40.01445600 31.29509000 49.26161900
H 40.26842000 32.71597700 44.28861300
H 41.06415000 30.45287800 44.78823400
H 38.73499000 31.43144700 46.50862000
H 39.72990500 30.05216300 46.96271600
H 41.75120300 31.47057800 47.02703700
H 40.80161200 32.88121800 46.52801200
H 40.99484300 34.12620700 48.32492500
C 39.22703300 28.08699900 40.23201900
C 40.15164600 26.86684800 40.43110000
O 40.74631600 26.34922900 39.50166800
C 39.95239000 29.34910500 39.73513500
C 38.90739000 30.46214400 39.58479600
C 40.68694500 29.10241700 38.41959600
C 39.48864000 31.76374100 39.04622900
H 38.49326400 27.78706500 39.48058700
H 40.68311300 29.65401500 40.49255700
H 38.12050100 30.11843300 38.90763000
H 38.44829900 30.63996900 40.55858300
H 39.96610600 28.99542000 37.60914200
H 41.35721900 29.93102700 38.20727000
H 41.26445700 28.18583000 38.49365600
H 40.32604800 32.09253100 39.65634800
H 39.83762700 31.63868200 38.02472300
H 38.72527300 32.53950600 39.03813500
N 40.24397600 26.35617000 41.68707300
C 41.06010800 25.19097000 42.06391800
C 42.17317300 25.59781500 43.01985600
H 39.77438700 26.83301400 42.44118300
H 41.46987400 24.79637200 41.13306000
H 42.79181300 26.36868700 42.56672500
H 41.75648400 25.98416100 43.94835100
H 42.79640600 24.73822900 43.25134700
C 47.07606100 32.79493700 40.18000200
C 46.76180600 33.23207400 38.72448900
O 47.34672500 32.68472800 37.80124200
C 47.89813000 33.85218500 40.93348000
C 48.56071200 33.21439200 42.15163200
C 48.96269800 34.48195800 40.03710800
H 46.15255500 32.57696200 40.71960300
H 47.22904400 34.64340200 41.28237600
H 47.82290400 32.70577600 42.76592400
H 49.30355000 32.48831900 41.82654200
H 49.05254600 33.97979600 42.74848100
H 49.57135100 35.17379900 40.61620600
H 49.60714800 33.71491100 39.61389300
H 48.50887900 35.02977200 39.21401700
N 45.84531000 34.19489000 38.45286300
C 45.51401000 34.62197900 37.09603100
C 44.76574300 35.93772000 37.21845700
C 44.06798900 35.76623800 38.55861600
C 45.16014000 35.06783900 39.35493500
H 44.89072800 33.85097300 36.62924200
H 45.45805100 36.77755000 37.27209200
H 44.08056900 36.09472700 36.38782900
H 43.77231700 36.70638400 39.01884300
H 43.18416200 35.13383700 38.45446900
H 45.84815400 35.82673400 39.75520900
H 44.76299300 34.51187500 40.20998700
C 40.54998700 33.82397300 32.70503700
C 40.79090100 33.68880600 34.20363800
C 41.90001400 32.69207200 34.56075600
C 42.25363500 32.82011900 36.04058100
C 41.49471300 31.25378500 34.24966600
H 41.47119300 34.09707200 32.19392100
H 41.06352400 34.67028900 34.60084100
H 39.86427000 33.38292700 34.69492500
H 42.78870600 32.93869600 33.96773200
H 42.54917800 33.84135400 36.27111800
H 41.39505000 32.57060100 36.65941900
H 43.06717000 32.14808300 36.29998300
H 40.59049200 30.99177300 34.79631100
H 41.30610400 31.11912200 33.18815600
H 42.28705800 30.56899100 34.54091400
C 45.94600900 30.63599100 35.28696900
C 45.81044400 30.19448100 36.74069400
O 44.49648300 30.33827100 37.24685300
H 45.67670300 31.68461700 35.19147300
H 46.13287700 29.14893600 36.84245500
H 46.44805100 30.82381800 37.36213800
H 43.91763800 29.73652900 36.74076700
C 55.42102900 35.46311000 36.33819300
C 54.69031800 36.43183400 37.25497600
C 53.17171200 36.50182500 37.05949900
C 52.49053900 35.17276000 37.37572800
C 52.59732600 37.60264600 37.95407900
H 55.11991200 34.43503700 36.52387100
H 54.89500700 36.14893800 38.29227600
H 55.09778900 37.42854400 37.06913700
H 52.97526600 36.75754300 36.01246000
H 51.41025400 35.27086400 37.29318900
H 52.81189500 34.39565400 36.68840800
H 52.72619500 34.85708300 38.39044300
H 51.52080700 37.68850600 37.82783700
H 52.79187900 37.37392600 39.00079000
H 53.04766800 38.56691500 37.72333600
C 44.33938000 34.34567100 44.36091000
N 49.79485600 39.99477700 39.84511200
O 43.95081100 28.90894500 42.71460500
S 48.22334700 37.40725000 42.58104800
C 45.45178800 33.39194400 44.79927200

N	43.03275300	32.09731200	39.28967200	H	46.97533700	30.51121000	34.96702600
O	45.64574000	37.72167500	41.85439800	H	45.29572800	30.04303400	34.64511800
C	43.02725500	33.58141100	44.04162900	H	40.40826900	24.44183600	42.52175800
O	50.92545300	41.04820300	41.50704600	H	38.70400900	28.32053600	41.15978900
C	43.15683500	32.50927900	42.98146900	H	40.26572400	39.69330400	47.29489500
O	43.69070100	36.19666800	42.95414700	H	39.68896700	38.46399600	46.15769900
C	43.45246200	31.19414400	43.36541500	H	46.43136400	34.69786600	36.50314400
C	43.61961400	30.21190700	42.38937000	H	44.37467400	36.87891300	53.55263800
C	43.49238300	30.50519900	41.03594400	H	44.50806900	35.12783800	53.47559800
C	43.19932300	31.81816500	40.63677000	H	51.73704800	33.44611900	49.30995700
C	43.02366900	32.81187300	41.62296500	H	51.06249400	35.07381900	49.37986200
C	44.76585400	35.25220400	43.20306500	H	48.15207600	38.50708800	50.04272000
C	46.07495100	35.98361700	43.43911500	H	47.04276100	38.10962100	51.36301900
C	46.42651600	37.02890000	42.55796000	H	44.07409300	45.06819400	41.45482400
C	48.34293000	38.92993100	41.56973000	H	43.52343700	45.97175700	40.03863700
C	49.54881100	38.79506500	40.63113700	H	55.21880500	35.70313100	35.29701600
C	50.52899800	41.02027600	40.33045200	H	56.49360500	35.53844700	36.49997400
C	50.87396100	42.11520600	39.34569100	H	40.18561300	32.89244200	32.28020500
H	44.10065700	34.99984500	45.20821900	H	39.80859100	34.59588600	32.51011200
H	43.91381400	28.82309500	43.67962200	H	47.44493700	29.98376400	52.16244900
H	45.07343300	32.74248600	45.59464800	H	48.86547400	30.20290100	51.13507400
H	45.79020100	32.75583000	43.97435200	H	37.54190600	33.60480800	42.62111200
H	46.31220800	33.93525700	45.19853700	H	49.76763900	39.60607900	33.22093100
H	42.27160100	34.31899200	43.76357700	H	50.93508000	44.36348200	32.77730300
H	42.69902300	33.11909200	44.97896500	H	39.37460400	29.92197200	44.57008500
H	44.10303500	36.88551200	42.38194900	H	51.63394300	39.86302200	47.62914200
H	43.58001100	30.95234800	44.41811100	H	53.45195000	43.14031800	43.83190300
H	43.59708900	29.71896500	40.29426200	H	47.66228200	31.88195200	40.08108800
H	42.78062800	33.82979200	41.32534600	H	44.14337400	41.86426700	41.07545200
H	44.85093000	34.62276100	42.30496600	H	55.60177200	42.08152000	33.02575400
H	46.90516700	35.33072800	43.70115300	N	44.85557900	40.47515300	42.43714100
H	46.06648700	36.77451000	44.83159400	H	45.12769500	39.50693300	42.58711000
H	48.46491000	39.79791300	42.21943400	N	52.81056100	40.50528700	34.21285800
H	47.39731200	39.02774600	41.03064800	H	52.48004300	41.08790100	34.97531200
H	50.44574100	38.58509600	41.22192500	H	54.25207000	45.23553700	35.77576800
H	49.39995100	37.96373200	39.93634500	C	47.80890600	37.74860800	34.19929900
H	50.30841100	42.04665700	38.41244600	H	46.84927600	37.23404100	34.18162600
H	50.69359900	43.09012700	39.80747200	H	47.76465300	38.57165200	33.48178700
H	51.94208200	42.04836900	39.10086600	H	48.57410300	37.04475100	33.87365900
H	49.61207800	39.95298000	38.84944600	C	40.38708700	33.88855600	50.33041700
H	43.14798900	33.06541800	39.02565900	H	41.34654700	34.13193800	50.78799100
H	43.51523400	31.47381300	38.64875200	H	39.73082800	34.75847800	50.35885800
O	47.24131500	30.41664500	43.49764000	H	39.92706600	33.06171600	50.86786600
H	47.08167800	30.05117500	42.60367700				
H	46.89187400	29.76443900	44.10785000				
O	46.77929800	38.49141200	38.18556200				
H	47.71313100	38.75029300	38.10010100				
H	46.63082100	38.24857800	39.10260700				
O	42.82700300	28.42970200	36.02751100				
H	41.92392800	28.70544200	36.20943100				
H	42.94646900	27.58769500	36.47406200				
O	49.79867300	30.80897200	44.38935500				
H	48.92710700	30.66823300	43.96696600				
H	50.14085000	31.62536000	44.02180000				
O	46.44877700	29.18967300	41.20947900				
H	46.30895900	29.63089700	40.36800000				
H	45.57962500	28.89724900	41.51586300				

Coordinates of DH2-IM1_a system

C	39.95266300	33.05301900	50.87560800
C	39.71041100	34.74266300	50.36331900
C	41.34550100	34.15657000	50.77670500
C	40.38708100	33.88856600	50.33043200
N	48.56076300	37.02118500	33.89442800
C	47.79106900	38.55936000	33.46724200
N	46.83801400	37.25601200	34.18125100
H	47.80897400	37.74857400	34.19935800
H	54.25225600	45.23552300	35.77584500
H	52.48040500	41.08638300	34.97658700
H	52.81081500	40.50515800	34.21310500
H	45.13710500	39.50477600	42.57852700

H	44.85847000	40.47337000	42.43597500	H	46.89056400	35.30344600	43.64403400
C	55.60005500	42.08240600	33.02358500	H	44.81353400	34.61092100	42.23174600
C	44.09743400	41.85120700	41.08703900	H	42.81060900	33.83886600	41.22224700
C	47.64823900	31.87273200	40.08283300	C	43.71864000	29.75984700	40.14591300
C	53.45186000	43.14348300	43.83230100	H	43.54850600	30.91739700	44.28828400
C	51.63210000	39.86264000	47.62954200	H	44.10324500	36.89197900	42.33938500
H	39.37485600	29.92252200	44.56874800	C	42.66762500	33.07966900	44.86600700
H	50.93476500	44.36389800	32.77738100	C	42.25340100	34.29324200	43.65799000
H	49.76766000	39.60496700	33.22111600	C	46.27633400	33.91489300	45.14123300
H	37.57051500	33.62690400	42.69114600	C	45.77196900	32.73802000	43.90762800
H	48.86107500	30.17122000	51.12568400	C	45.03704500	32.71675600	45.51958800
H	47.44218900	29.98408500	52.16158400	H	43.91043600	28.80139800	43.52432200
H	39.78104200	34.25884700	32.07062100	H	44.05960400	34.97087200	45.13196300
H	40.58249000	32.75519300	32.51039400	H	50.86208600	42.14153100	39.35570200
H	56.02922500	36.05029500	35.65461300	H	50.52052600	41.03874200	40.33350700
H	55.34453000	34.44958400	35.95249800	H	49.53890000	38.81046300	40.61855500
C	43.52132400	45.97984800	40.04687400	H	48.33558100	38.93246200	41.56182700
C	44.07718500	45.06318300	41.45259600	H	46.41186500	37.01396200	42.51424100
O	47.16319900	38.12580600	51.26003800	H	46.06496300	35.94679000	43.35150200
C	48.21066000	38.57234100	49.90609300	H	44.74566600	35.23660200	43.13299200
C	51.07104200	35.07746300	49.35963600	H	43.06299100	32.82028300	41.50943600
C	51.73578900	33.44495100	49.31120800	C	43.28681600	31.84708700	40.51221800
H	44.47003600	35.11675900	53.45043900	C	43.57351400	30.52948300	40.89783800
H	44.37229400	36.86855400	53.56478200	O	43.65203000	30.21208400	42.24967700
H	46.42560300	34.64788400	36.49060400	C	43.45038200	31.17692300	43.23662300
H	39.67680000	38.48879300	46.15220700	C	43.68086900	36.19686200	42.89884900
H	40.28644600	39.67556900	47.31793500	N	43.16021300	32.49723900	42.86676900
H	38.69144100	28.33482300	41.14875800	O	50.92594900	41.05613000	41.50738200
H	40.40974700	24.50176100	42.61055600	H	43.00701100	33.55499600	43.93902200
H	45.27041200	30.08002300	34.63831600	H	45.63481300	37.73186600	41.82327900
N	46.96585100	30.50295700	34.94057900	H	43.17728700	32.15484000	39.16307600
C	45.63893900	28.89538100	41.43266800	H	45.42188000	33.37025800	44.73058600
C	46.39933200	29.62305000	40.30243700	C	48.21734100	37.39467500	42.54977400
O	46.51599400	29.19042100	41.15190800	C	43.97686000	28.90461900	42.56267600
C	50.13984200	31.60958800	44.01868300	O	49.78192300	40.01879700	39.84375200
C	48.92241400	30.65718100	43.95936500	C	44.31208600	34.32283500	44.28331600
C	49.79045600	30.79775100	44.38952600	H	51.35856200	35.54194700	36.15589800
H	42.42722800	27.99302100	36.37958500	H	51.50534200	36.79182800	37.39549100
H	41.87205600	29.25631300	35.69119800	H	50.98720000	35.16470100	37.83602600
H	42.66768500	28.73289400	35.81502200	N	53.34130000	36.63324100	39.12401800
H	46.62266300	38.28971900	39.08990500	C	54.50254900	35.29857700	39.08144500
H	47.70635900	38.79689700	38.09134600	C	52.82742800	34.99738800	39.53649600
H	46.76996500	38.54820600	38.17676800	O	53.20235000	34.26136100	37.21130600
H	46.89342300	29.73805100	44.06390700	C	53.58134200	36.11518500	35.47189800
H	47.10661900	30.04682400	42.56725500	C	54.13403000	37.12821400	36.79817300
H	47.24587700	30.40236200	43.46872900	C	55.92923000	35.42689700	37.29968400
N	43.66820200	31.52200300	38.53570100	H	51.64833300	35.73331400	37.18640900
C	43.35837600	33.12108800	38.93006600	H	53.47159300	35.57968200	38.88104000
C	49.58964200	39.98806700	38.84942300	H	53.10437900	35.33255200	37.41911400
O	51.92946900	42.07594800	39.10735100	H	54.03581300	36.09162100	36.46468100
C	50.68356600	43.11307300	39.82528600	H	55.42102400	35.46347700	36.33845200
C	50.29365300	42.08027800	38.42363800	H	43.91906400	29.76599700	36.68749800
C	49.38995600	37.98618600	39.91520700	H	46.48257200	30.74067500	37.36074200
H	50.43762600	38.59599200	41.20513500	H	46.13613600	29.08941900	36.78303300
H	47.38811000	39.03696000	41.02702000	H	45.69697800	31.69268800	35.23710800
H	48.45954400	39.79285700	42.22114500	N	44.52333600	30.28512200	37.25170700
H	46.06723900	36.79643600	44.83042200	C	45.82858700	30.14293900	36.72446800

C	45.94597100	30.63598800	35.28698200	H	38.43894700	30.24148300	38.78747000
O	42.16118600	31.78444100	35.91163600	C	40.77675400	29.53689600	40.61387800
C	41.61813800	31.66550800	34.23893000	C	38.50342200	27.87139600	39.44419300
C	40.43117300	31.69889900	35.55046400	C	39.86484300	31.77786700	39.25749500
C	41.76768300	33.77106300	37.25091900	C	40.87944400	28.99693000	38.53871000
H	40.06043400	33.92775200	36.86151300	N	39.13615900	30.48390400	39.59442000
H	41.15511600	35.27042300	36.53590100	C	40.07951300	29.29360500	39.80440400
H	42.29998200	33.98529500	34.78841400	N	40.47086300	26.16331200	39.46825600
H	39.29336400	33.64696400	34.44039300	H	40.05309500	26.79803600	40.42026300
H	40.13388700	35.18902700	34.29925300	H	39.22704500	28.08695200	40.23203600
H	41.50942700	34.25334100	32.42340500	H	40.97251600	34.13087900	48.31895400
H	41.38771700	32.09314500	35.21121600	H	40.80051600	32.88183900	46.52873500
N	41.06458100	34.18602700	36.53357900	H	41.75144400	31.47096200	47.02303000
C	41.32841400	33.61789200	35.13995400	H	39.72882300	30.05251200	46.96295700
C	40.24597000	34.10926300	34.17149200	C	38.73440300	31.43232100	46.50838100
C	40.54998400	33.82398200	32.70505400	C	41.06432700	30.45201800	44.79045400
C	44.72577700	34.50878500	40.18872900	C	40.25116200	32.72505000	44.30523000
C	45.86474500	35.79104200	39.78995400	C	40.03518400	31.28888900	49.26646200
H	43.19511300	35.24862300	38.44100000	C	40.57312600	33.45581200	48.95247200
H	43.86880300	36.77979900	39.01710900	C	40.42316000	32.17450300	48.53248400
H	44.14993900	36.15577500	36.38482600	C	40.75833100	31.92570500	47.05302300
H	45.55418700	36.77752300	37.27428600	C	39.73035100	30.99543200	46.41481800
H	44.84398500	33.87988900	36.64247600	O	40.01596500	30.72400700	44.94018700
H	45.15990200	35.06768200	39.35479800	H	39.71692200	31.89690500	44.09973500
H	44.11334000	35.82699300	38.55297600	H	39.30520800	36.45804600	39.80339000
H	44.82551200	35.96959300	37.21684300	H	38.66471400	34.82456200	39.91971200
H	45.51431300	34.62213200	37.09610300	H	40.40433300	35.09619100	40.02978200
H	45.84149700	34.19106000	38.45116600	H	40.17725300	36.89940700	43.36589800
H	48.54758700	34.98586800	39.18366100	H	40.11171800	37.67701700	41.78482100
C	49.62251000	33.65520600	39.60206600	H	41.31893400	36.43025000	42.10946700
C	49.61550400	35.13131600	40.58194400	H	38.29689800	35.98203100	42.05237200
O	49.08043400	33.96539400	42.73177900	C	40.56840000	33.96210100	42.21340900
C	49.30553000	32.46262200	41.82077700	C	39.67951100	34.58725600	43.61612400
C	47.83065100	32.71173500	42.76116000	C	38.44931700	33.00394700	41.29942500
C	47.26878600	34.65029200	41.26460200	O	39.42942900	35.49690400	40.29770300
N	46.15486900	32.59357900	40.72990500	O	40.29140800	36.73406600	42.29650200
C	48.99370300	34.44193500	40.01370400	H	39.31694100	35.66037900	41.81103100
N	48.57537900	33.20346000	42.14158700	H	39.60514500	34.34750300	42.55175100
H	47.92039000	33.84316600	40.92023100	H	38.15771800	30.94648700	42.79124600
H	47.32799000	32.66537200	37.80042600	H	38.79877300	31.93555300	43.10174500
H	46.75436700	33.22395200	38.72377100	C	38.54596500	33.27306200	42.34797700
H	47.07596800	32.79489100	40.18000600	C	43.11632300	36.97968600	44.28172400
H	42.86595900	24.69537200	43.12313600	O	41.19405800	37.37916900	47.82140700
H	41.94899400	26.01838500	43.84922400	C	42.49758800	38.51023500	47.39027400
N	42.88322500	26.29666600	42.37328100	C	40.98239600	39.59407500	45.68681200
C	41.36750600	24.72959400	41.12427900	C	42.87578900	37.60600800	45.03617400
C	39.94501000	26.95094300	42.45652000	C	41.70871200	35.85377200	45.86766900
C	42.26771300	25.57634900	42.90674500	H	42.06399600	37.02006200	45.92037500
C	41.06009800	25.19097700	42.06391000	H	41.61666100	37.97881400	47.01062300
H	40.28267900	26.38397100	41.69424800	H	40.57808600	38.99771500	46.50978500
H	39.14756700	32.58196300	39.10710200	H	45.15971900	31.57710100	47.84387800
H	40.44882500	31.67836200	38.34808200	H	45.52194700	32.11900400	50.02206800
H	40.53853700	32.05424600	40.06364400	H	43.15655400	34.45715700	47.36486600
H	41.41505700	28.05791900	38.64571200	H	45.19174400	33.76716300	51.79379400
H	41.59755800	29.79075600	38.35387500	H	42.84742800	36.14318900	49.13645000
H	40.20231800	28.91079900	37.68975400	H	43.69164200	37.09059700	51.25311100
H	38.55148500	30.62545200	40.50508400	H	42.64219500	35.91900800	52.03115700

N 45.63713800 36.12316800 52.58398200
C 44.44519500 32.23015600 47.61657600
C 44.33957700 33.16045000 48.58473000
C 44.92894300 33.00056300 49.83401800
C 43.60257500 34.31811200 48.33832000
N 44.74143900 33.94048900 50.82924700
O 43.43369400 35.25562200 49.33834700
H 43.97781600 35.07813900 50.60707600
H 43.66920900 36.08604500 51.68714600
H 44.59753900 36.04161100 52.89443800
H 49.28134400 30.46763300 46.12077700
H 46.99632000 31.50927200 45.97640000
H 49.58523700 29.28356000 48.38538700
H 45.99814400 29.65922000 50.16484300
C 47.30911600 28.47223800 50.18717000
C 47.58088800 31.38250200 51.09101200
O 48.59628200 30.42635800 46.87408500
C 47.36563600 30.96205500 46.81932300
C 46.68168800 30.72465100 47.91366700
C 48.70027600 29.80260400 48.08199600
C 47.50316200 29.99363100 48.72258400
H 47.07881800 29.53464100 50.07716100
H 47.78502100 30.31786700 51.18510800
H 48.90474700 43.18007400 35.71114600
H 48.24417900 44.76512500 36.11756700
H 49.94763500 44.41302200 36.41613200
H 48.53636400 44.85935900 32.37343300
H 47.39918000 44.94561800 33.71861800
H 48.13279500 43.40209700 33.28338300
H 49.63129000 45.82965700 34.37497600
H 50.65443800 42.99316800 33.88187800
N 52.24064100 45.42709800 34.44848500
C 49.11875000 44.24644200 35.73227500
C 48.31102000 44.47199700 33.36427600
H 49.45985300 44.74752300 34.33145600
H 50.73096100 44.07796900 33.80907700
H 51.93835600 44.47844300 34.61337800
H 56.76208500 44.67067700 40.73819800
H 54.81044000 47.44932500 38.37129000
C 54.92914500 43.41762900 39.46364100
C 52.83974100 43.98297000 38.18356700
O 52.61079700 45.64990700 37.60465400
C 54.57667500 43.61196900 36.44071700
C 56.05618700 46.37620800 39.70820800
C 56.08052100 45.11299800 40.04000800
H 55.13150100 44.40604400 39.39329000
H 55.04861100 46.49800700 38.80444400
H 54.45369200 45.28254500 38.59151600
H 53.33300800 44.83808100 37.72101000
H 52.24783000 42.64275900 35.88253800
H 52.60095400 43.77253700 35.57207100
H 53.83086000 44.39220100 36.32312700
H 52.25159900 45.93429000 44.29620600
N 53.57141700 47.08733600 44.10348300
C 53.92809900 45.40672200 44.48130200
C 52.82003500 47.77186700 41.84060300
C 51.43091900 46.68546200 41.93749300
C 52.55669300 46.57305100 40.57904900
H 54.36175500 45.84966500 42.09267500
H 51.80478400 44.21505500 42.42642700
H 52.88910300 44.18736400 41.03449800
H 54.75931600 43.48998300 42.67660400
H 52.53745600 41.65147700 41.99955700
H 53.26472300 46.06025800 43.92118800
H 52.47786400 46.75852000 41.64759700
C 53.32368000 45.75350600 42.42725700
C 52.84609000 44.33204300 42.11576300
C 53.69900700 43.24121000 42.76988400
C 53.50265500 41.96919200 42.12179700
C 55.42886800 37.97942900 39.09195000
H 56.80493600 39.08291700 39.31544600
H 56.05129200 37.51108300 41.38378100
H 56.47515500 39.21120400 41.67442300
H 53.67285000 38.07501100 41.28197400
H 54.23868100 39.09636200 42.61349400
H 53.01314300 40.18858900 40.40384300
H 55.80219300 38.83858000 39.66366800
H 55.78433000 38.54166800 41.16170900
H 54.35095300 38.88566500 41.55185000
H 55.62434900 41.83087200 41.34159500
C 54.48157900 41.41001300 41.40797500
C 54.06306200 40.11996800 40.69717000
O 54.90215200 39.95263500 39.51479100
H 57.22885400 42.10419000 35.33602800
H 58.29828300 40.94119600 36.10898300
H 58.57417200 42.67467600 36.32452600
H 58.34371100 40.80464400 38.68673000
C 57.15534700 41.72353700 39.63092000
C 58.47367300 42.55545100 38.81616500
C 56.40288000 42.86079300 37.53919100
C 56.33472400 39.80978100 37.28594000
C 54.20000100 41.56253500 36.32730400
H 57.81113200 41.90535400 36.23213600
H 57.77122800 41.72930700 38.73421900
H 56.92581300 41.90027600 37.47415100
H 54.12753500 41.84538900 38.64015700
H 54.90831700 40.89589600 38.57447900
H 55.85984200 40.78773100 37.37782900
H 55.00927800 40.96693100 36.19263600
H 54.38769500 42.80508400 34.08917300
H 53.93214300 42.26160200 32.46887600
H 54.42544800 39.91032800 33.07650400
C 54.55802200 42.04511900 33.33178200
N 56.03991900 39.44331600 34.89474700
O 55.17108900 40.27799500 35.04156800
S 54.23505500 40.65115000 33.86072200
C 47.26605900 38.30162500 36.16135700
N 51.31296300 38.61718900 35.67061600
O 50.42657900 37.62221400 34.50866600
C 50.20889100 40.68007600 34.58389300
O 49.33530900 39.06010800 37.14905300
C 48.05315700 38.23570700 35.52588400
O 49.23273800 38.64130100 35.99576000
C 50.41070700 38.56033900 35.05753300

H	51.04139600	34.98944100	47.18519200	C	45.30591100	44.83361600	39.66613900
H	50.38040600	33.35609200	47.11907900	C	46.47382000	44.16047300	40.39676700
H	48.90959500	35.76453000	48.26696200	C	47.18603300	43.17213700	39.47263900
H	48.78759100	34.44635900	45.52431100	C	47.48303500	45.18386800	40.91125500
H	47.60192800	35.61661600	46.11295100	H	44.91701800	46.51638200	40.98073000
H	49.28459900	36.09915100	45.86248000	H	44.70435800	44.05636700	39.18797500
H	47.93092800	32.96692200	47.52800400	H	45.69666300	45.48042000	38.87577800
H	48.05169400	33.62316700	49.16012800	H	46.06683200	43.61387800	41.25364600
H	46.89698200	34.30433000	48.02301700	H	47.68014000	43.70119500	38.65923600
C	51.33507200	40.09306100	46.60609100	H	47.93724800	42.61082900	40.02403500
C	49.98365800	40.82373200	46.63353800	H	46.48326200	42.46567500	39.03524200
O	49.07362000	40.42647000	47.36074000	H	47.01992100	45.86367500	41.62043600
C	51.27675700	38.88875300	45.65326200	H	48.30611800	44.67706100	41.41043800
C	51.14959200	39.34386700	44.20427000	H	47.88872200	45.76770800	40.08599800
C	52.52294000	38.02543000	45.83585700	C	50.44689000	39.75820200	34.05388700
H	52.12882400	40.77375700	46.29751400	C	51.89654400	39.81933400	33.48080400
H	50.39710600	38.28834200	45.91218900	O	52.17049100	39.23128900	32.45456100
H	50.23537200	39.90791300	44.04344500	C	50.41092100	38.56023300	35.05781000
H	51.99579500	39.96332600	43.91430600	C	49.23561700	38.61538500	36.00098600
H	51.12034100	38.47709600	43.54963100	N	48.05660300	38.20590500	35.53489900
H	53.41893300	38.59689300	45.60249700	O	49.34348200	39.00622000	37.16320100
H	52.60199500	37.66508600	46.85931400	H	50.20882800	40.68007700	34.58423200
H	52.48158500	37.16551200	45.17182300	H	50.43656800	37.62226400	34.50742000
N	49.83435500	41.92379400	45.87150100	H	51.31102000	38.62552200	35.67173400
C	48.55090000	42.65303800	45.72594700	H	47.27928200	38.23483000	36.18500400
C	47.59954400	41.72508700	45.00127400	C	54.23495400	40.65097200	33.86067300
O	47.95968500	41.07916900	44.03049400	C	55.16932200	40.27640100	35.04250700
C	48.78178700	43.93480500	44.91651400	O	56.03577000	39.43893900	34.89765200
C	47.46306200	44.65967600	44.65329100	C	54.55815500	42.04513600	33.33270000
C	49.75081600	44.86293100	45.64549300	H	54.42540300	39.91052900	33.07612800
H	50.51334200	42.09327200	45.14389100	H	53.93197200	42.26241000	32.47019300
H	48.20350700	42.87632800	46.73616600	H	54.38831300	42.80464400	34.09065500
H	49.21149700	43.63586400	43.95354500	N	55.00763900	40.96486300	36.19374100
H	46.74927500	44.02261700	44.13673200	C	55.86004500	40.78809000	37.37809000
H	47.02123900	45.00289700	45.58698300	C	54.90883600	40.89579600	38.57469600
H	47.64637900	45.53225600	44.03198900	O	54.12968400	41.84773800	38.63667600
H	50.70782600	44.38082800	45.82924000	C	56.92433500	41.90201900	37.47327900
H	49.92203300	45.75806900	45.05247000	C	57.76963400	41.73197800	38.73356600
H	49.33339900	45.16652100	46.60355800	C	57.80960300	41.90796800	36.23119400
N	46.36156000	41.62771900	45.49163600	H	54.20133300	41.56467100	36.32763600
C	45.44602200	40.77464000	44.76108200	H	56.33773200	39.81163800	37.28606400
C	45.06159000	41.37436000	43.39604200	H	56.40020800	42.86186600	37.53832500
O	44.82197400	42.57340400	43.25922800	H	58.47140500	42.55870000	38.81560000
C	44.20915600	40.71646300	45.67088200	H	57.15334400	41.72566700	39.62998200
C	44.28241400	42.03448400	46.44325200	H	58.34261500	40.80759600	38.68670400
C	45.77986300	42.23612600	46.68395400	H	58.57109500	42.67892100	36.32292800
H	45.90224700	39.79714400	44.59439500	H	58.29883400	40.94471900	36.10879700
H	43.28905600	40.62671900	45.09720300	H	57.22689200	42.10492600	35.33488300
H	44.27876800	39.86862900	46.35258700	N	54.90156400	39.95359000	39.51359100
H	43.91278200	42.84008200	45.80927600	C	54.06315000	40.11997100	40.69708600
H	43.70871800	42.01271000	47.36737200	C	54.48020300	41.41243200	41.40454100
H	46.03466500	43.29045500	46.76287800	O	55.62540400	41.82870000	41.34460100
H	46.12752300	41.70068400	47.57503000	C	54.36981700	38.89601000	41.55998600
C	44.41494300	40.80832300	41.09466800	C	55.80800600	38.57431100	41.16870900
H	45.20205500	41.24374100	40.46828700	C	55.80183200	38.83882100	39.66361900
H	44.03441000	39.90636900	40.61055400	H	53.01198300	40.17968200	40.40688500
C	44.40098600	45.64273700	40.59103800	H	54.25365000	39.11050700	42.62028700

H	53.70456500	38.07340600	41.29437600	N	47.99796600	29.57364200	46.77491000
H	56.48715800	39.26959800	41.66244600	H	47.42955500	31.32304800	50.96835500
H	56.10012100	37.55476100	41.41005900	H	47.43276800	28.29515600	50.53909000
H	56.79834600	39.07273100	39.29202600	H	45.99398800	29.32321800	50.51434500
H	55.41006800	37.97248700	39.12824600	H	49.13942600	28.51064900	48.23840600
N	53.50134300	41.97135600	42.11849200	H	46.39082400	30.74538600	46.03000000
C	53.69895500	43.24114000	42.76982500	H	48.50790500	29.43061700	45.90612200
C	52.85333500	44.33483500	42.11132000	C	44.59753900	36.04161000	52.89443300
C	53.32440700	45.75528800	42.43607200	C	43.36410800	35.38151500	52.28130000
C	52.48887800	46.76286500	41.64864400	C	43.72467600	34.56513000	51.07089900
C	53.24213800	46.05497900	43.93036600	C	43.54839500	35.06386500	49.78765200
H	52.53151900	41.68220600	41.96568900	C	44.24980300	33.28601500	51.21204100
H	54.76082800	43.48716700	42.68595600	C	43.84169400	34.29973600	48.67300800
H	52.90948500	44.19509400	41.03011900	C	44.55781500	32.51523800	50.10922000
H	51.80855000	44.21305000	42.40740300	C	44.33770600	33.00632600	48.82531800
H	54.36730200	45.85441700	42.11742300	O	44.56437100	32.25775000	47.72521000
H	52.58570400	46.58370800	40.58051100	H	45.06854900	36.70553700	52.17280700
H	51.43760200	46.68503400	41.92100100	H	42.89732900	34.73810500	53.03114000
H	52.82495500	47.77610800	41.85303700	H	42.64277200	36.15331800	52.00344900
H	53.89835800	45.40016100	44.49741900	H	43.14959000	36.05974000	49.65166600
H	53.54336500	47.08192900	44.12263500	H	44.40425100	32.88119500	52.20248600
H	52.22354600	45.92452400	44.28864500	H	43.68251900	34.69171800	47.68078700
C	53.83084400	44.39212600	36.32308800	H	44.95839400	31.51989500	50.22701900
C	52.60097600	43.77241200	35.57204000	H	45.11002700	31.46685600	47.96741600
O	52.24690900	42.64301100	35.88285400	C	40.57809100	38.99771100	46.50978300
C	53.33301400	44.83802800	37.72102100	C	40.41155700	37.46846700	46.49163700
C	54.45489800	45.28283800	38.59005400	C	41.64965900	36.85965800	45.87142800
C	55.05285300	46.49738300	38.79974800	O	42.53871300	36.33157100	46.53430000
N	55.13088600	44.40669600	39.39372700	O	41.70139800	37.03699800	44.56294600
C	56.08160300	45.11292400	40.03850500	H	41.46906800	39.28418800	47.08027600
N	56.06040600	46.37542900	39.70357700	H	40.29318800	37.07226000	47.50360600
H	54.57677700	43.61207000	36.44102000	H	39.53122700	37.19858400	45.89870000
H	52.61088900	45.64997000	37.60458800	H	42.68561200	36.89487900	44.24352300
H	52.84112300	43.98404400	38.18467100	C	38.54600700	33.27302200	42.34803200
H	54.92623900	43.41875700	39.46623100	C	38.88092600	31.89742800	43.00095800
H	54.81679200	47.44823300	38.36431200	O	38.48820300	30.85878900	42.49966900
H	56.76211900	44.67067700	40.73774800	C	39.81447000	33.99541600	41.89920400
N	51.93912500	44.47775500	34.61231000	C	39.53507200	35.34487100	41.22433100
C	50.73096500	44.07797300	33.80906500	C	40.81511700	36.17790100	41.17854200
C	49.46668000	44.77354500	34.31323100	C	38.98090200	35.15904100	39.81432800
C	48.31796400	44.49441700	33.34695600	H	37.89708700	33.05529700	41.50287600
C	49.11414500	44.30373700	35.72199100	H	40.45131300	34.16944600	42.76920100
H	52.24298400	45.42555500	34.44522100	H	40.36686200	33.35205200	41.21197200
H	50.64054300	42.99580000	33.90145600	H	38.79419800	35.88739900	41.82306500
H	49.65188400	45.85405600	34.33669100	H	41.59616400	35.63869400	40.64717700
H	48.12596800	43.42558600	33.28607300	H	40.63911400	37.11935500	40.66274500
H	47.41111900	44.98670400	33.68845500	H	41.16394800	36.40188300	42.18350400
H	48.55212600	44.85953400	32.34971000	H	39.69788500	34.62321500	39.19612300
H	49.94334200	44.47116300	36.40530800	H	38.05145900	34.59640300	39.83041600
H	48.24595400	44.84204300	36.09453200	H	38.78304100	36.12459800	39.35354500
H	48.88464900	43.24040800	35.71996800	N	39.60596800	31.90546600	44.14701200
C	47.78503000	30.31789900	51.18505900	C	40.01596200	30.72397300	44.93999900
C	47.06423800	29.29539600	50.30045200	C	39.76852800	30.95160500	46.41933300
C	47.26359700	29.54341800	48.84054700	C	40.75827000	31.92576800	47.05318900
C	48.27568400	29.10535200	48.02505400	C	40.25204200	32.28450800	48.46440600
N	46.37944800	30.26947400	48.09269400	N	40.75326800	33.42145100	49.00119400
C	46.85059100	30.26242400	46.86815500	O	39.41688300	31.61184900	49.03530500

H	39.95030700	32.78962600	44.48596700	H	44.82492300	34.51521000	40.23956900
H	41.07051900	30.52656300	44.74112300	C	40.54998700	33.82397300	32.70503700
H	38.75544800	31.33169600	46.56235800	C	40.74336200	33.67890800	34.21161700
H	39.82941000	29.99960400	46.94727800	C	41.89555300	32.74565700	34.60453000
H	41.75037300	31.48065500	47.14499900	C	42.16294200	32.85067400	36.10560600
H	40.85151600	32.84523800	46.47306300	C	41.60090000	31.29395300	34.23488400
H	41.53816500	33.88298200	48.56231100	H	41.47289000	34.15392600	32.23230400
C	39.22703300	28.08699900	40.23201900	H	40.94148000	34.66818800	34.63206200
C	40.39479900	27.13663200	40.58111200	H	39.81830500	33.31166100	34.66223200
O	41.50051900	27.23599800	40.06834400	H	42.79627500	33.06458300	34.06675600
C	39.58129300	29.08908800	39.13376600	H	42.37927900	33.88029300	36.38094700
C	38.59568000	30.26224700	39.15266700	H	41.29167500	32.52442100	36.66862000
C	39.60877800	28.39185500	37.77356300	H	43.00901700	32.22936100	36.39164900
C	39.10027400	31.45672600	38.35179800	H	40.68208800	30.96103300	34.71434700
H	38.36038700	27.48710300	39.94827700	H	41.49103200	31.17495300	33.16057600
H	40.57202300	29.49159100	39.36343900	H	42.41417800	30.65058700	34.56365800
H	37.62921900	29.93548600	38.76134200	C	45.94600900	30.63599100	35.28696900
H	38.45022100	30.57481400	40.18772800	C	46.25251100	30.29950200	36.74264800
H	38.61403200	28.03067800	37.51703300	O	45.17293700	30.58210500	37.61883900
H	39.93096700	29.07129800	36.98726700	H	45.69488400	31.68953000	35.19827800
H	40.28214500	27.53766800	37.79520200	H	46.54423300	29.24585200	36.83425100
H	40.06656300	31.77717700	38.73666900	H	47.07148600	30.93269300	37.08803000
H	39.20517500	31.21066100	37.29685700	H	44.47466400	29.91702500	37.51151000
H	38.40295100	32.28720800	38.43230000	C	55.42102900	35.46311000	36.33819300
N	40.11408700	26.16747000	41.48731500	C	54.68793700	36.43159100	37.25317800
C	41.06010800	25.19097000	42.06391800	C	53.16910800	36.49685200	37.05786100
C	41.51920400	25.62810500	43.44818100	C	52.49161400	35.16644100	37.37612400
H	39.21244400	26.20779100	41.93822700	C	52.59216100	37.59684700	37.95158700
H	41.90818400	25.14016600	41.37960700	H	55.12234000	34.43473800	36.52608200
H	42.01199200	26.59567000	43.38943700	H	54.89338900	36.15104800	38.29092900
H	40.67192700	25.70677400	44.12647400	H	55.09278800	37.42912800	37.06545600
H	42.22032800	24.90206300	43.85072200	H	52.97165100	36.75093100	36.01051900
C	47.07606100	32.79493700	40.18000200	H	51.41104700	35.26149500	37.29490500
C	46.82805600	33.29459800	38.73259500	H	52.81412800	34.38925200	36.68932900
O	47.49905500	32.83896200	37.81764200	H	52.72890000	34.85256900	38.39095800
C	47.93726700	33.76163400	41.00841600	H	51.51555300	37.67913300	37.82504700
C	48.64169600	32.98178900	42.11707700	H	52.78690300	37.36852800	38.99823900
C	48.96891600	34.49049100	40.14973900	H	53.04024500	38.56234000	37.72089600
H	46.12920700	32.60626400	40.68531300	C	44.75872100	34.40571600	44.38640400
H	47.28659400	34.50795900	41.47440900	N	49.92727500	40.05581900	39.74024900
H	47.92662800	32.37770000	42.66769600	O	43.20422800	28.93842600	43.73685500
H	49.39613500	32.32511300	41.68709400	S	48.49773100	37.57955100	42.65222400
H	49.13119500	33.66672000	42.80626700	C	45.78447200	33.27785000	44.55243200
H	49.61071300	35.10177700	40.78153600	N	42.72667300	31.61657900	39.79967100
H	49.58427900	33.77925800	39.60327500	O	45.94519200	37.72488800	41.76627300
H	48.48335000	35.14071300	39.42477600	C	43.31916200	33.84568300	44.21215900
N	45.85858200	34.20458300	38.45363600	O	50.92276800	41.23555100	41.39963500
C	45.51401000	34.62197900	37.09603100	C	43.20212200	32.61029400	43.34578500
C	44.68032500	35.88592000	37.22252700	O	44.12489200	36.89654300	43.92780100
C	44.00685800	35.66994000	38.56897100	C	43.25684400	31.35121000	43.95719200
C	45.16014000	35.06783900	39.35493500	C	43.14039300	30.19738200	43.17984600
H	44.94449200	33.81500500	36.62114100	C	42.96393900	30.27204400	41.80095800
H	45.31844500	36.76804700	37.27364500	C	42.93756500	31.52686900	41.17452300
H	43.98170900	35.99836100	36.39552700	C	43.05506000	32.69125200	41.96093500
H	43.63737800	36.58677300	39.02282700	C	45.12827700	35.43207700	43.32684900
H	43.18451400	34.95751800	38.47906200	C	46.45346500	35.91755700	43.23319300
H	45.81773600	35.87310400	39.71176100	C	46.74609400	37.04761200	42.45923000

C 48.57131700 39.04125600 41.55942400
C 49.72716800 38.87613000 40.56811100
C 50.57231300 41.14280800 40.21089500
C 50.89467800 42.21650500 39.19811700
H 44.74551800 34.96096100 45.33023100
H 43.29106100 29.03466200 44.69838300
H 45.48303200 32.66385600 45.40709800
H 45.83581600 32.63587500 43.67019600
H 46.78157600 33.66679300 44.75968200
H 42.67633100 34.64461500 43.82984600
H 42.95161500 33.59933500 45.21378300
H 44.35219700 37.48103600 43.17937200
H 43.40969000 31.27963900 45.03215100
H 42.83809400 29.35570000 41.23311600
H 42.99344300 33.66554600 41.48216600
H 44.54779700 35.39929000 42.40693600
H 47.21091300 35.55788200 43.91545000
H 45.02126200 37.24156300 45.17146700
H 48.71524000 39.93785500 42.16213100
H 47.60006900 39.10346300 41.06191900
H 50.65309400 38.67687800 41.11698800
H 49.54278400 38.02897700 39.90238000
H 50.31997500 42.12083000 38.27283900
H 50.71795100 43.20118300 39.63922600
H 51.95968100 42.13907100 38.94320000
H 49.74597600 39.97398500 38.74667000
H 43.16452200 32.41609100 39.35867900
H 42.94924500 30.76586800 39.29003000
O 46.37974200 30.26277500 42.78759000
H 46.31969400 30.13752200 41.82166600
H 45.58281100 29.85699000 43.13661500
O 46.77744300 38.41357600 38.23094300
H 47.70546100 38.69047500 38.16063900
H 46.60334500 38.23096400 39.15858200
O 42.93119100 28.91321500 38.31034100
H 42.22873400 29.04757100 37.67000900
H 42.55883400 28.28583700 38.95649000
O 48.71967100 29.61990700 44.05754400
H 47.86752500 29.80146700 43.61167100
H 49.36792500 30.14591800 43.58669900
O 45.76421700 29.68806600 40.18015000
H 45.70356200 30.17437400 39.33906800
H 45.00662400 29.09791300 40.18948600
H 46.82055200 30.43235700 34.67709200
H 45.11152500 30.04170400 34.91454100
H 40.55772400 24.22229400 42.09859300
H 38.97865900 28.63433700 41.14563900
H 39.71119900 39.48039000 46.97241300
H 40.68568800 39.38097000 45.49135200
H 46.42831100 34.76352100 36.51036400
H 44.32541900 36.62058500 53.77438000
H 45.32455300 35.28769400 53.18754400
H 51.88856500 33.70732600 49.08302800
H 50.80040000 34.95667500 49.68691000
H 48.27193400 38.13295700 49.91692000
H 47.25324900 38.22424300 51.36057200
H 44.08337100 45.02748000 41.42977600

H 43.51835200 45.98326300 40.05391900
H 55.21786400 35.70039900 35.29652500
H 56.49353900 35.54133900 36.49948300
H 40.25088000 32.88139900 32.25435200
H 39.77582700 34.55868900 32.49568000
H 47.60230500 30.10116100 52.23460700
H 48.85708900 30.28538800 51.00352700
H 37.99905700 33.87884500 43.07345700
H 49.76775000 39.60601200 33.22081500
H 50.94286800 44.34221100 32.77307500
H 39.41932500 29.89225900 44.56216200
H 51.52929200 39.74861600 47.62226800
H 53.44303000 43.14155800 43.83008500
H 47.60590200 31.85137800 40.05566200
H 43.61354400 41.54303900 41.19706500
H 55.60011400 42.08235900 33.02415200
N 44.90644700 40.44751900 42.41650400
H 45.35075000 39.53403400 42.49262000
N 52.81091900 40.50442300 34.21388700
H 52.48076400 41.08517100 34.97779600
H 54.25229800 45.23529800 35.77556400
C 47.80890600 37.74860800 34.19929900
H 46.84915800 37.23451700 34.17721000
H 47.76457900 38.57889600 33.49014400
H 48.57383500 37.04753000 33.86658200
C 40.38708700 33.88855600 50.33041700
H 41.20626400 33.73579800 51.03334600
H 40.13544600 34.94778800 50.28931500
H 39.52058600 33.31245500 50.64868200

Coordinates of DH2-IM2(a2) system

C 47.27571900 37.90672100 50.31331300
C 46.38948300 38.84155500 49.47798900
C 46.20647000 38.39183800 48.06579800
C 45.14269400 37.83629400 47.40953000
N 47.21189400 38.51560500 47.11417500
C 46.76584900 38.08832100 45.92566700
N 45.51283100 37.65798200 46.08904400
H 46.85278900 36.89720500 50.34408600
H 45.39843200 38.93163700 49.93518400
H 46.82610400 39.84911600 49.47188200
H 48.07880400 39.05391100 47.25189700
H 44.15043100 37.55591500 47.72225000
H 47.32672700 38.11154200 45.00063300
C 50.85397700 34.04402800 49.09596400
C 50.35272700 34.07844100 47.65812600
C 49.17852000 35.03811100 47.43580800
C 48.89766900 35.15628000 45.93917800
C 47.91939100 34.57871900 48.16864500
H 50.09882000 33.63820800 49.76374400
H 51.17682300 34.38445600 47.00865900
H 50.05048300 33.07344700 47.35797800
H 49.46362600 36.02714000 47.81528900
H 48.64145900 34.18081800 45.53145900
H 48.06848800 35.83743300 45.76160400
H 49.76700900 35.53627000 45.40685300
H 47.64181000 33.57461800 47.85684800

H 48.07250800 34.57135300 49.24390400
H 47.08255200 35.24172700 47.95576200
C 51.33510200 40.09310400 46.60609200
C 49.98913800 40.83234300 46.63353100
O 49.07362600 40.42520900 47.34930900
C 51.22252200 38.80715100 45.77364000
C 50.96375000 39.13665500 44.30759700
C 52.49598100 37.97840700 45.92374100
H 52.11485000 40.73527900 46.19606400
H 50.37932700 38.22144000 46.15778600
H 50.04192700 39.69999300 44.18990300
H 51.77870900 39.72403400 43.89016600
H 50.87550100 38.21831200 43.73189300
H 53.35942300 38.54086100 45.57502100
H 52.66206000 37.70294600 46.96270000
H 52.42216400 37.06654700 45.33600900
N 49.84799500 41.94467500 45.89161200
C 48.55101500 42.65298900 45.72600800
C 47.62426300 41.65669500 45.05601600
O 48.02233500 40.92421900 44.16191200
C 48.77677600 43.90646800 44.87289100
C 47.46262100 44.62784100 44.58687700
C 49.74914300 44.85515600 45.57237600
H 50.53210900 42.12521400 45.17174600
H 48.20779100 42.90932400 46.72927200
H 49.20302600 43.57740600 43.91845000
H 46.76387100 43.97703600 44.06840600
H 47.00993400 44.98576700 45.50996500
H 47.65357300 45.48954300 43.95252000
H 50.70704300 44.38134900 45.77319800
H 49.91992700 45.73032000 44.95010000
H 49.33148200 45.19095200 46.51961400
N 46.37827400 41.57888000 45.52608500
C 45.44561700 40.77484700 44.76099400
C 45.26126200 41.35436300 43.34505800
O 45.60869500 42.49470300 43.04408200
C 44.15000900 40.84794900 45.58273300
C 44.28654200 42.15352900 46.36576600
C 45.77981600 42.23600600 46.68397900
H 45.81481100 39.75641400 44.64492100
H 43.26773300 40.83871000 44.94805800
H 44.08650100 39.99913300 46.26295800
H 44.00889500 42.99331200 45.72852500
H 43.66813100 42.16953600 47.26056100
H 46.11002900 43.26701300 46.78276100
H 46.03551000 41.67468800 47.58979400
C 44.41506600 40.80795600 41.09453900
H 45.34313300 40.81449000 40.51238000
H 43.73881800 40.04648500 40.70692100
C 44.40094100 45.64289800 40.59109400
C 45.23378000 44.83376700 39.60049700
C 46.45685300 44.16228200 40.23649300
C 47.07639500 43.15691800 39.26559400
C 47.51188300 45.18510000 40.65078400
H 44.94719000 46.51345600 40.94475500
H 44.59828700 44.05591500 39.16927200
H 45.55916900 45.48208400 38.78216000
H 46.13016900 43.62502600 41.13105600
H 47.48576600 43.66734200 38.39506400
H 47.88011600 42.60920600 39.75261600
H 46.33322300 42.44095900 38.92124600
H 47.11115800 45.88249900 41.38071500
H 48.36467000 44.67951200 41.09859500
H 47.86035800 45.74983200 39.78670600
C 50.44685300 39.75805200 34.05377300
C 51.89797300 39.81598300 33.48311700
O 52.17441800 39.21745300 32.46394800
C 50.41070500 38.56033300 35.05753900
C 49.23718500 38.61066100 36.00396400
N 48.05862300 38.20289300 35.53633000
O 49.34647200 38.99490300 37.16890200
H 50.20809200 40.68056300 34.58257600
H 50.43573400 37.62385800 34.50512300
H 51.31378000 38.62062500 35.66982200
H 47.28110700 38.22825400 36.18644300
C 54.23505800 40.65115100 33.86072100
C 55.16863500 40.27541600 35.04275200
O 56.03339500 39.43616300 34.89865300
C 54.56158000 42.04443600 33.33248400
H 54.42431500 39.90961300 33.07693100
H 53.93746200 42.26222400 32.46865900
H 54.39146600 42.80469600 34.08967400
N 55.00878100 40.96663400 36.19298200
C 55.85984800 40.78772900 37.37781500
C 54.90997300 40.89651600 38.57490800
O 54.13022100 41.84678600 38.64140700
C 56.92641200 41.89992200 37.47326100
C 57.77222900 41.72904200 38.73309500
C 57.81117500 41.90380700 36.23089800
H 54.20235900 41.56635500 36.32569800
H 56.33437800 39.80960300 37.28576800
H 56.40392700 42.86068700 37.53805500
H 58.47481000 42.55507600 38.81454200
H 57.15695100 41.72353200 39.63023400
H 58.34463900 40.80434300 38.68552700
H 58.57417600 42.67323600 36.32225800
H 58.29841100 40.93959400 36.10848800
H 57.22853200 42.10180700 35.33484900
N 54.90255200 39.95293400 39.51503300
C 54.06303700 40.11994500 40.69721700
C 54.48518900 41.40660700 41.41289100
O 55.62981200 41.82203800 41.35154900
C 54.34623300 38.88180200 41.54785100
C 55.78058500 38.53829800 41.16098000
C 55.80220600 38.83859700 39.66364700
H 53.01437100 40.19381800 40.40171400
H 54.22997000 39.08736200 42.61001100
H 53.66937100 38.07226000 41.27086200
H 56.46990400 39.20675000 41.67697000
H 56.04701700 37.50727100 41.38158500
H 56.80585900 39.08391400 39.31878100
H 55.43066000 37.98085400 39.08865200
N 53.50591300 41.96655500 42.12608400
C 53.69900200 43.24121300 42.76987000

C	52.84329400	44.32690500	42.11107100	C	44.59747100	36.04155900	52.89439300
C	53.31645700	45.75095100	42.41767100	C	43.85089300	36.25216200	51.58358900
C	52.46635400	46.75037900	41.63556800	C	44.05657200	35.17950500	50.54245600
C	53.25770300	46.06236100	43.91064500	C	43.47016300	35.34379000	49.29102300
H	52.53968000	41.66082100	41.99066000	C	44.78911000	34.02299200	50.76624500
H	54.75881900	43.49245900	42.67727900	C	43.59114100	34.38994700	48.30158700
H	52.88726400	44.17826700	41.03034900	C	44.90740300	33.05265300	49.78763900
H	51.80213700	44.20769800	42.42100000	C	44.29666900	33.21420500	48.55052300
H	54.35402600	45.84964800	42.08209100	O	44.35547400	32.26051500	47.59144000
H	52.54477100	46.56189800	40.56752400	H	45.67049400	35.98122500	52.72575500
H	51.42002300	46.67431800	41.92655900	H	42.77901700	36.32219800	51.79671200
H	52.80500000	47.76554100	41.82513700	H	44.14926600	37.21328400	51.15344500
H	53.92429300	45.41347800	44.47244500	H	42.89307000	36.23475600	49.08655100
H	53.56055200	47.09122900	44.08911600	H	45.27130400	33.85579000	51.71667700
H	52.24542400	45.93391600	44.28693100	H	43.15306300	34.56084600	47.33057600
C	53.83086100	44.39220300	36.32312700	H	45.47559200	32.15516000	49.97840200
C	52.60019400	43.77243900	35.57298400	H	45.06523800	31.60591700	47.81534300
O	52.24378700	42.64446000	35.88793000	C	40.57831100	38.99795400	46.50986900
C	53.33300900	44.83808000	37.72101000	C	41.18876600	38.59222700	45.15695800
C	54.45418700	45.28418700	38.59018900	C	42.48487500	37.77258800	45.28822100
C	55.04973700	46.49984400	38.80000200	O	42.57683900	36.95213400	46.22496200
N	55.13280300	44.40904800	39.39300300	O	43.41661400	37.97238800	44.41548900
C	56.08278600	45.11721800	40.03730900	H	40.42410500	38.11136500	47.13018900
N	56.05826800	46.37957000	39.70283900	H	40.46468900	37.96760300	44.61568700
H	54.57725500	43.61248000	36.44043100	H	41.37537600	39.46292200	44.52046500
H	52.61048500	45.64952600	37.60441500	H	44.11757300	37.75578400	41.42436900
H	52.84037000	43.98358000	38.18440200	C	38.54601700	33.27310500	42.34803000
H	54.93042300	43.42096300	39.46532600	C	38.84067500	31.92988400	43.07217200
H	54.81125500	47.45036600	38.36539400	O	38.24795700	30.92383700	42.72501200
H	56.76509300	44.67632300	40.73569600	C	39.66427400	34.30060300	42.29222600
N	51.94080500	44.47566400	34.61093000	C	39.22961500	35.60624200	41.61011200
C	50.73096100	44.07796900	33.80907700	C	40.33975700	36.64451800	41.73646000
C	49.47566500	44.80255800	34.29383400	C	38.88587400	35.41021800	40.13598700
C	48.32736100	44.52483000	33.32668600	H	38.22747400	32.98783200	41.34799600
C	49.10860100	44.36367100	35.70878200	H	39.98162400	34.55398900	43.30733700
H	52.24867400	45.42130400	34.43863900	H	40.51854300	33.88019100	41.75912100
H	50.62405900	42.99930500	33.92186300	H	38.33893200	35.98077900	42.12884600
H	49.67819000	45.88015600	34.29895600	H	41.21624700	36.34521600	41.16846800
H	48.11815400	43.45836400	33.28363100	H	40.01452000	37.60953700	41.35726200
H	47.42703100	45.03769000	33.65476300	H	40.63854300	36.77443000	42.77337500
H	48.57225000	44.86848200	32.32444000	H	39.73562500	34.98773700	39.60425300
H	49.93769800	44.52686000	36.39329900	H	38.02925800	34.75371600	40.00926100
H	48.24960900	44.92531600	36.06781700	H	38.64356000	36.36861500	39.68214300
H	48.85861000	43.30503600	35.72366700	N	39.72354000	31.90293700	44.10237700
C	47.78505600	30.31783000	51.18514800	C	40.01589200	30.72403000	44.94015200
C	47.07193100	29.59234500	50.04339000	C	39.73094900	30.99682700	46.41208700
C	47.49124600	30.11883500	48.71211500	C	40.75840100	31.92564700	47.05305700
C	48.71687800	30.04103700	48.10297600	C	40.38474000	32.19079700	48.52248800
N	46.63526100	30.79995700	47.89560000	N	40.62048900	33.45033800	48.96255800
C	47.32709200	31.11979100	46.82809700	O	39.88474000	31.33523100	49.22374700
N	48.59604000	30.68405600	46.90670800	H	40.20593100	32.75097000	44.35058700
H	47.57596700	31.38506800	51.14834900	H	41.06359100	30.44497900	44.79144300
H	47.30056600	28.52493800	50.09887100	H	38.73565300	31.43504900	46.50709400
H	45.99177600	29.71243900	50.14159400	H	39.72691900	30.05508900	46.96161600
H	49.63344200	29.58909700	48.41943600	H	41.75021000	31.46798400	47.04361700
H	46.93613100	31.65646800	45.98787100	H	40.81484600	32.87835300	46.52364300
H	49.30329800	30.79453900	46.18126900	H	41.14178600	34.08820000	48.38018400

C	39.22704200	28.08693200	40.23201100	H	39.96618600	35.10785300	34.31350700
C	39.98305200	26.75580900	40.42134900	H	39.25057700	33.49967900	34.38693500
O	40.27392900	26.04927800	39.47335700	H	42.20672000	34.06310500	34.85200000
C	40.16808500	29.25044500	39.88084500	H	40.89917800	35.22873600	36.57537500
C	39.30786100	30.49177600	39.62183900	H	39.91178100	33.79275200	36.84577700
C	41.03852900	28.91993400	38.67142900	H	41.61396400	33.77842700	37.29101700
C	40.12785000	31.75864900	39.42666300	H	40.48982800	31.63267900	35.52111800
H	38.53231800	27.92991200	39.40621800	H	41.71240100	31.70618500	34.24469100
H	40.81915200	29.44940100	40.73969800	H	42.19726500	31.83748300	35.93480300
H	38.68974300	30.31663700	38.73720700	C	45.94600200	30.63597300	35.28695100
H	38.63960400	30.62706600	40.47351800	C	46.06492200	30.04414200	36.68616200
H	40.40964700	28.81737000	37.78818900	O	44.83466000	30.03046500	37.38493200
H	41.77141800	29.70566900	38.51055200	H	45.61972900	31.67092900	35.34827700
H	41.56376000	27.98156000	38.82782600	H	46.46202000	29.02116800	36.62466200
H	40.73758600	31.94741900	40.30635500	H	46.74565900	30.65667400	37.27963900
H	40.78871600	31.67729400	38.56928700	H	44.18597200	29.55117200	36.83435700
H	39.46937700	32.60853200	39.26802200	C	55.42102200	35.46347500	36.33845400
N	40.31388700	26.40297200	41.69167100	C	54.03296300	36.08646700	36.45925400
C	41.06010400	25.19096600	42.06392300	C	53.10376700	35.32886500	37.41703200
C	42.33425100	25.55236900	42.81358900	C	53.46497000	35.59140700	38.87786500
H	40.06905700	27.02613500	42.44553300	C	51.64536200	35.71634600	37.17633000
H	41.28449700	24.67673000	41.12815400	H	55.92760800	35.43293200	37.30077200
H	42.95252300	26.21384500	42.21176500	H	54.12630400	37.12544500	36.78657600
H	42.09675800	26.05493200	43.74943600	H	53.57968800	36.10210700	35.46587700
H	42.90007400	24.65234000	43.03864300	H	53.21038900	34.25672300	37.21897100
C	47.07593000	32.79486700	40.17995900	H	52.82415600	35.00911000	39.53680300
C	46.75184300	33.22148100	38.72224700	H	54.49760400	35.32023300	39.08288200
O	47.33429100	32.67148200	37.79929900	H	53.32604700	36.64615000	39.11115400
C	47.89064400	33.86198300	40.92382800	H	50.98594100	35.14584700	37.82624600
C	48.50293800	33.25638500	42.18400500	H	51.49258700	36.77496900	37.37776900
C	48.99059200	34.44537600	40.03913700	H	51.36128800	35.51619600	36.14603800
H	46.15774900	32.57381000	40.72553100	C	44.28551300	34.62519600	44.19229800
H	47.21788300	34.67113700	41.22262500	N	49.92473700	39.95394300	39.77684500
H	47.73700000	32.77957900	42.78929700	O	44.37562600	29.15148900	42.72203800
H	49.24117200	32.50652500	41.90727100	S	48.30050200	37.51669700	42.63523000
H	48.98972600	34.03144200	42.77356100	C	45.31957200	33.75134300	44.90139500
H	49.60658700	35.13659900	40.61245200	N	43.41967900	32.02830200	39.04014500
H	49.62385700	33.65028500	39.65176000	O	45.99895100	37.53712400	41.29513000
H	48.56754200	34.98120700	39.19213900	C	43.06230300	33.82656200	43.66315600
N	45.82694500	34.17633600	38.45349500	O	50.93326300	41.10300600	41.44911800
C	45.51426100	34.62197700	37.09597500	C	43.35449700	32.70070700	42.69503300
C	44.66488500	35.87850000	37.22298200	O	43.16551900	37.86312500	41.60289300
C	44.00775300	35.68799300	38.58232700	C	43.72267600	31.44123100	43.18785500
C	45.16000400	35.06791600	39.35507800	C	43.99037700	30.40609500	42.29181600
H	44.96658900	33.82110800	36.58313700	C	43.90268000	30.59671300	40.91633700
H	45.29480500	36.76695200	37.24751700	C	43.54172200	31.85375100	40.41109400
H	43.95175700	35.96854900	36.40662900	C	43.25197000	32.89820600	41.31697700
H	43.67193600	36.61715000	39.03648500	C	44.85784700	35.54968700	43.15903500
H	43.15664600	35.00914400	38.51290300	C	46.14773800	35.93735900	43.09466100
H	45.84149800	35.87448200	39.65679500	C	46.62445100	37.00168300	42.20697900
H	44.84837500	34.54826900	40.26436900	C	48.51878300	38.98380400	41.56370700
C	40.54997500	33.82397400	32.70503400	C	49.69077900	38.77808000	40.59818500
C	40.17105900	34.04458500	34.16540600	C	50.57862000	41.03265300	40.26071600
C	41.25407900	33.61838600	35.16396000	C	50.89479200	42.12292800	39.26324500
C	40.90040600	34.14095600	36.55547600	H	43.84875400	35.30905300	44.94072100
C	41.42396900	32.10087800	35.21544100	H	44.36735000	29.15316200	43.69155000
H	41.47734000	34.34199400	32.46862800	H	44.82942800	33.12105100	45.64904800

H 45.84434600 33.10156400 44.19374600
H 46.05597500 34.36263100 45.43153400
H 42.37362700 34.54336800 43.20247400
H 42.55969400 33.41161700 44.54487200
H 43.10792400 37.90190700 42.58246400
H 43.80098500 31.27514000 44.25940600
H 44.09457900 29.77406200 40.23417800
H 42.91028100 33.85913000 40.93891200
H 44.14120700 36.00379400 42.47967700
H 46.88605500 35.51529100 43.76816000
H 44.79945800 37.49119600 45.32627200
H 48.69949700 39.84306400 42.21066300
H 47.57202800 39.12757200 41.03884800
H 50.59988900 38.55681400 41.16677300
H 49.49379200 37.93743300 39.92729300
H 50.33671700 42.02428900 38.32813200
H 50.68568900 43.09831700 39.71103800
H 51.96541200 42.07969800 39.02356600
H 49.73485300 39.88524000 38.78272800
H 43.57238500 32.97403400 38.71799400
H 43.94444400 31.35894300 38.47927700
O 47.48062700 30.41402000 43.56003100
H 47.36975100 30.09702300 42.64065000
H 47.28868700 29.65515100 44.11464400
O 46.76942700 38.33418900 38.20472900
H 47.68988000 38.63829100 38.17768400
H 46.53084800 38.18680600 39.12500600
O 42.82513700 28.70776800 35.93115900
H 42.08508900 29.31326300 35.83882700
H 42.51071000 27.96215000 36.44967600
O 49.93534400 31.13421600 44.50478500
H 49.10318000 30.89461700 44.04760800
H 50.20507400 31.98000300 44.14424000
O 46.83760700 29.23984400 41.20189700
H 46.71227000 29.60983200 40.32440800
H 45.96028700 28.98169300 41.51747600
H 46.91366000 30.60649100 34.79626400
H 45.22663800 30.07046200 34.69622700
H 40.41720500 24.55498200 42.67999100
H 38.66470800 28.33932100 41.13114100
H 39.61866500 39.50625100 46.36927200
H 41.24422900 39.67757900 47.05505300
H 46.44212900 34.78276300 36.53782500
H 44.40524600 36.87575400 53.56617200
H 44.26717300 35.13001100 53.38632400
H 51.73995400 33.41771400 49.16923600
H 51.11404200 35.04461100 49.43586500
H 48.28227300 37.83867400 49.88730100
H 47.36642100 38.28013700 51.33820900
H 44.14336900 45.02799700 41.45043600
H 43.48225900 45.98780300 40.12135300
H 55.34955200 34.44776700 35.95643400
H 56.02797800 36.05011600 35.65345700
H 40.68268300 32.76725500 32.48779900
H 39.76842000 34.20667300 32.05285600
H 47.45047800 29.93244000 52.14531500
H 48.86091900 30.17802600 51.11052600

H 37.67854200 33.69703400 42.86311700
H 49.76871200 39.60420800 33.22041400
H 50.95149700 44.31888600 32.76913800
H 39.37106300 29.92914700 44.56228400
H 51.58169200 39.84195300 47.63836800
H 53.45126400 43.14623900 43.83237700
H 47.67031400 31.88692600 40.08400000
H 43.95770700 41.79891900 41.01671800
H 55.60411400 42.07986300 33.02580800
N 44.68425600 40.48127600 42.49006000
H 44.30533500 39.61852500 42.86446400
N 52.81008600 40.50885000 34.21178500
H 52.47851000 41.09669700 34.96980600
H 54.25160700 45.23560800 35.77559800
C 47.80897600 37.74857800 34.19935800
H 46.84788600 37.23727200 34.17712600
H 47.76624300 38.58025500 33.49204500
H 48.57208700 37.04649000 33.86461700
C 40.38710400 33.88855900 50.33042000
H 41.33544900 34.09055900 50.83099100
H 39.77298500 34.78915100 50.32957400
H 39.86461800 33.08554900 50.84621800

Coordinates of DH2-TS_{3a} system

C 47.27574800 37.90674300 50.31332200
C 46.25098400 38.70416900 49.48163200
C 46.25580200 38.41478000 48.01188900
C 45.31990100 37.84821500 47.18693000
N 47.31980100 38.76106800 47.18470700
C 47.04593900 38.43164600 45.91873700
N 45.83797500 37.87346700 45.90436800
H 47.09275700 36.83134800 50.22755700
H 45.23918400 38.50580100 49.84998800
H 46.42938300 39.77856000 49.62298900
H 48.12710200 39.34667300 47.46228300
H 44.35166800 37.41920200 47.38903400
H 47.66322500 38.60124800 45.04363300
C 50.85397000 34.04403100 49.09595600
C 50.35231600 34.17059600 47.66304900
C 49.15301100 35.11192600 47.50462600
C 48.82660200 35.27029700 46.02148100
C 47.92221800 34.60522000 48.25423000
H 50.11811600 33.55268900 49.72703700
H 51.16755700 34.54769700 47.04068500
H 50.08251000 33.18200800 47.28872300
H 49.42930000 36.09361800 47.91003400
H 48.51909100 34.31369600 45.60588100
H 48.01629800 35.98042300 45.87656500
H 49.68845100 35.62982700 45.46424200
H 47.65364100 33.60817800 47.91469600
H 48.10282000 34.56390000 49.32473300
H 47.06884400 35.25929400 48.08093800
C 51.33511000 40.09310100 46.60608000
C 50.00805600 40.85908200 46.69166500
O 49.19160400 40.59752400 47.57965400
C 51.17247300 38.79436500 45.80027600
C 50.84507400 39.09519300 44.34235600

C 52.45078100 37.96539400 45.90183900
H 52.10069100 40.71804500 46.14540500
H 50.34930900 38.21640500 46.23578000
H 49.90526000 39.63285200 44.25176300
H 51.63014100 39.68994500 43.87970000
H 50.74746400 38.16673900 43.78598000
H 53.29649800 38.51888700 45.49961700
H 52.66844700 37.70833100 46.93599700
H 52.34514600 37.04383400 45.33493900
N 49.77517700 41.82699300 45.79361100
C 48.55098500 42.65297200 45.72603300
C 47.39576000 41.75380200 45.28018800
O 47.58566000 40.86588100 44.46211700
C 48.79424200 43.77960200 44.70756900
C 47.57633400 44.68526300 44.54692300
C 49.99652300 44.62700100 45.12364100
H 50.37480100 41.87787400 44.98270600
H 48.37643200 43.05124100 46.72805200
H 49.00109700 43.29986600 43.74383700
H 46.68619800 44.12778000 44.26899400
H 47.38517000 45.23537100 45.46683200
H 47.76944800 45.41164500 43.76197500
H 50.91226000 44.04454400 45.18489300
H 50.14496800 45.42221900 44.39719800
H 49.81788400 45.08437300 46.09506700
N 46.19600400 41.96072900 45.83908000
C 45.02283600 41.27756800 45.31951700
C 44.53841700 41.97857300 44.03273800
O 44.81605200 43.15041600 43.77726700
C 43.99826700 41.41334800 46.44450000
C 44.33300400 42.78927400 47.01344800
C 45.85953900 42.84167300 46.94314800
H 45.26650800 40.24380000 45.07240600
H 42.97667800 41.34932400 46.07822900
H 44.15709800 40.63307700 47.19229000
H 43.91425900 43.55925100 46.36622800
H 43.96110800 42.93508800 48.02535700
H 46.20885700 43.85867800 46.77123500
H 46.31385300 42.45492000 47.86430400
C 43.29517400 41.59556800 41.94559400
H 44.06984800 42.16646800 41.42764100
H 43.05153400 40.69440500 41.37926200
C 44.40094600 45.64286400 40.59109600
C 45.18906000 44.57745400 39.83317200
C 46.38877800 44.03266700 40.61977000
C 46.91587300 42.75047700 39.97485900
C 47.51488600 45.06107000 40.70051800
H 44.99549600 46.54103100 40.73745100
H 44.51553600 43.74806100 39.60301700
H 45.53784600 44.98676800 38.88125500
H 46.05544200 43.80055700 41.63676800
H 47.26028900 42.94751300 38.96082300
H 47.74980900 42.35116600 40.54845600
H 46.14138000 41.98817200 39.93030300
H 47.18470100 45.96375400 41.20756200
H 48.36077000 44.65051300 41.24813500
H 47.85440900 45.33123900 39.70150700
C 50.44686000 39.75804000 34.05376000
C 51.89588700 39.82056500 33.47968600
O 52.16990900 39.23595200 32.45163800
C 50.41068600 38.56035000 35.05757100
C 49.23594200 38.61984400 36.00373400
N 48.05739200 38.20652000 35.53744500
O 49.34670000 39.02137900 37.16062500
H 50.20807400 40.68012900 34.58356900
H 50.43142200 37.62314700 34.50637500
H 51.31393400 38.61830000 35.66966600
H 47.28606500 38.21926600 36.19573400
C 54.23506000 40.65115300 33.86072100
C 55.17166700 40.27924400 35.04133200
O 56.04294800 39.44719700 34.89427100
C 54.55749300 42.04507800 33.33102700
H 54.42539100 39.91010500 33.07671500
H 53.93094300 42.26090100 32.46846000
H 54.38733300 42.80535900 34.08817900
N 55.00786300 40.96627000 36.19370600
C 55.85984500 40.78773000 37.37781600
C 54.91320900 40.89888600 38.57713700
O 54.13897100 41.85363400 38.64681400
C 56.92725500 41.89935000 37.47239500
C 57.77065700 41.73055600 38.73425800
C 57.81440700 41.90062900 36.23179300
H 54.19830800 41.56152400 36.32764700
H 56.33388600 39.80930200 37.28618400
H 56.40522900 42.86057400 37.53426200
H 58.47269000 42.55707400 38.81614200
H 57.15389800 41.72528100 39.63048400
H 58.34357800 40.80607100 38.68890200
H 58.57769000 42.66984900 36.32318800
H 58.30114400 40.93587800 36.11182000
H 57.23340700 42.09732200 35.33441800
N 54.90536700 39.95541200 39.51676300
C 54.06307000 40.11994200 40.69722400
C 54.48181100 41.40533000 41.41596300
O 55.63128500 41.81044200 41.37470800
C 54.34423100 38.88050200 41.54657600
C 55.77844600 38.53554600 41.16036700
C 55.80219000 38.83858900 39.66364200
H 53.01489700 40.19351800 40.39773700
H 54.22820400 39.08541600 42.60902700
H 53.66619600 38.07244700 41.26869100
H 56.46838300 39.20193000 41.67835800
H 56.04249800 37.50355500 41.37921800
H 56.80662700 39.08253900 39.31991600
H 55.42889500 37.98282800 39.08702000
N 53.49560900 41.97638500 42.11128000
C 53.69898500 43.24120800 42.76986100
C 52.87189100 44.35353500 42.11832600
C 53.41548000 45.75936400 42.39329400
C 52.56829600 46.78964000 41.64913700
C 53.45338400 46.08412300 43.88434000
H 52.52542100 41.68953700 41.95802200
H 54.76427000 43.47479600 42.69171100
H 52.88232300 44.19118600 41.03879800

H	51.83489300	44.28238500	42.45401500	C	44.11813500	33.32542800	48.52559000
H	54.43726100	45.81424900	42.00395100	O	44.14506900	32.38979600	47.55234400
H	52.57600000	46.58779500	40.58071700	H	45.65455300	35.99044300	52.64344300
H	51.53784600	46.76561300	41.99988800	H	42.69788500	36.28772300	51.93390900
H	52.96356100	47.78963500	41.80683200	H	43.98222200	37.26645800	51.24307800
H	54.10955800	45.40073900	44.41653400	H	42.82785400	36.39050500	49.14002100
H	53.82721500	47.09419000	44.03369400	H	45.11479500	33.85715900	51.70171500
H	52.45830800	46.02132000	44.31838400	H	43.00495800	34.72472700	47.34126600
C	53.83086100	44.39220300	36.32312700	H	45.27800200	32.20302500	49.91920600
C	52.60103000	43.77196300	35.57243600	H	44.83731600	31.71177000	47.77033900
O	52.24864300	42.64234200	35.88427800	C	40.57829400	38.99778100	46.50964200
C	53.33300800	44.83808000	37.72100900	C	41.21706100	38.90097700	45.11299800
C	54.45953500	45.28573100	38.58278200	C	42.47885100	38.05451800	44.98288300
C	55.06449700	46.49910000	38.77841700	O	42.42818800	36.83171600	45.44814200
N	55.14203800	44.41139700	39.38290000	O	43.48535000	38.50372200	44.40951600
C	56.10342400	45.11761400	40.01219600	H	40.30707600	38.00669800	46.88515800
N	56.08248100	46.37833300	39.67059900	H	40.48488300	38.46958200	44.41795300
H	54.57710800	43.61237000	36.44061300	H	41.46750800	39.89432200	44.73102300
H	52.60944600	45.64871900	37.60544300	H	44.16914400	38.15435000	41.21972200
H	52.84394300	43.98389500	38.18706100	C	38.54594500	33.27338400	42.34839000
H	54.93467100	43.42462000	39.46133700	C	38.80611200	31.94205000	43.10647400
H	54.82657900	47.44847000	38.34095200	O	38.13582500	30.96475600	42.82670100
H	56.79114500	44.67697000	40.70550000	C	39.62826100	34.33675100	42.40625400
N	51.93826700	44.47773500	34.61403000	C	39.22502800	35.64083500	41.70206200
C	50.73096100	44.07796900	33.80907700	C	40.28092800	36.71361800	41.96135500
C	49.45734200	44.73592200	34.34017500	C	39.04210200	35.45851500	40.19843200
C	48.30907200	44.46681900	33.37051200	H	38.33709200	32.97971900	41.32229200
C	49.11966400	44.21648200	35.73510700	H	39.83798800	34.58238100	43.45109600
H	52.24037800	45.42659600	34.45006500	H	40.53891500	33.94809400	41.94873100
H	50.66007400	42.99214200	33.87204700	H	38.27394000	35.97911400	42.13108700
H	49.62423600	45.81821700	34.39648900	H	41.21210600	36.47513900	41.45362800
H	48.13583500	43.39717800	33.27669200	H	39.94820000	37.68167500	41.59524500
H	47.39526100	44.93173100	33.73126700	H	40.48341400	36.79827600	43.02714800
H	48.53174900	44.86732400	32.38428100	H	39.95133000	35.05887400	39.75485000
H	49.94890800	44.37685700	36.41989800	H	38.21814800	34.78551100	39.97779000
H	48.24432600	44.72744700	36.12870200	H	38.82849700	36.41707500	39.73091700
H	48.90867000	43.14990000	35.70041900	N	39.74347400	31.89595500	44.08768900
C	47.78505700	30.31783000	51.18515100	C	40.01597600	30.72395800	44.94009900
C	46.94353700	29.73648500	50.04619100	C	39.72376600	31.00739700	46.40916100
C	47.31124000	30.30492500	48.71450500	C	40.75831800	31.92564200	47.05302200
C	48.53213700	30.30972300	48.09097200	C	40.39349500	32.18181400	48.52480200
N	46.40000600	30.91504400	47.89838100	N	40.59129800	33.45375200	48.95706400
C	47.06085700	31.27187200	46.82070400	O	39.92982800	31.31651700	49.23682600
N	48.35611900	30.92794800	46.88945600	H	40.32757200	32.70079900	44.24266800
H	47.66438000	31.39830100	51.23434600	H	41.06025300	30.43051100	44.79929700
H	47.08270600	28.65183900	50.02040500	H	38.73305700	31.45793300	46.49414100
H	45.88449900	29.92859800	50.22762800	H	39.70528200	30.06759600	46.96167300
H	49.48309700	29.93022800	48.40035600	H	41.74636300	31.46116000	47.03601900
H	46.62644300	31.78196500	45.98407800	H	40.81772700	32.87869900	46.52461700
H	49.06985000	31.10471600	46.17792700	H	41.10355800	34.09199100	48.36825800
C	44.59746300	36.04155600	52.89437600	C	39.22712200	28.08698900	40.23190800
C	43.75557100	36.27582400	51.64898900	C	39.93946900	26.73135800	40.42503100
C	43.94370100	35.24878700	50.56255900	O	40.13035600	25.97604700	39.49025300
C	43.36897600	35.46898300	49.31543900	C	40.21205000	29.23785000	39.97503100
C	44.64066000	34.06446200	50.75619300	C	39.39849600	30.50284700	39.67947600
C	43.44994700	34.53005800	48.30575100	C	41.15593100	28.90088300	38.82363100
C	44.73212700	33.11847900	49.75465600	C	40.25212900	31.75991400	39.58864000

H	38.57814500	27.96962800	39.36378000	H	41.94170200	31.37551900	32.71554600
H	40.80601300	29.40817200	40.88002600	H	42.79663100	30.67897700	34.08322400
H	38.85413900	30.36216700	38.74183500	C	45.94600500	30.63597500	35.28696900
H	38.66170000	30.62848000	40.47513000	C	46.07151400	30.16922600	36.73255100
H	40.58034300	28.79101500	37.90575000	O	44.83478600	30.17264800	37.41947900
H	41.90025700	29.68255800	38.69909200	H	45.55474300	31.64979000	35.25423000
H	41.66979800	27.96294700	39.01890400	H	46.50434700	29.15918900	36.75907600
H	40.75698000	31.93750600	40.53466600	H	46.72626200	30.85078200	37.27731400
H	41.01039200	31.67190400	38.81698800	H	44.21611800	29.60940600	36.91695500
H	39.62916600	32.61956800	39.35414000	C	55.42102400	35.46347500	36.33845500
N	40.34361600	26.41877500	41.68473700	C	54.02491200	36.06874300	36.45988500
C	41.06011600	25.19092200	42.06395600	C	53.11207800	35.31238800	37.43455400
C	42.43717200	25.51572700	42.62469900	C	53.47779500	35.60211100	38.88909100
H	40.18695200	27.08951400	42.42106100	C	51.64663300	35.67500400	37.19798700
H	41.13730500	24.59419700	41.15376400	H	55.93271100	35.45100700	37.29852000
H	43.02622800	26.05826500	41.88976600	H	54.10623300	37.11341900	36.77207700
H	42.35228300	26.12803500	43.52031700	H	53.56496300	36.06419100	35.46942100
H	42.95883600	24.59762700	42.88114500	H	53.23278300	34.23898100	37.25181100
C	47.07593000	32.79485700	40.17995100	H	52.84556200	35.02430000	39.55989200
C	46.81194200	33.27653900	38.72735600	H	54.51441000	35.34541200	39.09383500
O	47.44516300	32.77429900	37.80864900	H	53.32772600	36.65879000	39.10592600
C	47.74817400	33.84862500	41.06643200	H	51.00095300	35.10419400	37.86144400
C	48.02351400	33.25253700	42.44450100	H	51.47925200	36.73413800	37.38472300
C	49.04142500	34.35346100	40.43342500	H	51.35758700	35.45499300	36.17305700
H	46.13139600	32.48588800	40.63154400	C	44.10862800	35.06847600	44.17002400
H	47.07126900	34.69695200	41.19813600	N	50.04887700	39.98688000	39.74412200
H	47.09497700	32.90854400	42.89658900	O	44.64772600	29.60537400	43.48316400
H	48.70356700	32.40855800	42.36171300	S	48.29655000	37.60799700	42.57239100
H	48.46501600	34.00935900	43.08958700	C	45.04665600	34.43162100	45.18035800
H	49.48983300	35.12257400	41.05946300	N	43.50329700	31.88962700	39.44166600
H	49.75078600	33.53675700	40.31621800	O	45.97240300	37.80478300	41.24081500
H	48.84494500	34.77657700	39.45072600	C	42.89176100	34.22765800	43.77134000
N	45.85582300	34.19765700	38.45495100	O	50.90223900	41.22590800	41.43989700
C	45.51425700	34.62197200	37.09597600	C	43.25832500	32.98697400	42.97532100
C	44.62156900	35.84632400	37.22571700	O	43.21098900	38.26127300	41.40684500
C	43.97262800	35.62092300	38.58299100	C	43.71842500	31.83983100	43.63623500
C	45.16000500	35.06793400	39.35507900	C	44.13371900	30.74070800	42.88396900
H	44.99101500	33.79603500	36.59869000	C	44.07402700	30.74369400	41.49247000
H	45.22073000	36.75541100	37.26198400	C	43.60737900	31.88575200	40.82077800
H	43.90932700	35.91772000	36.40601800	C	43.19911000	33.00269100	41.58199400
H	43.58370600	36.53016500	39.03556200	C	44.66639800	35.89384700	43.18713700
H	43.16575100	34.88754600	38.51111700	C	45.97938300	36.37827600	43.18499600
H	45.80190400	35.90921300	39.64704000	C	46.51234500	37.27062800	42.22494400
H	44.87124000	34.54413900	40.27091700	C	48.58086200	39.05578900	41.49964400
C	40.54998200	33.82395600	32.70503500	C	49.78677100	38.82956100	40.58599000
C	40.69845600	33.44905900	34.17624600	C	50.60630900	41.10989700	40.23554100
C	41.95615200	32.62769900	34.48702600	C	50.90876500	42.19661000	39.23174500
C	42.09280000	32.44418400	35.99863400	H	43.22420800	36.20206000	44.95223500
C	41.92768700	31.26614900	33.79628300	H	44.61222100	29.72945600	44.44460100
H	41.44113600	34.33817000	32.35066300	H	44.50855000	33.76937100	45.85979400
H	40.73053100	34.36720500	34.76848600	H	45.82190400	33.82679500	44.68865800
H	39.81824800	32.88514800	34.49448600	H	45.57147500	35.17144400	45.79589700
H	42.82946000	33.18165400	34.12330500	H	42.21713700	34.85280000	43.17861800
H	42.13757600	33.41027900	36.49706900	H	42.34998300	33.92660000	44.67870400
H	41.23279400	31.90427400	36.39058700	H	43.20412000	38.31814600	42.37572300
H	42.99389400	31.88700000	36.24461300	H	43.77144300	31.81474400	44.72197800
H	41.02690700	30.71998800	34.07233200	H	44.36987800	29.86219700	40.93161000

H 42.82848000 33.88894200 41.07161200
H 44.01172700 36.23863400 42.38694800
H 46.68480700 35.98045300 43.90672900
H 45.35592000 37.59323400 45.04072000
H 48.74395200 39.93432700 42.12425100
H 47.66103100 39.19141900 40.92578800
H 50.67780900 38.62321000 41.18817400
H 49.61433800 37.97311600 39.92927900
H 50.35660300 42.07862500 38.29534800
H 50.68307000 43.17219400 39.67049300
H 51.98028200 42.16221800 38.99546000
H 49.84413200 39.91075400 38.75349600
H 43.50406200 32.79892600 39.00227500
H 44.07014000 31.22107000 38.92788800
O 49.56611000 30.15449800 42.63272300
H 48.64603800 29.87169200 42.45842400
H 50.12106300 29.41277800 42.38769000
O 46.75248200 38.26301400 38.25470500
H 47.66276500 38.58986400 38.24983400
H 46.48807600 38.16081000 39.17794800
O 42.91073100 28.65429000 36.04409900
H 42.18411800 29.27110700 35.92023700
H 42.57988000 27.93501700 36.58814100
O 50.15147800 31.56293300 44.86972100
H 49.96655700 31.01088700 44.08267600
H 50.19340100 32.46589100 44.54910600
O 47.07017200 29.31033200 41.97865800
H 46.81393400 29.69131900 41.13471500
H 46.27209100 29.30370700 42.52749400
H 46.92403000 30.62740200 34.81627600
H 45.27762600 29.97827900 34.73233400
H 40.46058400 24.64988700 42.80191800
H 38.61780300 28.32006500 41.10580100
H 39.67299000 39.60964300 46.46190100
H 41.26249200 39.46073100 47.22989200
H 46.42975200 34.81378700 36.52761800
H 44.45326100 36.86021300 53.59700000
H 44.30765900 35.12003600 53.39232600
H 51.76619000 33.45278800 49.12075200
H 51.07063700 35.02459600 49.51584500
H 48.29799000 38.10968900 49.97697600
H 47.20239200 38.19346500 51.36641100
H 44.10659300 45.26295300 41.56684500
H 43.50497600 45.91573700 40.03787400
H 55.36134800 34.44237500 35.96887000
H 56.01670900 36.05015900 35.64355300
H 40.39251200 32.94315300 32.08857500
H 39.69701300 34.48563300 32.57177300
H 47.47600300 29.89035300 52.13572600
H 48.83824800 30.09748500 51.03129400
H 37.61521900 33.66347200 42.77121400
H 49.76763400 39.60469500 33.22116700
H 50.93122000 44.37433700 32.77969400
H 39.36117200 29.93380000 44.56875500
H 51.63050800 39.85665500 47.62855700
H 53.43938500 43.13841800 43.82913600
H 47.73374900 31.93155500 40.08017500

H 42.40694800 42.23338800 42.03419300
H 55.59933600 42.08262600 33.02215500
N 43.78499600 41.17928400 43.25071600
H 43.66257000 40.21328300 43.54168800
N 52.81115000 40.50448000 34.21381800
H 52.48065600 41.08419200 34.97815500
H 54.25181300 45.23576300 35.77592600
C 47.80897800 37.74858100 34.19935200
H 46.83729400 37.25827700 34.17307900
H 47.79024200 38.57716300 33.48774300
H 48.55928000 37.02737500 33.87557200
C 40.38710600 33.88856600 50.33042200
H 41.34368700 34.09976100 50.81096600
H 39.76193700 34.78153900 50.34547300
H 39.88551500 33.07912900 50.85683800

Coordinates of DH2-IM3_a system

C 47.27576200 37.90675500 50.31332500
C 46.17401300 38.50398800 49.41688500
C 46.33131200 38.25649300 47.94919800
C 45.55983300 37.55679600 47.06147100
N 47.37288900 38.78550600 47.19488600
C 47.23860500 38.42397100 45.91862200
N 46.14643000 37.68045400 45.81610100
H 47.32227800 36.82188200 50.20120100
H 45.20379900 38.09582700 49.70948100
H 46.11702200 39.58560000 49.58557100
H 48.09817300 39.44152400 47.52411000
H 44.66470700 36.97895200 47.21461800
H 47.87526900 38.68929000 45.08735400
C 50.85394200 34.04405000 49.09590400
C 50.35252700 34.03279300 47.65791700
C 49.17526000 34.98150600 47.40746100
C 48.89382300 35.05444000 45.90893900
C 47.91788200 34.53750100 48.15308400
H 50.10481900 33.64800800 49.77666800
H 51.17528700 34.32491400 47.00105300
H 50.05763600 33.01798900 47.38577700
H 49.45716100 35.98171200 47.76042000
H 48.58524700 34.07877200 45.54140000
H 48.10165300 35.76627300 45.69464100
H 49.77789000 35.36919400 45.35958400
H 47.63024100 33.53407300 47.84905900
H 48.07819100 34.53362300 49.22784900
H 47.08532200 35.20605600 47.93932000
C 51.33507500 40.09311600 46.60608600
C 50.02050500 40.88006800 46.69902100
O 49.21768500 40.65158000 47.60858000
C 51.14986200 38.78787800 45.81581800
C 50.84683900 39.07637000 44.35049300
C 52.40717500 37.93048000 45.94117700
H 52.10446300 40.70300300 46.13169000
H 50.31004500 38.23371200 46.25062400
H 49.93193700 39.65181900 44.24028600
H 51.65900800 39.63160900 43.88568500
H 50.71554400 38.14366000 43.80847800
H 53.27020400 38.45942100 45.54280000

H 52.60702500 37.67913900 46.98034600 H 50.20823000 40.68001100 34.58396000
H 52.28507200 37.00597500 45.38267600 H 50.43152000 37.62313300 34.50621000
N 49.77922200 41.83111200 45.78433100 H 51.31411600 38.61840100 35.66921500
C 48.55098800 42.65295700 45.72601400 H 47.28796500 38.21231500 36.19841500
C 47.40468100 41.74426700 45.28004700 C 54.23507200 40.65115400 33.86072500
O 47.59327600 40.89098300 44.42613700 C 55.17267300 40.28012800 35.04078700
C 48.77174300 43.78619700 44.71189400 O 56.04529400 39.44958100 34.89271800
C 47.54233700 44.68265500 44.58961300 C 54.55639700 42.04527700 33.33077000
C 49.97853800 44.63571100 45.10851600 H 54.42558800 39.91028300 33.07658400
H 50.36175800 41.86324300 44.95999500 H 53.92921100 42.26072100 32.46856200
H 48.38116900 43.04373700 46.73147700 H 54.38622600 42.80542900 34.08803400
H 48.95974200 43.31506000 43.74020700 N 55.00841900 40.96652300 36.19332000
H 46.65232200 44.11925900 44.32310300 C 55.85985300 40.78773300 37.37781600
H 47.36463900 45.21542800 45.52240300 C 54.91149800 40.89811700 38.57638300
H 47.71082300 45.42313600 43.81231000 O 54.13531200 41.85124100 38.64497400
H 50.89640200 44.05462600 45.14628800 C 56.92669200 41.89971200 37.47329700
H 50.10945200 45.43643400 44.38468500 C 57.77010200 41.73049300 38.73505900
H 49.81892100 45.08536700 46.08681500 C 57.81394000 41.90227500 36.23272500
N 46.21802100 41.89571700 45.88221900 H 54.19764700 41.56000100 36.32818500
C 45.05221000 41.19696900 45.36751000 H 56.33421600 39.80946700 37.28630600
C 44.54642300 41.91536600 44.09865000 H 56.40425700 42.86066800 37.53579700
O 44.76845500 43.10178700 43.89246200 H 58.47204300 42.55706700 38.81732300
C 44.03881800 41.29924700 46.50621800 H 57.15313500 41.72488700 39.63111000
C 44.35871900 42.66948300 47.09748200 H 58.34308500 40.80605200 38.68937200
C 45.88289300 42.75204400 47.00517600 H 58.57709600 42.67155400 36.32485000
H 45.31144800 40.16904400 45.10770200 H 58.30082300 40.93769800 36.11191800
H 43.01443500 41.22756800 46.14925500 H 57.23295800 42.09965300 35.33548300
H 44.21657800 40.50689200 47.23672800 N 54.90491700 39.95499400 39.51649000
H 43.91654300 43.44411900 46.47182700 C 54.06308000 40.11994500 40.69722600
H 43.99941400 42.78884100 48.11744500 C 54.48112000 41.40677400 41.41370600
H 46.20923000 43.77841900 46.84277600 O 55.62914300 41.81582700 41.36682800
H 46.36022800 42.36096600 47.91266700 C 54.34608200 38.88195900 41.54808800
C 43.34054300 41.55723900 41.98566100 C 55.77995600 38.53694400 41.16066100
H 44.12485500 42.08552200 41.44185900 C 55.80217100 38.83858800 39.66363700
H 43.03668300 40.67402200 41.42655000 H 53.01462200 40.19178600 40.39876800
C 44.40094400 45.64287700 40.59110700 H 54.23144400 39.08860900 42.61036500
C 45.19344900 44.56067300 39.86209200 H 53.66782700 38.07327900 41.27271700
C 46.38311300 44.02569100 40.67034000 H 56.47037600 39.20388100 41.67734100
C 46.92265000 42.73976500 40.04335900 H 56.04441300 37.50518000 41.38017000
C 47.50573300 45.05740400 40.75803300 H 56.80624700 39.08236600 39.31869000
H 44.99743400 46.54111500 40.72863300 H 55.42850100 37.98213700 39.08827500
H 44.51926800 43.72963700 39.64008400 N 53.49636000 41.97557200 42.11256100
H 45.55395600 44.95137000 38.90679500 C 53.69898000 43.24120700 42.76985300
H 46.03613600 43.80103700 41.68461800 C 52.86830500 44.35128300 42.11883200
H 47.28993700 42.93194100 39.03650200 C 53.40788900 45.75867300 42.39352200
H 47.74253100 42.34132600 40.63729800 C 52.55929500 46.78623000 41.64720100
H 46.14894500 41.97766500 39.98415700 C 53.44216400 46.08449200 43.88443200
H 47.16869200 45.96175600 41.25759000 H 52.52711000 41.68023500 41.96830800
H 48.34699600 44.65129300 41.31586200 H 54.76360200 43.47675300 42.68888100
H 47.85466200 45.32371700 39.76129100 H 52.87861000 44.18891100 41.03928600
C 50.44687400 39.75807700 34.05381200 H 51.83170400 44.27736100 42.45524600
C 51.89568500 39.82107800 33.47942300 H 54.43017300 45.81587200 42.00582800
O 52.16914300 39.23846900 32.44998200 H 52.56959500 46.58378000 40.57891800
C 50.41060400 38.56028000 35.05754200 H 51.52826100 46.75949100 41.99605300
C 49.23683600 38.61775600 36.00563900 H 52.95147900 47.78741600 41.80511400
N 48.05814800 38.20274800 35.53902800 H 54.09895100 45.40296900 44.41825100
O 49.34809000 39.01715700 37.16257000 H 53.81328600 47.09554500 44.03394400

H	52.44634800	46.01948300	44.31649400	H	43.13022500	34.68793900	47.31848500
C	53.83086100	44.39220500	36.32312600	H	45.23813600	32.12532900	49.98857800
C	52.60113400	43.77202500	35.57219500	H	44.88676700	31.65360600	47.80176500
O	52.24919500	42.64218700	35.88302400	C	40.57824500	38.99752500	46.50925000
C	53.33300800	44.83808000	37.72100900	C	41.16864800	38.90860400	45.09263700
C	54.45920300	45.28380300	38.58407900	C	42.39060200	38.02832700	44.93432100
C	55.06504300	46.49647300	38.78141500	O	42.20331500	36.74399500	45.23391000
N	55.13995200	44.40819900	39.38417800	O	43.46209100	38.43862600	44.51796300
C	56.10122500	45.11291500	40.01516700	H	40.26182600	38.01648600	46.86756400
N	56.08191200	46.37402000	39.67467000	H	40.40652300	38.52003700	44.40956700
H	54.57683400	43.61212300	36.44070100	H	41.45463900	39.89552900	44.72764500
H	52.61014300	45.64937000	37.60561500	H	44.20836900	38.08810600	41.24453900
H	52.84262400	43.98363400	38.18627400	C	38.54583300	33.27358300	42.34884100
H	54.93157000	43.42150900	39.46170600	C	38.80708400	31.93835600	43.10053500
H	54.82845500	47.44644200	38.34448800	O	38.14528700	30.95832700	42.81172700
H	56.78766600	44.67093500	40.70887300	C	39.64618300	34.31982200	42.38449300
N	51.93791900	44.47831200	34.61417900	C	39.25161400	35.63453500	41.69612900
C	50.73096100	44.07796900	33.80907500	C	40.32912400	36.68679100	41.95109900
C	49.45632400	44.73245000	34.34199500	C	39.04548900	35.46568400	40.19414400
C	48.30810600	44.46288500	33.37239200	H	38.31113200	32.98387300	41.32725800
C	49.12038000	44.20968200	35.73609000	H	39.88638600	34.55841600	43.42461300
H	52.23928900	45.42754100	34.45107100	H	40.53823500	33.91783700	41.90256800
H	50.66210400	42.99189400	33.87008100	H	38.31201500	35.98433900	42.14097700
H	49.62112100	45.81498400	34.40025600	H	41.25377900	36.42733700	41.44176600
H	48.13698700	43.39306700	33.27674000	H	40.01594600	37.66081800	41.58375100
H	47.39352500	44.92533000	33.73440800	H	40.53492000	36.76762300	43.01645700
H	48.52954000	44.86558700	32.38676300	H	39.94458500	35.06143300	39.73452100
H	49.94967400	44.37034000	36.42073200	H	38.21286100	34.80098200	39.98110200
H	48.24419300	44.71810800	36.13113000	H	38.83314800	36.42933700	39.73663900
H	48.91170700	43.14272500	35.69955800	N	39.73705900	31.89509500	44.08884300
C	47.78505800	30.31783000	51.18515200	C	40.01606000	30.72396700	44.94006200
C	46.96591900	29.66510200	50.06914700	C	39.72559500	31.00620600	46.40798800
C	47.32331300	30.19616300	48.71997800	C	40.75822700	31.92562100	47.05297700
C	48.52727100	30.13815700	48.06667900	C	40.36310900	32.19654600	48.51500500
N	46.42124900	30.84017400	47.92082400	N	40.63009900	33.44998800	48.96452300
C	47.07038400	31.15469200	46.82297700	O	39.81326400	31.36265600	49.20236900
N	48.34954800	30.75209800	46.86319700	H	40.30829100	32.70684100	44.25465400
H	47.62790200	31.39474700	51.19262700	H	41.06120100	30.43459500	44.79658100
H	47.14014900	28.58572800	50.08540300	H	38.73465300	31.45573500	46.49486400
H	45.90097800	29.83250200	50.23997300	H	39.70733400	30.06660000	46.96064500
H	49.46642600	29.71671800	48.35756300	H	41.74511100	31.45823900	47.05478400
H	46.63693200	31.67216300	45.99100200	H	40.82806900	32.87521600	46.51939100
H	49.04877500	30.88880500	46.12839300	H	41.22464100	34.04783000	48.41102700
C	44.59746500	36.04155600	52.89438100	C	39.22721700	28.08713700	40.23176900
C	43.69766700	36.20648300	51.67658500	C	39.95291400	26.73854400	40.42298900
C	43.92645200	35.19268700	50.58493100	O	40.17697000	25.99937100	39.48254100
C	43.41813800	35.43041800	49.31249300	C	40.20171000	29.24276400	39.95392400
C	44.59367800	33.99469400	50.80390600	C	39.37609400	30.50079200	39.66183500
C	43.52898800	34.49150200	48.30377400	C	41.13361500	28.90847500	38.79204100
C	44.71714900	33.05151800	49.80383700	C	40.21980700	31.76372100	39.56034500
C	44.16126100	33.27229400	48.54880100	H	38.56832200	27.96044000	39.37238400
O	44.20020500	32.33868100	47.57820100	H	40.80658300	29.42178700	40.85005000
H	45.64439700	36.02173100	52.60004400	H	38.82468200	30.35335000	38.72936900
H	42.65257000	36.13771900	51.99840800	H	38.64540800	30.62415300	40.46346300
H	43.83177400	37.21078300	51.26366000	H	40.54869000	28.79310200	37.88067200
H	42.90516700	36.36384400	49.11439400	H	41.87130500	29.69491000	38.65907900
H	45.01705700	33.77643200	51.77089700	H	41.65583700	27.97461300	38.98335000

H	40.73095400	31.94627000	40.50202900	H	46.80055000	30.73188000	37.25547500
H	40.97315000	31.67985300	38.78326300	H	44.31714600	29.43550400	36.88938200
H	39.58862500	32.61838100	39.32921400	C	55.42102600	35.46347600	36.33845700
N	40.33229400	26.41278700	41.68693800	C	54.02714400	36.07376400	36.45996300
C	41.06012200	25.19087300	42.06400000	C	53.11080100	35.31928300	37.43276900
C	42.38431100	25.53448200	42.73028200	C	53.47657200	35.60486000	38.88807700
H	40.14373200	27.06687500	42.43070700	C	51.64708400	35.68852800	37.19603200
H	41.21637100	24.63586800	41.13770600	H	55.93211700	35.44786500	37.29879600
H	42.99533300	26.14287600	42.06841800	H	54.11213800	37.11759400	36.77394200
H	42.21657800	26.08798600	43.65223900	H	53.56781400	36.07262700	35.46917600
H	42.92709100	24.62361400	42.96797700	H	53.22734400	34.24569400	37.24808200
C	47.07595700	32.79483100	40.17995000	H	52.84199900	35.02780900	39.55727800
C	46.78250500	33.24786900	38.72479100	H	54.51224900	35.34451900	39.09311000
O	47.38145700	32.71413600	37.80065200	H	53.32952800	36.66150500	39.10693400
C	47.81126600	33.85562500	41.00646400	H	50.99866400	35.12088000	37.85936000
C	48.21532100	33.25861800	42.35158300	H	51.48456500	36.74824200	37.38342200
C	49.03989600	34.37800500	40.26763300	H	51.35736400	35.47051100	36.17081100
H	46.14063200	32.52445600	40.67391100	C	44.22789700	34.70878000	43.97564600
H	47.13781400	34.69500400	41.19864600	N	50.00737100	39.96378300	39.78501300
H	47.33506900	32.89968100	42.88102400	O	44.52143300	29.28356600	43.11953800
H	48.89475000	32.42262500	42.20401300	S	48.32663000	37.49363800	42.57947600
H	48.70237800	34.01870900	42.95880200	C	45.12453900	34.07715500	45.01117400
H	49.54523600	35.12994400	40.87068500	N	43.52156600	31.81033500	39.19849700
H	49.73383000	33.56526900	40.06255100	O	45.97069100	37.74592700	41.31277300
H	48.75451900	34.82884400	39.31957300	C	42.95857600	33.95532400	43.62205800
N	45.84626600	34.19021600	38.45465200	O	50.90842300	41.18061500	41.46632900
C	45.51425500	34.62195100	37.09596200	C	43.25775800	32.72960700	42.77570500
C	44.61676100	35.84337500	37.22676100	O	43.26619500	38.23359700	41.46113800
C	43.97067400	35.61949800	38.58586400	C	43.67243700	31.53909100	43.38194900
C	45.16002600	35.06800800	39.35508500	C	44.05057600	30.46459800	42.57906800
H	44.99911500	33.79848400	36.58564300	C	44.00492900	30.54201400	41.19301700
H	45.21360600	36.75401700	37.26171600	C	43.59271600	31.73126400	40.57570500
H	43.90315300	35.91242100	36.40786800	C	43.20806200	32.81641300	41.38826600
H	43.58323200	36.52990200	39.03732100	C	44.69576100	35.68500000	43.14807300
H	43.16354400	34.88569400	38.51845700	C	46.00351500	36.26305700	43.20854800
H	45.80654200	35.90743100	39.64116300	C	46.51492900	37.16714400	42.26817600
H	44.87666900	34.54731000	40.27412600	C	48.57940800	38.97885700	41.55110600
C	40.54999400	33.82394400	32.70504300	C	49.77030800	38.79019300	40.61393900
C	40.71079700	33.42564400	34.16847300	C	50.58711600	41.07401600	40.27297600
C	41.94693700	32.56110700	34.44604200	C	50.87754500	42.16789300	39.27509600
C	42.11461700	32.36900900	35.95318800	H	42.98581000	36.21719600	44.90470100
C	41.85520900	31.20269900	33.75466700	H	44.47950200	29.34109000	44.08068500
H	41.44995000	34.31696600	32.34289400	H	44.56304600	33.45235500	45.70563700
H	40.78251200	34.33478000	34.77107300	H	45.88349700	33.43520500	44.54641100
H	39.81874500	32.88590400	34.49534700	H	45.67038500	34.81594400	45.60461100
H	42.82934300	33.08603800	34.06186600	H	42.29046200	34.62043200	43.07182600
H	42.20385100	33.33126100	36.45281500	H	42.43634600	33.64344100	44.53594500
H	41.24770100	31.85622300	36.36565200	H	43.25070800	38.20733400	42.42325200
H	43.00320200	31.78251800	36.17393800	H	43.72620800	31.46325500	44.46455600
H	40.94894400	30.68218400	34.06025300	H	44.28011600	29.68145000	40.59276100
H	41.83647800	31.31424100	32.67425000	H	42.87525800	33.74009600	40.92338100
H	42.71506500	30.58863400	34.01155600	H	44.03208100	36.05469300	42.36874200
C	45.94600000	30.63599100	35.28700200	H	46.74913200	35.75550400	43.81059200
C	46.15287000	30.06455100	36.68453900	H	45.83493700	37.28665100	44.89867900
O	44.94878500	29.95790900	37.41970800	H	48.73470000	39.84295500	42.19309900
H	45.53035800	31.63843100	35.35103600	H	47.65060900	39.11620500	40.99772600
H	46.62763300	29.07572300	36.61410400	H	50.67290100	38.58099700	41.19323400

H 49.59747000 37.94352000 39.94808800
H 50.32237500 42.05930500 38.34204200
H 50.65236300 43.13751300 39.72118900
H 51.94553000 42.14193200 39.03288100
H 49.80041400 39.89439500 38.79746800
H 43.57762500 32.73906400 38.81224800
H 44.08665700 31.14801400 38.67763200
O 49.44567200 30.03934200 42.45446900
H 48.53472700 29.77418700 42.22017700
H 50.00997600 29.32105800 42.16473300
O 46.76082500 38.23045100 38.29038800
H 47.66976000 38.55982500 38.27524700
H 46.51036300 38.12357300 39.21713800
O 42.92201800 28.60702500 36.02492300
H 42.22454900 29.26658600 35.97346800
H 42.58252100 27.88214700 36.55611000
O 50.07324100 31.31592900 44.76504500
H 49.85307900 30.80692900 43.95891500
H 50.14101200 32.23012800 44.48253200
O 46.99798600 29.17530100 41.62979900
H 46.74535900 29.54672700 40.78032600
H 46.18393800 29.10283100 42.14801700
H 46.90012200 30.69084700 34.77250700
H 45.26763300 30.00438100 34.71430700
H 40.43141100 24.59997900 42.73703300
H 38.62775900 28.32293900 41.11160800
H 39.70817000 39.65583000 46.50653000
H 41.30383300 39.40316300 47.21927400
H 46.43369900 34.82152900 36.53649800
H 44.44890400 36.87449600 53.57874800
H 44.36541400 35.12547800 53.43070700
H 51.74677700 33.42984400 49.18567500
H 51.10328900 35.05667500 49.40755700
H 48.25741200 38.31784000 50.06436000
H 47.07231500 38.13996600 51.35991000
H 44.09197500 45.28214000 41.56966100
H 43.51328400 45.90946700 40.02167100
H 55.35776500 34.44305100 35.96753700
H 56.01930300 36.04880400 35.64461900
H 40.35766800 32.95617400 32.08001900
H 39.71445900 34.51144500 32.59364500
H 47.49046300 29.91708800 52.15195400
H 48.84533900 30.12805300 51.03861900
H 37.63084100 33.67712500 42.79288400
H 49.76748600 39.60502000 33.22125800
H 50.93019300 44.37664300 32.78015000
H 39.36464100 29.93100300 44.56875300
H 51.63704100 39.86370100 47.62829900
H 53.44187000 43.13890600 43.82976200
H 47.70558000 31.91054700 40.08268600
H 42.49329600 42.23950800 42.10103000
H 55.59806300 42.08339800 33.02134700
N 43.83869100 41.11342000 43.27877100
H 43.77691500 40.13454000 43.51998600
N 52.81138700 40.50352900 34.21430300
H 52.48114400 41.08155500 34.97999800
H 54.25207200 45.23572400 35.77601900

C 47.80898400 37.74856600 34.19935900
H 46.83808200 37.25672700 34.17249500
H 47.78828300 38.57950200 33.49055200
H 48.56022700 37.02967700 33.87269400
C 40.38711300 33.88857500 50.33041900
H 41.32917200 34.01488100 50.86642400
H 39.83917700 34.83091400 50.32222100
H 39.79136300 33.11950500 50.81768300

Coordinates of DH2-TS4_a system

C 47.27575500 37.90674500 50.31333700
C 46.06895000 38.17413100 49.39703200
C 46.33953200 37.97527800 47.93790800
C 45.70178400 37.20840500 46.99307400
N 47.35866500 38.62220100 47.25159600
C 47.32207300 38.25373800 45.95809800
N 46.32135400 37.39945600 45.77147600
H 47.62212700 36.87394500 50.20758600
H 45.24669700 37.50317200 49.66702700
H 45.70762300 39.19843900 49.56558200
H 48.02440300 39.30958000 47.62181500
H 44.85245500 36.55091000 47.09733200
H 48.00420300 38.59137400 45.19213200
C 50.85397600 34.04402900 49.09596200
C 50.43742200 33.94251200 47.63539000
C 49.26643400 34.86100500 47.27185300
C 49.07529500 34.86882300 45.75738100
C 47.97337800 34.42892700 47.96110100
H 50.06757300 33.68385000 49.75417200
H 51.29355800 34.20743100 47.01006400
H 50.16648800 32.90999200 47.40562300
H 49.51360600 35.87973300 47.59548800
H 48.78785900 33.87765400 45.41371600
H 48.30214900 35.57580000 45.47020700
H 49.99436200 35.15793900 45.25246200
H 47.73737800 33.39659500 47.71400200
H 48.05721100 34.50814700 49.04167600
H 47.14079300 35.05303000 47.64345900
C 51.33509700 40.09310100 46.60606900
C 50.02120100 40.88666500 46.70290600
O 49.17738500 40.59189800 47.54876900
C 51.15345900 38.81387300 45.77514600
C 50.92438600 39.14401900 44.30442500
C 52.38225500 37.92054500 45.93267800
H 52.11732400 40.71176200 46.16510900
H 50.28368100 38.27033800 46.16154500
H 50.04626800 39.76829600 44.16274000
H 51.78091000 39.66882000 43.88667200
H 50.77747200 38.22709000 43.73891900
H 53.27574200 38.43831800 45.59051600
H 52.52669900 37.63461000 46.97210600
H 52.26376900 37.01536400 45.34224400
N 49.83451400 41.92565100 45.86582200
C 48.55100900 42.65298200 45.72605700
C 47.64552500 41.71691300 44.91473300
O 48.10197500 41.11410000 43.95336100
C 48.78153600 43.97153700 44.98321100

C 47.45909300 44.69355900 44.73317400
C 49.73141200 44.86791400 45.77416500
H 50.45095500 42.01057500 45.06974200
H 48.16378100 42.81679200 46.73280400
H 49.23160500 43.72418500 44.01484900
H 46.76060100 44.07109200 44.17866100
H 47.00189000 44.98943600 45.67570000
H 47.64031700 45.59500600 44.15373400
H 50.68830500 44.38047100 45.94442400
H 49.90444600 45.79513600 45.23338000
H 49.29808300 45.11543700 46.74112100
N 46.38795100 41.52355300 45.32280300
C 45.51759500 40.66296100 44.53724300
C 45.05081800 41.39129500 43.26363400
O 44.86465400 42.60800000 43.24229800
C 44.32794600 40.41142500 45.46329000
C 44.23692200 41.72624400 46.23175800
C 45.70212400 42.09649700 46.46454200
H 46.05057500 39.75129700 44.25815200
H 43.42443200 40.17488900 44.90597800
H 44.54868300 39.58335400 46.13988200
H 43.77049400 42.48135900 45.59988600
H 43.67792500 41.64104100 47.16140700
H 45.83873300 43.17643700 46.51141700
H 46.08688800 41.64377200 47.38770300
C 44.21925300 40.96113900 40.97503300
H 44.97712900 41.08308800 40.19190600
H 43.50001000 40.19742100 40.66645100
C 44.40094100 45.64285500 40.59109400
C 45.32747800 44.81596700 39.70373700
C 46.47470100 44.15349800 40.47567200
C 47.20899300 43.14851400 39.58807600
C 47.47095100 45.18450100 41.00024200
H 44.90717400 46.52525300 40.97384500
H 44.73688900 44.03180300 39.22329300
H 45.73962300 45.44879400 38.91285300
H 46.04551300 43.62022800 41.32949200
H 47.72289800 43.66112800 38.77624000
H 47.94516800 42.59739800 40.16920900
H 46.51559500 42.43409000 39.14982100
H 46.99097900 45.87308900 41.68941600
H 48.28170700 44.68496700 41.52623300
H 47.89648700 45.75761200 40.17734900
C 50.44686000 39.75804500 34.05376600
C 51.89716600 39.81787900 33.48117500
O 52.17177000 39.22546500 32.45777100
C 50.41068200 38.56034600 35.05756300
C 49.23408100 38.62323300 36.00002500
N 48.05603300 38.21248800 35.53267800
O 49.33862600 39.02541700 37.15870800
H 50.20867700 40.68032400 34.58331700
H 50.43271300 37.62296200 34.50700300
H 51.31276800 38.61971100 35.67111100
H 47.27553800 38.24762800 36.17871300
C 54.23506200 40.65115200 33.86072100
C 55.17009500 40.27708100 35.04211100
O 56.03793600 39.44120400 34.89588200
C 54.55938500 42.04490900 33.33212000
H 54.42525500 39.91011200 33.07665500
H 53.93407300 42.26202500 32.46896500
H 54.38925800 42.80492300 34.08951500
N 55.00835300 40.96602400 36.19318200
C 55.85984300 40.78773000 37.37781700
C 54.91050300 40.89688300 38.57546300
O 54.13260900 41.84875300 38.64152000
C 56.92604200 41.90029900 37.47251300
C 57.77267600 41.72946500 38.73179300
C 57.81006900 41.90516200 36.22959900
H 54.20028100 41.56340800 36.32698300
H 56.33479000 39.80976600 37.28598400
H 56.40317000 42.86081500 37.53801300
H 58.47521900 42.55559200 38.81301600
H 57.15767100 41.72380500 39.62911600
H 58.34506400 40.80475200 38.68384600
H 58.57330100 42.67439000 36.32116500
H 58.29698000 40.94092800 36.10603100
H 57.22692600 42.10403900 35.33405900
N 54.90225100 39.95281100 39.51476400
C 54.06307800 40.11994400 40.69722800
C 54.48704200 41.40705700 41.41193700
O 55.63043900 41.82584100 41.34326700
C 54.34563300 38.88170900 41.54764400
C 55.77977000 38.53736300 41.16076400
C 55.80218300 38.83858800 39.66364100
H 53.01445100 40.19453700 40.40245200
H 54.22985100 39.08775900 42.60976500
H 53.66776500 38.07285600 41.27144700
H 56.46967100 39.20477600 41.67742400
H 56.04521000 37.50588300 41.38059200
H 56.80597000 39.08429800 39.31927900
H 55.43095000 37.98098800 39.08821900
N 53.51079600 41.96316200 42.13133500
C 53.69898100 43.24120600 42.76985800
C 52.84156900 44.31844800 42.09984700
C 53.27872600 45.74795900 42.43186900
C 52.44078700 46.73793100 41.62479800
C 53.15634200 46.04698700 43.92349400
H 52.54432300 41.65348800 41.99879800
H 54.75823100 43.49609000 42.68123500
H 52.91537800 44.18056000 41.01941900
H 51.79554900 44.17610000 42.38266300
H 54.32620200 45.86666000 42.13565200
H 52.56418300 46.55962900 40.55924500
H 51.38568300 46.63989900 41.87482800
H 52.75239100 47.75778100 41.83490500
H 53.81586600 45.40948100 44.50621900
H 53.42713900 47.08134000 44.12107700
H 52.13347200 45.89079600 44.25855500
C 53.83086100 44.39220300 36.32312700
C 52.60100800 43.77238400 35.57228700
O 52.24798400 42.64255500 35.88331100
C 53.33300700 44.83808000 37.72100900
C 54.45287900 45.28505500 38.59141900
C 55.04404900 46.50225700 38.80491100

N 55.13200200 44.41076400 39.39467600 O 42.37160700 38.06956300 44.44050000
C 56.07774200 45.12081600 40.04283500 H 41.09338100 39.87462100 46.10825800
N 56.05043300 46.38371000 39.71042300 H 42.32646000 38.10572400 47.44682400
H 54.57698600 43.61223900 36.44067000 H 41.04696400 36.95552800 47.12716300
H 52.60989300 45.64906800 37.60419000 H 43.99111000 37.73177000 41.46952000
H 52.84074100 43.98332700 38.18429500 C 38.54587300 33.27344000 42.34872000
H 54.93253500 43.42179100 39.46542300 C 38.83825400 31.93606700 43.08103200
H 54.80382600 47.45271700 38.37097700 O 38.22200000 30.93843000 42.75254600
H 56.75914800 44.68080600 40.74261600 C 39.53252100 34.41961100 42.49845900
N 51.93873400 44.47781000 34.61325000 C 39.00261900 35.71553300 41.86605300
C 50.73096100 44.07796900 33.80907600 C 39.90351700 36.89154900 42.23366500
C 49.46086100 44.75064100 34.32987600 C 38.90203400 35.60568200 40.34696100
C 48.31163900 44.47449400 33.36334200 H 38.41896300 33.00289900 41.30331400
C 49.11908200 44.25339300 35.73187600 H 39.71584200 34.61886800 43.55855800
H 52.24094000 45.42653500 34.44852500 H 40.47876900 34.15125700 42.02621800
H 50.65254800 42.99343000 33.88363200 H 38.00086100 35.90531000 42.27029600
H 49.63389600 45.83261500 34.37078700 H 40.88453300 36.77722900 41.78173000
H 48.13174600 43.40468500 33.28502900 H 39.47801100 37.82421000 41.87206600
H 47.40055800 44.95033100 33.71659800 H 40.02380600 36.97269900 43.31223100
H 48.53754200 44.85914500 32.37156100 H 39.87130100 35.35028700 39.92432700
H 49.94805500 44.42088000 36.41542300 H 38.17944600 34.85056200 40.04964300
H 48.24496600 44.77373500 36.11581200 H 38.58742800 36.55723400 39.92492900
H 48.90391100 43.18723300 35.71338200 N 39.74197600 31.90014400 44.09326900
C 47.78505800 30.31782900 51.18515300 C 40.01599300 30.72395100 44.94004500
C 47.05640900 29.53569000 50.08995700 C 39.72743600 31.00641200 46.40477900
C 47.42235400 30.01705000 48.72555800 C 40.75827800 31.92565700 47.05299600
C 48.60330500 29.86031200 48.04679300 C 40.29902600 32.23792900 48.49029700
N 46.55751800 30.72920600 47.94469500 N 40.69788100 33.43839500 48.98158500
C 47.20384200 30.98754500 46.83154700 O 39.58295300 31.48528500 49.11616100
N 48.44747500 30.48364400 46.84467300 H 40.25829700 32.73576200 44.31258900
H 47.54822400 31.37785300 51.11760800 H 41.06009600 30.42954400 44.79584700
H 47.31159800 28.47678100 50.17725400 H 38.73736900 31.45720900 46.49335400
H 45.97708700 29.63504900 50.21789800 H 39.70523700 30.06746200 46.95820500
H 49.51068100 29.36420200 48.32066500 H 41.73766200 31.44550200 47.10148900
H 46.79381700 31.53363900 46.00695800 H 40.86230000 32.86361700 46.50478300
H 49.12635900 30.55831100 46.08600000 H 41.43628000 33.93915100 48.50745900
C 44.59746400 36.04155500 52.89437700 C 39.22717100 28.08708000 40.23180100
C 43.54770600 36.00887100 51.78903300 C 39.96601600 26.74594200 40.42140500
C 43.84929400 35.03092600 50.68334800 O 40.22862000 26.02553000 39.47609200
C 43.44531300 35.30975500 49.38360900 C 40.19556900 29.24175400 39.92014400
C 44.49310300 33.82172000 50.91795100 C 39.37088900 30.50534800 39.64676400
C 43.63953100 34.40431100 48.35591600 C 41.09383800 28.90394000 38.73288200
C 44.70602100 32.91403800 49.89991300 C 40.21791800 31.76853300 39.55726800
C 44.26225600 33.18280000 48.60925300 H 38.55115200 27.95045400 39.38740800
O 44.38948600 32.29404300 47.60429600 H 40.82625700 29.42058600 40.79840200
H 45.59305700 36.15734600 52.47168700 H 38.81509400 30.37012600 38.71516700
H 42.57818200 35.75387400 52.23065700 H 38.64499900 30.62206000 40.45339000
H 43.44608700 37.00899200 51.35857800 H 40.48401600 28.78085900 37.83892900
H 42.94986600 36.24868300 49.17209300 H 41.82216600 29.69449900 38.57551700
H 44.82820500 33.57227800 51.91243300 H 41.62581000 27.97382800 38.91406000
H 43.32286100 34.63212400 47.34863700 H 40.71270600 31.95383000 40.50754200
H 45.21070800 31.98061700 50.09576900 H 40.98424700 31.68385000 38.79280200
H 45.06571400 31.60284900 47.84085500 H 39.59311100 32.62524400 39.31361500
C 40.57829500 38.99766100 46.50942700 N 40.31723100 26.40464800 41.68937600
C 41.55135700 37.83673500 46.71442400 C 41.06012300 25.19089100 42.06399000
C 42.28792300 37.41020700 45.45894800 C 42.32738300 25.55177200 42.82513200
O 42.86991700 36.20923400 45.62397300 H 40.09063800 27.03841600 42.44006800

H	41.29155300	24.67919200	41.12857200	H	55.92783100	35.43588600	37.30074800
H	42.94574000	26.22458100	42.23604200	H	54.12052600	37.12123100	36.78483100
H	42.08066800	26.04102600	43.76574300	H	53.57649600	36.09369500	35.46621100
H	42.89772700	24.65294700	43.04331100	H	53.21662800	34.24971100	37.22344100
C	47.07593600	32.79485700	40.17995100	H	52.82633400	35.00745700	39.53956100
C	46.75504400	33.21882700	38.72313900	H	54.49970100	35.32092000	39.08546300
O	47.32145800	32.65993100	37.79505700	H	53.32473900	36.64396900	39.10995800
C	47.90343500	33.84866900	40.92609100	H	50.99061300	35.12955200	37.83218700
C	48.38682600	33.26775300	42.25177700	H	51.48806800	36.76047900	37.37950200
C	49.09366000	34.31205600	40.09044100	H	51.36051700	35.49892300	36.14992500
H	46.15084700	32.59141700	40.72236200	C	44.42037300	34.31677500	43.78567000
H	47.27027700	34.71511700	41.13833100	N	49.93539300	39.97568900	39.77321900
H	47.53962600	32.96731300	42.86261700	O	44.30994500	28.90792900	42.71014000
H	49.00727900	32.39356400	42.07096300	S	48.33357600	37.44697600	42.55047500
H	48.96524500	34.01190700	42.79557000	C	45.29563500	33.54774800	44.73736800
H	49.67928900	35.04224100	40.64623400	N	43.58055800	31.70613700	38.91563200
H	49.73099500	33.46685000	39.84002700	O	45.82962500	37.82977900	41.69669700
H	48.75947300	34.77087200	39.16238500	C	43.09406500	33.66222900	43.43672900
N	45.83928400	34.18440600	38.45578900	O	50.95087400	41.09622500	41.46153700
C	45.51425800	34.62196000	37.09596900	C	43.30123700	32.45476200	42.53706600
C	44.57647200	35.81516300	37.22645600	O	43.01429600	37.72580800	41.48406800
C	43.95050300	35.58623000	38.59498500	C	43.61672200	31.20546700	43.08694800
C	45.16000600	35.06795000	39.35509400	C	43.93196800	30.14737400	42.23154800
H	45.03547000	33.79001100	36.56541700	C	43.92185400	30.30314500	40.84893800
H	45.14175600	36.74685500	37.23785900	C	43.60634800	31.55151100	40.29290200
H	43.85141200	35.85034800	36.41590600	C	43.27778600	32.61781300	41.15373900
H	43.53893800	36.48547000	39.04700000	C	44.80484100	35.46888500	43.18810300
H	43.16545200	34.82884600	38.54149900	C	46.11263700	36.11803600	43.36778200
H	45.80461200	35.92072800	39.61192600	C	46.53582900	37.13686100	42.45180400
H	44.90344200	34.56144400	40.28872500	C	48.51248000	38.94963700	41.52098700
C	40.54998900	33.82395000	32.70503200	C	49.70196000	38.78241600	40.57079000
C	40.69815000	33.38593900	34.15772600	C	50.58907200	41.04528400	40.27400900
C	41.91763300	32.49228300	34.41357400	C	50.90266600	42.15204800	39.29352900
C	42.09581900	32.28070200	35.91631800	H	43.40608400	35.96185500	44.82548600
C	41.78989000	31.14279800	33.71054700	H	44.24427800	28.92084200	43.67727800
H	41.45815800	34.31408000	32.35968700	H	44.71984700	33.18758500	45.59811000
H	40.78511700	34.27799500	34.78334700	H	45.70546200	32.65602400	44.24417300
H	39.79582300	32.85459000	34.46911200	H	46.12902300	34.14213400	45.11767200
H	42.80742800	33.00209500	34.02573200	H	42.45278400	34.39358400	42.93369300
H	42.20619700	33.23466600	36.42700700	H	42.58936500	33.34809200	44.36123000
H	41.22486700	31.77798900	36.33201800	H	42.80199300	37.95500600	42.40622000
H	42.97682000	31.67760600	36.12017500	H	43.64783800	31.07079800	44.16592100
H	40.88140500	30.63429100	34.02877700	H	44.15233000	29.46164200	40.20313000
H	41.75272400	31.26542700	32.63183800	H	43.00840200	33.58410500	40.73560100
H	42.64323900	30.51077600	33.94535700	H	44.10201400	35.95577600	42.51280600
C	45.94601200	30.63597600	35.28696700	H	46.92783800	35.44630700	43.63840200
C	46.27285800	29.95927900	36.61268400	H	46.12675500	36.84737500	44.64766900
O	45.12984500	29.73731500	37.41719200	H	48.66490100	39.81604500	42.16578200
H	45.51383600	31.61724700	35.46543100	H	47.56920100	39.07383000	40.98453700
H	46.77799200	29.00140400	36.42550300	H	50.60708800	38.56693500	41.14801400
H	46.93259000	30.60483500	37.19523700	H	49.53069400	37.94980600	39.88275200
H	44.46779700	29.25994300	36.88013200	H	50.33275200	42.07479900	38.36354000
C	55.42102400	35.46347500	36.33845500	H	50.70683300	43.12037900	39.76189200
C	54.03074300	36.08142000	36.45925900	H	51.97006500	42.10360700	39.04109900
C	53.10560500	35.32186800	37.41940000	H	49.73694700	39.92865000	38.78026300
C	53.46637200	35.58906500	38.87943200	H	43.73385700	32.65342200	38.59614400
C	51.64530000	35.70224200	37.17953500	H	44.16440600	31.04500200	38.40359700

O 49.24328400 29.94973200 42.17867300
H 48.34760700 29.66999800 41.91072100
H 49.83754700 29.28668000 41.82343800
O 46.74624500 38.40656700 38.16558400
H 47.67305100 38.69414800 38.14052700
H 46.50006300 38.29792200 39.08796100
O 42.98485500 28.57553700 36.03944700
H 42.31406000 29.26452400 36.04073400
H 42.62246100 27.83631700 36.53454300
O 50.02168700 30.96105900 44.58977900
H 49.71156100 30.54543600 43.76137300
H 50.22189400 31.87136900 44.36410200
O 46.86226600 28.99877200 41.22140700
H 46.60696100 29.30781000 40.34764600
H 46.04106300 28.84094200 41.70497500
H 46.85618000 30.76073300 34.70903500
H 45.24067100 30.03317700 34.71608900
H 40.41264100 24.55234600 42.67287800
H 38.64691200 28.33357000 41.12117300
H 40.10966100 39.27144100 47.45927000
H 39.78776700 38.72691800 45.80275700
H 46.43541100 34.85834500 36.55364600
H 44.40625400 36.87662200 53.56504300
H 44.57628800 35.12996300 53.48497500
H 51.74329300 33.44446500 49.27642100
H 51.07910200 35.07586500 49.35899200
H 48.11324600 38.57190800 50.07240300
H 47.00364600 38.08034500 51.35883000
H 44.06554400 45.04548400 41.43579200
H 43.52993800 45.97051000 40.02763300
H 55.35315200 34.44699300 35.95768500
H 56.02585400 36.05146500 35.65265900
H 40.34946800 32.97532300 32.05667500
H 39.72422100 34.52513900 32.60709100
H 47.48926600 29.95723900 52.16739600
H 48.86113800 30.20111100 51.08115900
H 37.56498900 33.58186100 42.72374200
H 49.76784600 39.60456100 33.22101300
H 50.93574400 44.36183600 32.77699400
H 39.36257700 29.93560700 44.56282900
H 51.61713800 39.82912500 47.62592400
H 53.44512700 43.15072900 43.83118400
H 47.65311700 31.87519800 40.09285500
H 43.71654400 41.91782600 41.12448000
H 55.60159200 42.08148700 33.02440700
N 44.81292500 40.54933200 42.23464800
H 45.10874000 39.58167900 42.30872500
N 52.81051500 40.50641000 34.21228200
H 52.47960700 41.09023700 34.97360100
H 54.25199000 45.23559100 35.77573800
C 47.80898000 37.74858200 34.19935500
H 46.84456500 37.24338900 34.17722400
H 47.77451000 38.57401400 33.48414700
H 48.56840400 37.03821300 33.87334500
C 40.38710800 33.88856600 50.33042000
H 41.27002300 33.83297000 50.96907400
H 40.02241100 34.91495400 50.29825100

H 39.61339800 33.23178100 50.72248100

Coordinates of DH2-P(a3) system

C 47.27571900 37.90672000 50.31331300
C 46.54519800 39.04557900 49.58910200
C 46.20876200 38.63065900 48.19955600
C 45.10218400 38.03732400 47.65081400
N 47.15436800 38.61755500 47.19402400
C 46.60235100 38.04941000 46.09431200
N 45.35232400 37.67457800 46.33874000
H 46.65664900 37.00360900 50.32969500
H 45.62497200 39.30943100 50.12298700
H 47.17640400 39.94332800 49.57122800
H 48.04376400 39.11269500 47.24441100
H 44.14597100 37.83989200 48.10984700
H 47.13684800 37.95163700 45.16103000
C 50.85397600 34.04402800 49.09596300
C 50.21600700 34.02379500 47.71231700
C 49.00165000 34.94932100 47.58058700
C 48.56811400 35.02510400 46.11824600
C 47.83031700 34.47684500 48.43782400
H 50.17444300 33.64729900 49.84528300
H 50.96555100 34.32787900 46.97697900
H 49.91012100 33.00309200 47.47063500
H 49.29344600 35.95430400 47.90841600
H 48.34746500 34.02664500 45.74622200
H 47.67376700 35.63723500 46.02648000
H 49.35008100 35.46072000 45.49894000
H 47.55839200 33.45660800 48.17760500
H 48.07763200 34.50930800 49.49524800
H 46.96120800 35.11157200 48.27685300
C 51.33510200 40.09310400 46.60609300
C 50.00806900 40.86739500 46.67147800
O 49.13438700 40.52985200 47.46320600
C 51.14291700 38.77644200 45.83820100
C 50.80188100 39.04328100 44.37520700
C 52.40433700 37.92290700 45.94844600
H 52.10653200 40.69637900 46.12632800
H 50.31271200 38.22887400 46.29901600
H 49.87909100 39.61031400 44.28157400
H 51.59718400 39.60209300 43.88565300
H 50.67207500 38.10010900 43.84847800
H 53.25569900 38.44484500 45.51628100
H 52.63137200 37.69644100 46.98769200
H 52.27149600 36.98422400 45.41565400
N 49.84461000 41.93546300 45.86280500
C 48.55101800 42.65299300 45.72600600
C 47.61162400 41.68908400 45.02957400
O 47.99127300 40.99984700 44.09409300
C 48.77755100 43.92688800 44.90339500
C 47.46326300 44.65088000 44.62378600
C 49.74807700 44.85754700 45.62784300
H 50.47155100 42.03674900 45.07790600
H 48.21803100 42.88091500 46.73909100
H 49.20952800 43.61935200 43.94416900
H 46.76773600 44.00742400 44.09136900
H 47.00511700 44.99125400 45.55082300

H	47.65512000	45.52447000	44.00583000	O	54.13747300	41.85156900	38.64421800
H	50.69919200	44.36898600	45.82523000	C	56.92638800	41.90016000	37.47137600
H	49.93023500	45.74424500	45.02523700	C	57.77279900	41.73023000	38.73094600
H	49.32564400	45.17583800	46.57895400	C	57.81039100	41.90353100	36.22849000
N	46.37326900	41.59376300	45.51599200	H	54.20203000	41.56665200	36.32604900
C	45.44561700	40.77484700	44.76099300	H	56.33452400	39.80966700	37.28555200
C	45.25741000	41.34620100	43.34568800	H	56.40364100	42.86077800	37.53608100
O	45.55489000	42.50112700	43.05072200	H	58.47555800	42.55620800	38.81144300
C	44.15243400	40.84329100	45.58802300	H	57.15774400	41.72569400	39.62825900
C	44.28575700	42.15100300	46.36921000	H	58.34495900	40.80531800	38.68406300
C	45.77981400	42.23600600	46.68398300	H	58.57305800	42.67342400	36.31880400
H	45.82646000	39.75504900	44.67053900	H	58.29809000	40.93947000	36.10658000
H	43.26622500	40.82636500	44.95654700	H	57.22712800	42.10053800	35.33260700
H	44.11268700	39.99606200	46.27335400	N	54.90151900	39.95200900	39.51413600
H	44.00443100	42.98937800	45.73126600	C	54.06303600	40.11994700	40.69721500
H	43.67051200	42.16561500	47.26662200	C	54.48409000	41.40883600	41.40957700
H	46.10968200	43.26609700	46.79184600	O	55.62838100	41.82543900	41.34510200
H	46.03737500	41.66432900	47.58255700	C	54.34980800	38.88465600	41.55081400
C	44.41506500	40.80795900	41.09453900	C	55.78364700	38.54155200	41.16172300
H	45.33317600	40.91178500	40.50711000	C	55.80220600	38.83859500	39.66364800
H	43.79559900	40.01658500	40.67254200	H	53.01379700	40.18991600	40.40316000
C	44.40094200	45.64289800	40.59109400	H	54.23623100	39.09399900	42.61254800
C	45.25292500	44.83944400	39.61207200	H	53.67273900	38.07370500	41.27859900
C	46.46954200	44.17321800	40.26582700	H	56.47336900	39.21178300	41.67485600
C	47.11469800	43.17917300	39.29974900	H	56.05146000	37.51126500	41.38418300
C	47.50914100	45.20093500	40.70593600	H	56.80506700	39.08391400	39.31642400
H	44.93615300	46.51747100	40.95154600	H	55.43025900	37.97941500	39.09112900
H	44.62813000	44.05879800	39.17030400	N	53.50529000	41.96859000	42.12241400
H	45.58753000	45.49067600	38.79974600	C	53.69900300	43.24121400	42.76987200
H	46.13024600	43.62803300	41.15088700	C	52.84554300	44.32873600	42.11110500
H	47.53805000	43.69881900	38.44144100	C	53.31438300	45.75193300	42.42756500
H	47.91241800	42.63277900	39.79817900	C	52.46814600	46.75368600	41.64416200
H	46.38328400	42.46132000	38.93425100	C	53.24354300	46.05525900	43.92163200
H	47.09124900	45.88760800	41.43632400	H	52.53899700	41.66173100	41.99053100
H	48.35906200	44.69822500	41.16221500	H	54.75930900	43.49137000	42.68028800
H	47.86614700	45.77680900	39.85271700	H	52.89539300	44.18524800	41.02987900
C	50.44685400	39.75805100	34.05377200	H	51.80312500	44.20628600	42.41518000
C	51.89785900	39.81517400	33.48315600	H	54.35422600	45.85397700	42.09978900
O	52.17462900	39.21462200	32.46504600	H	52.55455700	46.57060800	40.57573300
C	50.41070500	38.56033400	35.05753600	H	51.42000100	46.67407400	41.92746000
C	49.23605200	38.61007100	36.00406000	H	52.80340100	47.76860700	41.84117300
N	48.05856100	38.19812400	35.53716500	H	53.91009900	45.40741700	44.48458600
O	49.34358200	38.99656900	37.16789400	H	53.53847700	47.08509600	44.10795800
H	50.20843800	40.68051900	34.58274200	H	52.22961100	45.91767200	44.28997600
H	50.43644400	37.62377000	34.50528500	C	53.83086100	44.39220300	36.32312700
H	51.31321500	38.62114600	35.67059200	C	52.60059100	43.77236300	35.57271600
H	47.28171100	38.21712800	36.18900400	O	52.24491200	42.64379400	35.88633600
C	54.23505700	40.65115100	33.86072100	C	53.33300900	44.83808000	37.72101000
C	55.16742900	40.27458000	35.04355700	C	54.45429100	45.28806900	38.58815400
O	56.03127600	39.43416000	34.89963800	C	55.04843200	46.50538900	38.79242900
C	54.56246800	42.04448200	33.33321700	N	55.13500600	44.41713200	39.39374100
H	54.42469900	39.90972900	33.07690100	C	56.08444100	45.12932700	40.03433800
H	53.93890000	42.26294200	32.46915000	N	56.05804400	46.39026800	39.69468400
H	54.39224200	42.80446900	34.09062500	H	54.57738600	43.61266100	36.44069900
N	55.00756300	40.96563700	36.19369000	H	52.60860200	45.64784600	37.60426400
C	55.85984800	40.78772900	37.37781500	H	52.84293000	43.98297300	38.18570000
C	54.91260700	40.89771000	38.57635300	H	54.93474800	43.42897800	39.47093600

H	54.80808200	47.45381100	38.35419000	O	38.32881100	30.90535400	42.66296800
H	56.76788500	44.69231900	40.73404300	C	39.65454500	34.30393100	42.21907500
N	51.94056900	44.47596800	34.61115600	C	39.13780500	35.63541400	41.65541000
C	50.73096100	44.07796900	33.80907700	C	40.24727200	36.68115900	41.70110200
C	49.47453300	44.79917100	34.29598500	C	38.63007400	35.49665600	40.22260500
C	48.32592800	44.51997700	33.32960400	H	38.16449400	32.99260600	41.36853000
C	49.10980400	44.35781300	35.71075800	H	40.09683600	34.50520100	43.19865000
H	52.24707600	45.42235200	34.44055200	H	40.43598400	33.91656700	41.56446600
H	50.62599700	42.99887300	33.91961100	H	38.30876300	35.97511400	42.28835000
H	49.67466500	45.87722300	34.30216500	H	41.04318300	36.42274600	41.00832900
H	48.11890000	43.45311500	33.28582800	H	39.86619900	37.65878700	41.41789000
H	47.42483700	45.03066000	33.65899700	H	40.67200700	36.75680700	42.69948900
H	48.56920600	44.86503500	32.32742600	H	39.41679500	35.10630100	39.58067300
H	49.93892700	44.52287100	36.39477100	H	37.77014300	34.83514300	40.16560400
H	48.24936400	44.91647900	36.07096400	H	38.33192400	36.46961600	39.83902600
H	48.86302400	43.29843800	35.72503500	N	39.72189300	31.90695600	44.10649100
C	47.78505600	30.31782700	51.18513700	C	40.01588800	30.72402000	44.94015300
C	46.83043000	29.70987800	50.15104500	C	39.73514400	30.99568200	46.40719400
C	47.20376400	30.03168300	48.73926600	C	40.75841000	31.92565800	47.05304600
C	48.23879500	29.53334200	47.98981300	C	40.28300900	32.24899600	48.48409600
N	46.48223600	30.89916900	47.96638800	N	40.72872400	33.42050400	48.99597300
C	47.07212900	30.91755500	46.79414400	O	39.51879500	31.52287600	49.08577900
N	48.14290300	30.10946000	46.75760400	H	40.15117000	32.76921400	44.39961100
H	47.79942100	31.40220800	51.09671700	H	41.06322100	30.44395900	44.78766100
H	46.82608800	28.62347300	50.27228000	H	38.73980900	31.43229600	46.50739900
H	45.81696200	30.07224200	50.33246700	H	39.72901100	30.05385400	46.95601400
H	49.00898200	28.83270400	48.23614200	H	41.73986600	31.45156800	47.11170400
H	46.74757400	31.50697800	45.96019000	H	40.86438800	32.86019700	46.49983800
H	48.70727000	29.92599600	45.92910900	H	41.47974800	33.91422500	48.53161600
C	44.59747000	36.04156000	52.89438800	C	39.22704100	28.08693200	40.23201100
C	43.75575700	36.28908800	51.64917600	C	39.95150300	26.73882900	40.42643400
C	43.96017400	35.28889900	50.53996800	O	40.19598400	26.00637000	39.48511300
C	43.37396700	35.52369300	49.30111300	C	40.21436600	29.22332400	39.91358600
C	44.71243300	34.13279500	50.69329700	C	39.40833200	30.48981600	39.60721600
C	43.53399100	34.64875800	48.24247600	C	41.13684500	28.85952200	38.75211300
C	44.86439500	33.23853800	49.65234500	C	40.27755300	31.73121400	39.46061500
C	44.27886900	33.48300900	48.41620200	H	38.54955000	27.95430700	39.38838400
O	44.40068300	32.61047900	47.39024100	H	40.83102700	29.41029400	40.80055100
H	45.65633000	36.02089900	52.64740400	H	38.83456900	30.33476800	38.69019100
H	42.69680900	36.28984000	51.92928900	H	38.70163300	30.64554300	40.42324400
H	43.98179400	37.28620700	51.25902300	H	40.55358600	28.73092800	37.84177800
H	42.76906600	36.40969100	49.16473200	H	41.87377000	29.64561500	38.60800900
H	45.18915100	33.91057200	51.63428900	H	41.65357200	27.92715600	38.96370300
H	43.11594900	34.87519800	47.27225100	H	40.87859300	31.87058000	40.35624900
H	45.45496400	32.34547400	49.78148700	H	40.94781100	31.64764500	38.60987000
H	45.05715300	31.91637500	47.64696300	H	39.65341100	32.60980300	39.31562700
C	40.57831000	38.99795500	46.50986900	N	40.31994000	26.40711300	41.69176000
C	40.81539200	38.32834200	45.14019700	C	41.06010400	25.19096600	42.06392300
C	42.27421300	37.99825200	44.87442000	C	42.32805300	25.54756500	42.82587800
O	42.80600500	37.23360100	45.81383600	H	40.10617900	27.04701900	42.44093700
O	42.89819800	38.40148000	43.89479000	H	41.28918500	24.67988400	41.12758600
H	40.90923900	38.34403100	47.32090700	H	42.94797700	26.22314000	42.24148800
H	40.24624600	37.39073800	45.09898500	H	42.08167400	26.03151700	43.76928700
H	40.46709000	38.96431100	44.32269800	H	42.89760900	24.64720500	43.03965700
H	43.98207300	37.74660900	40.97450300	C	47.07593600	32.79488300	40.17995000
C	38.54602000	33.27310700	42.34802900	C	46.78099100	33.24523200	38.72775700
C	38.87365200	31.92378600	43.04716400	O	47.38050100	32.70623500	37.80508000

C	47.77418300	33.85923600	41.03931400	H	50.99291800	35.15341000	37.85876200
C	48.43407100	33.17631600	42.23629900	H	51.50031000	36.77704700	37.39517300
C	48.81927200	34.63297400	40.23796000	H	51.35588900	35.51080300	36.17292400
H	46.14836300	32.48130300	40.66063700	C	44.40007400	34.30050700	43.34568000
H	47.02728900	34.56688700	41.41233200	N	49.92408200	39.95818500	39.76863400
H	47.73249300	32.50734000	42.72589100	O	44.41150300	28.72995300	42.67195500
H	49.28797900	32.58963500	41.90353000	S	48.01361400	37.74546500	42.63818600
H	48.78151300	33.91493600	42.95548900	C	45.33923500	33.60398100	44.28940900
H	49.35655800	35.32166300	40.88794800	N	43.88174700	31.27599800	38.65109300
H	49.53528300	33.94684300	39.79030100	O	45.85212000	37.64443700	41.09825000
H	48.35495900	35.20434900	39.43697700	C	43.14590000	33.51063500	42.99794900
N	45.84391500	34.18480900	38.45574100	O	50.92530000	41.11197700	41.44271400
C	45.51425100	34.62197300	37.09596700	C	43.42457300	32.25021100	42.20223300
C	44.52124800	35.76981300	37.22540000	O	43.01094400	37.84128300	40.95629700
C	43.92254100	35.52788100	38.60305800	C	43.71171800	31.04287800	42.84774300
C	45.16001100	35.06788900	39.35510000	C	44.07500500	29.93061300	42.08451500
H	45.08345600	33.77423000	36.54938800	C	44.14932500	29.99494100	40.69574100
H	45.04168300	36.72690900	37.21878300	C	43.84722200	31.19880400	40.04403700
H	43.78391300	35.75999800	36.42587200	C	43.46699900	32.31422500	40.81142400
H	43.47214500	36.41262800	39.04417700	C	44.56922300	35.53248500	42.84018100
H	43.17596800	34.73262200	38.56315600	C	45.65812300	36.48909500	43.23605900
H	45.78594700	35.94157600	39.57326000	C	46.36373000	37.27519100	42.14752900
H	44.93554500	34.57225100	40.30166200	C	48.37775500	39.12577100	41.49267300
C	40.54997700	33.82397500	32.70502900	C	49.59688600	38.82429600	40.61617300
C	40.08461000	34.04310600	34.14041200	C	50.59050200	41.03052000	40.24915300
C	41.14599300	33.71563200	35.19748700	C	50.93889100	42.10283700	39.24316400
C	40.67864300	34.21616000	36.56333100	H	43.82063300	37.22944500	45.74420200
C	41.43859300	32.21832000	35.26948200	H	44.27967200	28.81350800	43.62908700
H	41.45066800	34.40054300	32.50327700	H	44.84913300	33.41178200	45.25399600
H	39.79580500	35.09093100	34.25551600	H	45.61877500	32.62628300	43.88044100
H	39.19697300	33.43530900	34.32961900	H	46.25376600	34.16437800	44.48524800
H	42.07208000	34.23895500	34.92986900	H	42.46615200	34.15855600	42.43758700
H	40.55228700	35.29668700	36.56044500	H	42.64492400	33.23651100	43.93731800
H	39.72642900	33.75919300	36.82325700	H	42.77716100	38.05779200	41.87540200
H	41.40021900	33.95654700	37.33378300	H	43.68233100	30.97956400	43.93346100
H	40.52966700	31.66873300	35.50467700	H	44.44817900	29.11646700	40.13357700
H	41.83264900	31.84907700	34.32659100	H	43.21074900	33.24416000	40.31292500
H	42.17213500	32.01159800	36.04643800	H	43.81152400	35.93846200	42.17468100
C	45.94600200	30.63597700	35.28695800	H	46.40785700	36.01760400	43.87398100
C	46.73480600	29.99381300	36.41750400	H	45.19733600	37.27783200	43.85135700
O	45.90333500	29.48570800	37.44961800	H	48.56017500	40.00473800	42.11314400
H	45.37691600	31.48146200	35.66473300	H	47.47740800	39.28834700	40.89724500
H	47.36401300	29.18386600	36.02505300	H	50.45949800	38.59524800	41.24959700
H	47.36540000	30.75176500	36.88642400	H	49.40721200	37.96435900	39.96802900
H	45.24531700	28.87930500	37.05596400	H	50.40879300	41.98909700	38.29359300
C	55.42102200	35.46347500	36.33845400	H	50.71403600	43.08458400	39.66933700
C	54.03177700	36.08320300	36.46457400	H	52.01602900	42.06009400	39.03637100
C	53.10907500	35.32819000	37.43081200	H	49.73767200	39.88241100	38.77440600
C	53.48095400	35.59427400	38.88830900	H	44.01912500	32.22115400	38.31169700
C	51.64933200	35.71698200	37.19944400	H	44.57140100	30.65434700	38.22906000
H	55.93328800	35.43883300	37.29788300	O	47.21400400	29.76635000	42.30629300
H	54.12453600	37.12360200	36.78711000	H	47.46419200	29.68095200	41.36887100
H	53.57279100	36.09372300	35.47371300	H	46.45194200	29.18785100	42.41019100
H	53.21391500	34.25537600	37.23426800	O	46.72555800	38.30248600	38.14978100
H	52.84492700	35.01453700	39.55415800	H	47.64011900	38.62042100	38.17749200
H	54.51497700	35.32339400	39.08661500	H	46.42665100	38.17619300	39.05662600
H	53.34368200	36.64946800	39.11962300	O	43.68537500	28.02699100	36.62349800

H 42.97139600 28.59790100 36.92366400
H 43.46139600 27.13908000 36.91154100
O 49.19800800 29.84537000 44.16679600
H 48.46291300 29.75956900 43.52488300
H 49.82560900 30.44446600 43.76014100
O 47.72631500 29.45334800 39.59707800
H 46.97816400 29.39431700 38.98103700
H 48.39760300 29.95557600 39.12997100
H 46.62895900 30.99065400 34.52143900
H 45.25614500 29.91789400 34.84568800
H 40.41178100 24.55220200 42.67188100
H 38.65247600 28.34870300 41.12025000
H 39.51315000 39.20814500 46.64400100
H 41.12413900 39.94442300 46.58621200
H 46.42980300 34.90703400 36.56744600
H 44.43207900 36.84042300 53.61470500
H 44.32624100 35.10157800 53.36866000
H 51.75638100 33.43676800 49.10355300
H 51.12318300 35.06007100 49.37784200
H 48.20991800 37.66067500 49.79868100
H 47.51976600 38.18363800 51.34533400
H 44.13692600 45.02611800 41.44710300
H 43.48603900 45.98090300 40.10898100
H 55.35060400 34.44583500 35.96119900
H 56.02208700 36.04913900 35.64752200
H 40.76420200 32.77516600 32.51700700
H 39.77776000 34.14087100 32.00792200
H 47.46453900 30.05388700 52.18959500
H 48.79600100 29.94785100 51.03195500
H 37.71401200 33.69771200 42.91918400
H 49.76833400 39.60434200 33.22067600
H 50.95060700 44.32153100 32.76955200
H 39.37204000 29.93022300 44.55847100
H 51.62984600 39.87901800 47.63371300
H 53.44781000 43.14407100 43.83114100
H 47.72723800 31.92921700 40.08229200
H 43.88279900 41.76414700 41.05931400
H 55.60520600 42.07961900 33.02716100
N 44.73286600 40.45042700 42.47320100
H 44.33130700 39.60547600 42.86114400
N 52.80977600 40.50935300 34.21063800
H 52.47809700 41.09749000 34.96843300
H 54.25153100 45.23568600 35.77560100
C 47.80897600 37.74857700 34.19936000
H 46.84857500 37.23589200 34.17553800
H 47.76407000 38.58275500 33.49492400
H 48.57294800 37.04914000 33.86048500
C 40.38709400 33.88856100 50.33044000
H 41.27038600 33.89440900 50.97082200
H 39.97305000 34.89554600 50.27273800
H 39.64345500 33.20625200 50.73680400

Coordinates of DH3-R(b1) system

C 33.62303800 49.71499500 40.56399100
C 34.78552100 48.84296000 41.07765500
C 35.76231700 48.51339400 39.99477400
C 36.94670400 49.09472200 39.60695400
N 35.49852400 47.56975000 39.01565200
C 36.49813600 47.61858200 38.09818500
N 37.39651800 48.54063500 38.42018900
H 34.00447900 50.64717400 40.13379200
H 35.31623400 49.36825600 41.88012800
H 34.38214200 47.92104600 41.51693700
H 34.73466300 46.89626100 39.03779200
H 37.47771600 49.90759800 40.08379800
H 36.52973300 46.98570100 37.22367300
C 32.46001800 48.55411000 33.93702400
C 31.47078200 48.16473500 32.83461100
O 31.24012400 47.00776400 32.54711100
C 33.72878500 47.69789500 33.88064700
C 34.39945600 47.80715900 32.51396700
C 34.68279200 48.10422600 34.99952000
H 32.71714900 49.61256600 33.85483500
H 33.43494700 46.65655000 34.02264800
H 33.75542400 47.38837100 31.74489600
H 34.60254900 48.84606400 32.26155400
H 35.34001000 47.26117600 32.51126100
H 34.18570700 48.05399500 35.96617200
H 35.54340400 47.44287900 35.02391500
H 35.03663300 49.12325700 34.85510400
N 30.86309900 49.20406100 32.21180100
C 29.90300800 49.06899700 31.12400500
C 30.42030100 49.71884300 29.84737400
H 31.09808200 50.14590000 32.48323000
H 28.95406200 49.52394500 31.42508600
H 31.35837800 49.26022400 29.54428900
H 29.69576800 49.59080600 29.04835200
C 32.22225900 44.40446800 37.53274600
C 33.32381500 44.47608100 38.56455200
O 33.57301000 45.48260900 39.21473800
C 32.66850800 44.88263300 36.14095600
C 33.85315300 44.06913500 35.62388200
C 31.48183600 44.78783600 35.18405800
H 31.85230100 43.37991600 37.46151500
H 32.97735700 45.92846300 36.22912100
H 33.60145400 43.01001200 35.57840900
H 34.11788900 44.39496100 34.62070300
H 34.72640900 44.19821900 36.25987600
H 30.62565400 45.32868700 35.58082000
H 31.71643800 45.21076200 34.21072800
H 31.19174200 43.74844700 35.04397400
N 33.97629900 43.31838100 38.76027000
C 34.98913600 43.15273900 39.78018000
C 36.28800800 43.80978400 39.31822700
O 36.60795100 43.78961400 38.13352500
C 35.19469500 41.64425400 40.02590400
C 36.22948000 41.37024000 41.11259100
C 33.86801100 41.00375100 40.43415400
H 33.90161500 42.58507300 38.07322700

H	34.61408800	43.63580100	40.68684900	N	40.80598400	34.48340400	33.11519100
H	35.54549600	41.20390800	39.08526600	C	40.05798600	33.70300700	32.13499900
H	35.89988300	41.77862900	42.06564100	C	38.67307000	34.31456700	31.75958700
H	36.35186100	40.29632900	41.23163700	O	38.16698700	34.03391000	30.69281900
H	37.20014900	41.78930400	40.86886300	C	39.83061000	32.28033400	32.63392500
H	34.01106700	39.94031000	40.60217300	H	40.56114500	34.34507700	34.08378300
H	33.50604800	41.44871100	41.35911000	H	40.64825700	33.70402500	31.21375900
H	33.10027700	41.13066000	39.67536900	H	40.78276500	31.78615600	32.81328300
N	37.07065000	44.39023900	40.23476600	H	39.25430000	32.28830800	33.55799800
C	38.42831000	44.78735600	39.88884400	H	39.27941600	31.71922300	31.88465800
C	39.31287600	43.54771900	40.07961300	N	38.05208200	35.11160800	32.65848900
O	39.24112300	42.87205100	41.09527000	C	36.72502100	35.69199700	32.43700300
C	38.79142600	45.89590200	40.88843400	C	36.59265200	36.91309700	33.37817200
C	37.58482700	46.00819100	41.82779600	O	37.25544200	36.96679400	34.40778700
C	36.82749800	44.69559100	41.62760300	C	35.63370300	34.66664900	32.75098900
H	38.45287900	45.12604700	38.85030500	H	38.46933200	35.35173700	33.54768300
H	39.69326100	45.62506600	41.43676000	H	36.66650000	35.99122400	31.38619600
H	38.96886900	46.82879000	40.36079400	H	35.71704000	33.83989100	32.05041500
H	37.88051700	46.14844400	42.86478400	H	35.75580700	34.28925800	33.76335600
H	36.95831500	46.84800800	41.52726800	H	34.64483800	35.10864200	32.66357000
H	37.25154800	43.90735400	42.25693700	N	35.73040300	37.89161600	33.04580300
H	35.76448400	44.80059500	41.83468900	C	35.40898000	39.00997600	33.95000800
N	40.12880500	43.23688600	39.06439200	C	34.37464100	38.46660400	34.99751100
C	40.87619100	41.99718500	39.03612100	O	33.46434100	37.74546700	34.61220100
C	42.17097600	42.00613700	39.95540700	C	34.77295400	40.04498000	33.03200500
O	43.26364200	41.99838900	39.42625800	C	34.04013800	39.17660700	32.01199600
H	40.20717100	43.85062900	38.26681800	C	34.98801900	37.99542300	31.79970800
H	40.22684400	41.18533600	39.37644400	H	36.30959400	39.34943600	34.46091900
H	41.21965700	41.81259000	38.02115000	H	34.10488000	40.71410700	33.57069500
N	41.96379500	41.97031000	41.28616400	H	35.55069900	40.63820900	32.54744200
C	43.00086800	41.96993800	42.34376000	H	33.10640500	38.82101600	32.44520000
C	43.11443700	43.32718300	43.04614700	H	33.82554700	39.70361000	31.08511200
C	43.56342500	44.40648500	42.06618900	H	34.43994500	37.07807400	31.58369000
C	41.80086900	43.71197600	43.72532200	H	35.68480900	38.19154500	30.97576200
H	41.00350100	42.04819800	41.60328600	N	34.52632300	38.81961000	36.28250000
H	43.94259800	41.71692200	41.85462000	C	33.67301200	38.34296700	37.38797600
H	43.88336200	43.21423500	43.81888500	C	34.50918100	37.61317300	38.43240800
H	42.80987300	44.57805100	41.30170900	C	33.67736100	37.09603600	39.61195100
H	43.73849300	45.34494800	42.58453000	C	32.77337300	35.93659900	39.20092800
H	44.48167100	44.11076300	41.56596400	C	34.60917900	36.64928700	40.73705600
H	41.00764100	43.84048900	42.99216500	H	35.31937900	39.39045900	36.56246700
H	41.49366400	42.94427300	44.43212000	H	32.91788000	37.69151000	36.94979200
H	41.91958800	44.64709800	44.26819000	H	35.01736800	36.76954900	37.96272700
C	42.64000100	35.88800000	33.97600000	H	35.27254400	38.30341000	38.80053900
C	41.91194700	35.21362000	32.80463900	H	33.04593600	37.91275300	39.98244600
O	42.29184900	35.35111300	31.66142800	H	32.22145900	35.56880500	40.06261600
C	42.58983900	37.41074400	33.79874300	H	32.05235800	36.24362800	38.44809000
C	41.14592900	37.90654400	33.84941600	H	33.36244300	35.11521200	38.80048200
C	43.43481800	38.10296000	34.86497600	H	34.03539600	36.30134900	41.59237100
H	42.19900300	35.60219500	34.93242400	H	35.24158300	35.83331300	40.39541300
H	43.00228400	37.63875600	32.81073200	H	35.24907400	37.46686700	41.06353600
H	40.68523900	37.66199600	34.80473500	C	37.50699300	33.10202000	36.06397300
H	41.11415300	38.98654400	33.71912900	C	36.44537300	33.17982600	37.16090400
H	40.55732200	37.45120300	33.05648900	C	35.20225300	33.83195500	36.65569600
H	44.46552400	37.76016600	34.82211600	C	35.06059600	35.06448500	36.07384300
H	43.42872400	39.18066400	34.71589300	N	33.99148600	33.20601600	36.68527300
H	43.04400700	37.89322500	35.85885900	C	33.14491100	34.03253400	36.13373100

N 33.74064900 35.17888900 35.74155900
H 37.76292900 34.10263200 35.72059000
H 36.18653400 32.17909800 37.50704200
H 36.84418300 33.74443800 38.00928000
H 35.77157500 35.83715700 35.86495300
H 32.09934200 33.83701300 36.00469800
H 33.33228400 35.98124300 35.27628800
C 39.42300000 57.74198000 33.26698500
C 39.58066500 57.24383000 34.70549300
C 40.77920900 56.34714900 34.83118400
C 42.04952900 56.88639000 34.99903800
C 40.64650200 54.96764900 34.75162500
C 43.15774000 56.06551900 35.10006600
C 41.75498600 54.14316000 34.84743900
C 43.01805600 54.68836400 35.02908800
H 39.29958100 56.89988100 32.58746800
H 39.69268100 58.10304300 35.36924000
H 38.68109600 56.69986000 35.00049700
H 42.16639200 57.95852000 35.06638500
H 39.66405900 54.53561100 34.63003100
H 44.13765800 56.49435500 35.24536100
H 41.61917500 53.07087800 34.79549000
H 43.89339500 54.06341100 35.14261600
C 37.11203800 56.39803700 28.57292200
C 38.37067200 55.59031300 28.30398400
C 39.62169600 56.23974100 28.89723200
C 40.84822200 55.43672600 28.47983600
C 42.18735800 56.01977800 28.90896100
N 43.24857900 55.29383200 28.17196500
H 37.19571200 57.39126700 28.13927000
H 38.25373800 54.58654900 28.72036700
H 38.50294700 55.48889800 27.22418300
H 39.70538100 57.26320900 28.52961600
H 39.54082700 56.27829500 29.98447600
H 40.75988500 54.42764500 28.88164000
H 40.85210100 55.37513500 27.39051900
H 42.23962900 57.07932800 28.65250300
H 42.34586300 55.90786000 29.98293700
H 44.18483300 55.65146600 28.36166900
H 43.20295700 54.25894700 28.36276600
C 36.61904300 54.49330100 33.09101000
C 36.89789800 53.41238100 34.12671800
C 36.02378900 52.15998500 34.00017700
C 34.55851900 52.46569800 34.29900000
C 36.17506800 51.49950600 32.63130800
H 35.58927200 54.83298100 33.15421700
H 37.94446500 53.10305500 34.05383400
H 36.75288200 53.82941400 35.12454600
H 36.37854100 51.45551100 34.76135700
H 33.98481600 51.54247200 34.34672000
H 34.46801500 52.97087000 35.25717600
H 34.12388400 53.09540900 33.52621600
H 35.66259200 50.54132200 32.61929900
H 35.74397200 52.11988900 31.84913400
H 37.22419200 51.32401200 32.40060900
C 34.87001100 55.58592500 39.66095800
C 34.66597900 54.96726400 38.26806600
C 35.63733600 53.85081500 37.95340000
C 35.22194700 52.51816000 37.85244300
C 36.99763400 54.11732600 37.74579100
C 36.11483600 51.48866600 37.55228900
C 37.90651500 53.10283400 37.45776800
C 37.47323700 51.77257600 37.35931400
O 38.39631400 50.81357600 37.04889000
H 35.87936300 55.99954500 39.76448200
H 33.64004600 54.58720300 38.18866300
H 34.75838500 55.75999400 37.51238600
H 34.17150200 52.27549900 37.99739600
H 37.35793400 55.14210800 37.80874000
H 35.76222400 50.46766100 37.46170600
H 38.95465400 53.34093100 37.30183300
H 38.06062400 49.91496000 37.30193700
C 43.15299600 48.32598900 42.97598700
C 41.70396500 47.94635100 42.67938100
C 41.22692200 48.44130100 41.30798000
C 41.71922200 47.61837500 40.14226300
O 42.77357500 47.01340300 40.09078100
O 40.84968300 47.64314500 39.10662000
H 43.82312000 47.87940700 42.23635400
H 41.58020000 46.85838200 42.74508900
H 41.04814100 48.38240600 43.44202100
H 40.13621700 48.50040000 41.26197600
H 41.59970900 49.46484000 41.14114400
H 41.23836300 47.15465200 38.33874800
C 47.52200100 51.20007000 43.95317400
C 47.35522300 51.09394600 42.41742600
O 47.29593300 52.08111300 41.71352200
C 48.97024600 50.91039500 44.33708200
H 47.25492000 52.21796000 44.23062300
H 49.10467500 51.03325000 45.40904300
H 49.25172200 49.89355700 44.06999600
H 49.63861400 51.59843600 43.82512700
N 47.26251400 49.83817800 41.89852800
C 47.36511100 49.46697600 40.46364400
C 46.96040700 50.64625800 39.58277600
O 47.78214600 51.14843100 38.82876900
C 46.55888000 48.19059200 40.22784900
C 46.76445000 47.56214400 38.84362300
C 48.23369600 47.25366900 38.55917100
C 45.94140100 46.27494600 38.76550400
H 47.37644100 49.05935000 42.53070200
H 48.42548300 49.28303600 40.24725800
H 46.85958700 47.45731100 40.98171900
H 45.49503800 48.39133900 40.36974600
H 46.41079600 48.26810800 38.08525700
H 48.80483300 48.16477900 38.40066700
H 48.67694500 46.69962200 39.38405700
H 48.31797100 46.64431900 37.66248100
H 45.91924500 45.89322500 37.74713900
H 46.38340500 45.51013300 39.39964300
H 44.91994400 46.43360500 39.10271500
N 45.67466300 51.02420900 39.59443700
C 45.28727400 52.28018200 38.96834400
C 44.02593500 52.85801800 39.61286800

C	42.76682600	52.20666100	39.14341600	H	48.47378900	51.32759300	24.71167800
C	42.08495600	52.45920100	37.98106600	H	47.61466100	49.00644200	26.31577100
N	42.10205100	51.25126800	39.85824700	H	46.17314000	51.60900700	25.64203400
C	41.04631500	50.94705600	39.14633500	H	44.98739100	49.06739700	26.84649800
N	40.99340100	51.64364700	37.99593100	H	44.16510500	50.62354400	26.75927500
H	45.05340000	50.66840800	40.30538500	H	44.58187300	49.75162500	25.27309200
H	45.13111400	52.12821900	37.89370200	H	47.63315200	51.61186600	27.67097700
H	44.10449600	52.76602500	40.69683100	H	45.92312300	51.79158200	28.09257000
H	43.97748200	53.91950500	39.36322900	H	46.72977100	50.23599200	28.30907300
H	42.28651300	53.14921200	37.18923200	C	43.56029300	53.60977000	24.06911000
H	40.29521600	50.23204900	39.41271200	C	42.51383600	53.67160900	25.16001800
H	40.24906300	51.55758000	37.31603300	O	42.28400900	54.71192100	25.77278900
C	50.19704000	52.45997700	36.13906600	H	44.39443100	52.99685700	24.40535300
C	49.82438700	53.32111100	34.91917000	H	43.91425400	54.61305200	23.85401300
O	50.41956200	53.24259500	33.86500700	N	41.84328200	52.53282800	25.39816700
C	49.26141800	51.23676600	36.05298600	C	40.86989800	52.33908200	26.46798200
O	47.90388100	51.58641200	36.21914800	C	41.64213500	52.26809500	27.81699100
H	51.23217000	52.14260400	36.04789800	O	42.78943800	52.70650500	27.89858200
H	49.35149200	50.78420300	35.06012900	C	40.03259500	51.09910700	26.19029200
H	49.55212900	50.49833200	36.80638900	H	42.14548100	51.69349100	24.92641100
H	47.74298300	51.59591500	37.18667800	H	40.24240100	53.23820300	26.50407000
N	48.73621200	54.11909500	35.08998400	H	40.59999100	50.19330400	26.39542600
C	47.94892900	54.69299900	33.99800400	H	39.13304600	51.09260700	26.79957600
C	46.79181500	53.74897700	33.65749800	H	39.72036200	51.09298100	25.14847300
O	46.07661300	53.35322000	34.80340900	N	40.96926600	51.81060200	28.86844900
H	48.23823100	54.03394100	35.96430100	C	41.58973200	51.44967200	30.14996600
H	48.60834200	54.81397300	33.13890900	C	42.14782200	50.02508200	29.91745800
H	46.08426800	54.26034700	32.99985500	O	41.50438200	49.22083600	29.26704200
H	47.18984200	52.86996400	33.13914600	C	40.49668500	51.47539400	31.22603300
H	46.63496300	52.72454700	35.29569200	C	40.99294500	50.85977900	32.52708300
C	53.17046300	51.34362300	28.66622800	C	40.02195000	52.90920300	31.45383500
C	52.04774300	51.75708800	27.68105400	H	40.10752400	51.30879100	28.70308000
O	51.30501000	52.68989900	27.91623100	H	42.39175700	52.15402200	30.37605400
C	53.04501400	49.89396800	29.13591000	H	39.65927700	50.87021300	30.85771800
C	51.67570200	49.60588100	29.74070600	H	41.85175100	51.40693500	32.89972500
H	54.13150700	51.50100200	28.17323600	H	40.20364800	50.89868500	33.27404900
H	53.22293700	49.20834900	28.30358400	H	41.28468900	49.82352100	32.37911000
H	53.82128200	49.70882800	29.88217800	H	39.61028000	53.33841600	30.54323300
H	50.90347400	49.66141400	28.97636000	H	39.24678600	52.92886200	32.21387900
H	51.66056600	48.60729100	30.17262100	H	40.84789800	53.53028700	31.79408100
N	51.96602300	51.07588000	26.49892700	N	43.38417800	49.81010800	30.37556900
C	50.85931000	51.25119300	25.54578200	C	43.97236300	48.49204900	30.32013600
C	49.72432100	50.29639000	25.95230100	C	43.14739500	47.52966400	31.19634300
O	49.87836200	49.40254800	26.75619200	O	42.47857800	47.93542000	32.13046700
C	51.33039900	51.02089600	24.10802200	H	43.84677700	50.48625000	30.97696000
C	51.74025800	49.57723800	23.83469100	H	43.96401100	48.13312800	29.28750600
H	52.44220200	50.18967200	26.43483400	H	44.99545000	48.54548100	30.69057200
H	50.51577600	52.28329600	25.67963600	N	43.19579500	46.24188800	30.83164100
H	50.52098500	51.29909500	23.42904600	C	42.59683600	45.16868500	31.60592300
H	52.17322100	51.68605100	23.91154100	C	43.74220600	44.20886500	31.96559700
H	52.62764000	49.30654000	24.40073500	O	44.66855000	44.05373700	31.18647000
H	50.93983900	48.89110400	24.10216800	C	41.52911000	44.43132800	30.79227100
N	48.54701300	50.54282400	25.33897400	C	40.36524400	45.32959500	30.35611800
C	47.33668100	49.80713600	25.62811100	C	39.39700600	44.51855700	29.49754800
C	46.26258000	50.70525200	26.26033400	C	39.63808900	45.93257500	31.55648000
C	44.91231900	49.99287200	26.28174400	H	43.84363700	45.92323900	30.12323000
C	46.66547500	51.11541200	27.67326700	H	42.16908900	45.62271100	32.50098400

H	42.00946500	44.00671000	29.90800100	C	39.21189400	47.14031500	36.07007800
H	41.14368900	43.60173900	31.38980200	C	38.65229600	45.73630800	35.73192800
H	40.76457700	46.15248100	29.75499000	C	38.63611700	43.05665500	35.10391400
H	39.90815400	44.09114100	28.63848800	C	37.61653000	41.07933100	36.27297800
H	38.96317000	43.70543100	30.07635900	C	38.63461300	40.13381500	35.65659100
H	38.58916900	45.14940300	29.13527100	C	38.24550700	48.21152400	34.13450300
H	39.34997200	45.15670200	32.26489800	H	45.55025200	50.06156000	36.21150000
H	40.26948800	46.65913900	32.06012000	H	44.08015100	48.20588900	37.95167300
H	38.73863300	46.44649300	31.22598700	H	40.40251600	49.45797400	35.20657900
N	43.68289600	43.59192000	33.15043600	H	38.08835900	43.59466900	34.32707600
C	44.76613000	42.72340300	33.59799800	H	39.63911800	40.32635200	36.05222300
C	44.52642200	42.58068900	35.09543900	H	39.21291700	48.41503100	33.65917600
C	43.00455600	42.65086400	35.19569300	H	45.52392300	48.48972000	35.46729800
C	42.64150800	43.70899400	34.15370600	H	42.58282700	49.11946100	38.02342000
H	45.72847000	43.17087900	33.34489600	H	40.93251000	49.16007700	36.84703500
H	44.93021500	41.65457300	35.49505800	H	39.29707600	42.32361400	34.64178900
H	44.97359800	43.41503300	35.63518800	H	38.34791000	39.10978500	35.90195700
H	42.57024900	41.68859500	34.92197400	H	37.81669300	47.30046400	33.70756300
H	42.66517900	42.92319600	36.19169400	H	44.13585700	49.95577500	38.04596600
H	41.65520900	43.53985700	33.71761500	H	38.68654800	40.22532300	34.56573600
H	42.65282900	44.70733000	34.60550800	H	37.57568400	49.05115400	33.94379800
C	47.86100900	44.55308900	30.49698900	H	43.45938400	53.44268500	33.12022300
C	47.34454900	45.97168200	30.74190100	H	37.08082100	43.00039700	36.52752500
C	47.82067200	46.48044900	32.06990400	H	42.40134600	46.77904900	36.39622500
C	48.97604100	47.24817200	32.16805900	H	47.59764400	50.54994600	30.52249900
C	47.13456000	46.15740600	33.23424100	H	47.83559500	49.20802500	31.48095200
C	49.42974300	47.69192000	33.39948700	H	43.60050000	51.62293700	34.57981500
C	47.59195300	46.58963500	34.46719600	H	46.60447800	48.77236500	33.45467000
C	48.73827000	47.36360000	34.55316900	H	45.62763000	52.02880500	30.80386400
H	47.45035600	43.87384700	31.23811200	H	42.62328500	49.10677200	34.25669000
H	47.69261200	46.63134000	29.94426100	H	40.88100400	47.02538100	34.66653400
H	46.25406200	45.94318900	30.72748400	H	39.13196200	47.25568500	37.15899800
H	49.52819800	47.49274500	31.27076400	H	32.93151200	49.96083900	41.37676500
H	46.23134600	45.56817800	33.16486900	H	33.05956100	49.18759600	39.78669200
H	50.32434400	48.29426100	33.45848400	H	31.95679200	48.39537400	34.89332600
H	47.05060500	46.32602600	35.36533700	H	29.75441300	47.99716900	30.97972600
H	49.08892000	47.71305900	35.51207700	H	31.40838500	45.04521000	37.87726300
C	44.52356400	51.92281100	32.65119100	H	42.73393400	41.18835900	43.05755300
N	37.72913500	42.41220600	36.00306000	H	43.67716700	35.55275400	33.94740500
O	43.79468000	53.04230100	32.29836800	H	33.17935300	39.21051200	37.83612400
S	39.77343600	44.31726800	35.85306200	H	37.13167700	32.52828000	35.21899600
C	44.32011400	51.25450800	33.85740400	H	38.40728400	32.61849400	36.43978700
N	47.14491700	49.83498800	31.08065800	H	38.55260500	58.38757700	33.18098900
O	37.49854600	45.58708100	35.39363100	H	40.30271300	58.30365700	32.96052600
C	45.07405200	50.11000900	34.14865200	H	36.24425700	55.90807100	28.13935000
O	36.70614100	40.66414400	36.99170200	H	36.94641000	56.50520700	29.64264100
C	46.00662000	49.64711100	33.22323000	H	36.80573000	54.13553000	32.08103000
O	38.35255100	48.12647500	35.55360500	H	37.26424000	55.35173500	33.26715800
C	46.22547000	50.32464900	32.01173000	H	34.74096300	54.83005900	40.44340500
O	41.46881200	46.58127100	36.60110600	H	34.15222100	56.39363200	39.84165900
C	45.46039400	51.46555600	31.71852300	H	43.45800900	47.98601100	43.97264600
C	44.97896300	49.44320800	35.50376700	H	43.27965700	49.41521900	42.94015700
C	43.59728700	49.20966700	36.10045000	H	46.84606900	50.49955900	44.44625200
C	43.58672700	49.12003900	37.60319300	H	46.12146100	52.97737400	39.09768600
C	42.50108000	49.07218800	35.33630100	H	50.03880600	52.98826100	37.07784400
C	41.08569600	48.85511600	35.80863900	H	47.57533700	55.66467900	34.32785800
C	40.68668700	47.37781400	35.68807200	H	53.09047400	52.02286600	29.51398000

H 46.95473900 49.36482200 24.70085600
H 43.14719000 53.16891000 23.16578700
H 44.69714600 41.75791800 33.08523300
H 48.94696400 44.52491600 30.55561600
H 47.55307300 44.20641200 29.51443500
H 30.58449400 50.78441200 29.99775800
H 51.96641800 49.44926100 22.77902100
H 51.44749500 50.32765900 30.52198000
H 43.02212900 55.32270700 27.14318200

Coordinates of DH3-TS1_b system

C 33.62300700 49.71499400 40.56400200
C 35.10936200 49.43980000 40.87267500
C 35.84098200 48.62773200 39.84292600
C 37.07940000 48.78898200 39.26897200
N 35.32749700 47.47121000 39.26863400
C 36.22056900 46.97796800 38.39139800
N 37.29932500 47.75483400 38.37859400
H 33.51335500 50.25591600 39.61978100
H 35.64506100 50.39004300 40.97416000
H 35.17842100 48.94025200 41.84912200
H 34.46535800 46.98359400 39.52959900
H 37.81421500 49.56374000 39.41848200
H 36.07548400 46.09528600 37.78832400
C 32.45997400 48.55401900 33.93699500
C 31.46014800 48.14875100 32.84957100
O 31.17155600 46.99212900 32.62345600
C 33.64997400 47.60066500 34.05331600
C 34.43492400 47.54066500 32.74695300
C 34.54642000 48.04325600 35.20640100
H 32.81774800 49.56967600 33.74866400
H 33.26428100 46.60055700 34.25952300
H 33.79961100 47.18269500 31.94074100
H 34.81908300 48.52366900 32.47870200
H 35.27617200 46.86002600 32.85100400
H 33.98232300 48.10011600 36.13613800
H 35.36556800 47.34380400 35.34238200
H 34.96434200 49.02757200 35.00174400
N 30.89602000 49.18922200 32.18500700
C 29.90301200 49.06898300 31.12403700
C 30.42199400 49.64637500 29.81397500
H 31.18429800 50.12776500 32.41350300
H 28.98750000 49.58430000 31.43158500
H 31.32621700 49.12754500 29.50538100
H 29.67182500 49.53080400 29.03702300
C 31.93206100 44.72386600 38.16110300
C 33.07476100 44.64455900 39.14568400
O 33.43307600 45.59768900 39.83233100
C 32.37576100 45.11944100 36.73975200
C 33.37579300 44.12270600 36.15914700
C 31.13557400 45.21905500 35.85271700
H 31.41885200 43.76136900 38.12023700
H 32.85727400 46.10105200 36.79355600
H 32.94361200 43.12371500 36.11796000
H 33.64082500 44.41408800 35.14584400
H 34.29117900 44.09163300 36.74561500
H 30.42597300 45.93536100 36.26127400

H 31.39112700 45.53617400 34.84498500
H 30.64142900 44.25209900 35.78589500
N 33.63713200 43.43348600 39.25422800
C 34.73505500 43.14454900 40.15422100
C 36.00995300 43.77526400 39.59424100
O 36.16567400 43.84898100 38.37898200
C 34.90282300 41.61544300 40.26486400
C 36.00907800 41.23427000 41.24387500
C 33.59113300 40.97869600 40.72413200
H 33.44073500 42.74138400 38.54829100
H 34.47886800 43.56982000 41.12837900
H 35.17015500 41.23961800 39.27015600
H 35.77430400 41.59127800 42.24454400
H 36.09647200 40.15142500 41.28459900
H 36.97381000 41.63217500 40.94643900
H 33.72112700 39.90435200 40.81723500
H 33.30342900 41.37197100 41.69726500
H 32.77587600 41.16361400 40.02936900
N 36.93674100 44.22378500 40.44732100
C 38.26847600 44.59367000 39.98864700
C 39.17549800 43.35914400 40.11000700
O 39.10352800 42.60409100 41.06813800
C 38.73603900 45.69435400 40.95895100
C 37.62370100 45.80056300 42.00962700
C 36.85145300 44.48790100 41.86724100
H 38.22199100 44.92907400 38.95091600
H 39.68339400 45.41190500 41.41774200
H 38.87700700 46.63379600 40.43254800
H 38.01437800 45.93315100 43.01566500
H 36.96752700 46.64040200 41.77733900
H 37.34985200 43.68609500 42.41939700
H 35.82028400 44.57957300 42.20045200
N 40.04336900 43.17797400 39.10892500
C 40.87620300 41.99718900 39.03613600
C 42.16347300 42.06282600 39.96003500
O 43.25563500 42.16864200 39.44072600
H 40.09730700 43.84614600 38.35174600
H 40.28465300 41.12928800 39.34171000
H 41.23556200 41.87708200 38.01683900
N 41.96031100 41.94560000 41.28830100
C 43.00086300 41.96993400 42.34375200
C 43.04078100 43.31023000 43.08639700
C 43.43335900 44.44293200 42.14239800
C 41.70664300 43.60464800 43.77066700
H 40.99845800 41.92107900 41.60645900
H 43.95269200 41.78647700 41.84354900
H 43.81264100 43.21524200 43.85873800
H 42.66831900 44.60907300 41.38802300
H 43.56972500 45.36818200 42.69522500
H 44.36082200 44.20600100 41.62804200
H 40.91139900 43.71369000 43.03653000
H 41.43742700 42.80107900 44.45265500
H 41.77386300 44.52843100 44.34116100
C 42.64000100 35.88799900 33.97600200
C 41.92225600 35.20252500 32.80527200
O 42.31340200 35.32581900 31.66430200
C 42.46014600 37.40841300 33.86545400

C	40.98476600	37.78709300	33.98035800	H	33.44234500	35.10486700	38.81547000
C	43.28273700	38.12140900	34.93589300	H	34.04255900	36.33311600	41.60615800
H	42.26100300	35.53109200	34.93513600	H	35.27756200	35.89205400	40.42839500
H	42.82198900	37.71038600	32.87728200	H	35.22797100	37.53014100	41.08221500
H	40.57230800	37.46000600	34.93298200	C	37.50698900	33.10202100	36.06397100
H	40.86584600	38.86639100	33.91163400	C	36.43952700	33.16057800	37.15633600
H	40.40740300	37.33127300	33.17956400	C	35.19821700	33.81765200	36.65310200
H	44.33565100	37.86553600	34.84719800	C	35.06031800	35.05508100	36.08095600
H	43.18472600	39.20029900	34.83565800	N	33.98677100	33.19235200	36.67221000
H	42.94260400	37.83888700	35.93030400	C	33.14362600	34.02449800	36.12353200
N	40.80936300	34.48158500	33.11365600	N	33.74219400	35.17349400	35.74398000
C	40.05798700	33.70300700	32.13499700	H	37.76099000	34.10834500	35.73642500
C	38.67462200	34.31816300	31.75974100	H	36.18118200	32.15422400	37.48633300
O	38.17132900	34.04346700	30.68989100	H	36.83235800	33.71345800	38.01520000
C	39.82643400	32.28138400	32.63556000	H	35.77270500	35.82882400	35.88108600
H	40.55221700	34.36072500	34.08132300	H	32.09847300	33.83096800	35.98780000
H	40.64817400	33.70121400	31.21377600	H	33.33878400	35.97952100	35.28019400
H	40.77730200	31.78474600	32.81496000	C	39.42299800	57.74198100	33.26698400
H	39.25089000	32.29222100	33.56007100	C	39.55793900	57.26908800	34.71629600
H	39.27308500	31.72100600	31.88731200	C	40.74637400	56.36367300	34.87319500
N	38.05105400	35.11045400	32.66097300	C	42.01800600	56.89511400	35.05498100
C	36.72502100	35.69198600	32.43699700	C	40.60410700	54.98429400	34.80775000
C	36.58724800	36.90933000	33.38239300	C	43.11823100	56.06726300	35.18190400
O	37.23802800	36.95334800	34.41946600	C	41.70445700	54.15255700	34.92932800
C	35.63224300	34.66644500	32.74565900	C	42.96887200	54.69063500	35.12356400
H	38.46275700	35.34453400	33.55438800	H	39.30237000	56.88856300	32.60123600
H	36.67025100	35.99374100	31.38678800	H	39.67000200	58.13934200	35.36545800
H	35.71799300	33.83962400	32.04541400	H	38.64927800	56.73980800	35.01039000
H	35.74992300	34.28929600	33.75869000	H	42.14209900	57.96706700	35.11135400
H	34.64403300	35.10920000	32.65430300	H	39.62096200	54.55693400	34.67487600
N	35.73182000	37.89246100	33.04534500	H	44.09933500	56.49006900	35.33613200
C	35.40898500	39.00997000	33.95000900	H	41.55967200	53.08110200	34.88512800
C	34.37685000	38.46492900	34.99879900	H	43.84004800	54.06219800	35.25250100
O	33.47288900	37.73412000	34.61478800	C	37.11203900	56.39803700	28.57292200
C	34.77270400	40.04571900	33.03345500	C	38.37020900	55.58500300	28.31868600
C	34.04406100	39.17770300	32.01020200	C	39.62365200	56.25365500	28.88463700
C	34.99812300	38.00218500	31.79485300	C	40.84971400	55.44524600	28.47669700
H	36.30975400	39.34844200	34.46199900	C	42.19022300	56.04677100	28.87518500
H	34.10291400	40.71216000	33.57348000	N	43.24560000	55.31706200	28.13391800
H	35.55000100	40.64133500	32.55121900	H	37.19058900	57.37815200	28.10949100
H	33.11213300	38.81581100	32.44224000	H	38.25833300	54.59321000	28.76396900
H	33.82717300	39.70657800	31.08487500	H	38.49527800	55.45337600	27.24131500
H	34.45572400	37.08401100	31.56811400	H	39.70015900	57.26775100	28.49031400
H	35.69945800	38.20814200	30.97707000	H	39.55194000	56.31968800	29.97122000
N	34.52381100	38.82249400	36.28255900	H	40.77060500	54.44659500	28.90561100
C	33.67300700	38.34296000	37.38797200	H	40.84274900	55.35543500	27.38937900
C	34.51701700	37.63478800	38.44110400	H	42.22959200	57.10218100	28.59987800
C	33.68695700	37.10071100	39.61413700	H	42.36596900	55.95480400	29.94836000
C	32.82365900	35.91135700	39.20105300	H	44.18315200	55.67781700	28.31054100
C	34.61661100	36.69125700	40.75508000	H	43.20264500	54.28336700	28.33358200
H	35.29867600	39.41844800	36.56423600	C	36.61905500	54.49337200	33.09102200
H	32.92854100	37.67688400	36.95339400	C	36.90996300	53.34934800	34.05391500
H	35.04846200	36.80259700	37.97697000	C	35.99004400	52.13371600	33.89472500
H	35.26060500	38.34396300	38.81342400	C	34.55859200	52.46569400	34.29897700
H	33.02568200	37.90053000	39.96946000	C	36.03182800	51.55603000	32.48110100
H	32.27068100	35.53401100	40.05802500	H	35.60123300	54.85248600	33.21180600
H	32.10481500	36.19031700	38.43536500	H	37.94315600	53.01709100	33.91960500

H	36.81913500	53.71239300	35.08043500	H	46.23012900	48.28242500	38.15605400
H	36.35930600	51.36956100	34.58820100	H	48.63149900	48.05933000	38.35105200
H	33.95270000	51.56184700	34.31650600	H	48.47919200	46.61154700	39.35628400
H	34.53874900	52.90459000	35.29384600	H	48.03298700	46.55823900	37.65594200
H	34.10482200	53.16271000	33.59869800	H	45.61795200	45.92352400	37.87558200
H	35.47782300	50.62054400	32.44169500	H	46.11788600	45.54951400	39.51941400
H	35.57979700	52.24099600	31.76812300	H	44.69482400	46.54300300	39.24668000
H	37.05658400	51.35692800	32.17261300	N	45.67364200	51.02509700	39.59520800
C	34.86999100	55.58600100	39.66099800	C	45.28727500	52.28015200	38.96829800
C	34.41331100	54.29778300	38.96374900	C	44.09831400	52.92493800	39.68382600
C	35.50933900	53.43395800	38.36247200	C	42.78251800	52.34991100	39.27573400
C	35.21563600	52.13497800	37.91971500	C	42.13242700	52.52859300	38.08225700
C	36.82636400	53.87857700	38.20286200	N	42.02721900	51.55183500	40.08600800
C	36.18466300	51.30652900	37.35576600	C	40.95115800	51.26729600	39.40014000
C	37.80941700	53.06781700	37.63661200	N	40.96593300	51.82929300	38.17460300
C	37.49873800	51.77034900	37.21652400	H	45.05838800	50.67888500	40.31583900
O	38.50785800	51.01192700	36.68822000	H	45.05286600	52.11246600	37.91047900
H	35.34704300	56.27938000	38.95950800	H	44.22664900	52.82072700	40.76157600
H	33.84586200	53.68902300	39.68054200	H	44.09956200	53.99011500	39.44397400
H	33.69223300	54.56132600	38.17586900	H	42.39990300	53.09818300	37.21832300
H	34.19825000	51.76125800	38.01187200	H	40.14056100	50.66038100	39.74783100
H	37.10462000	54.87658000	38.52548600	H	40.25314200	51.71964000	37.46561900
H	35.93375000	50.30016800	37.03396500	C	50.19703900	52.45998000	36.13907200
H	38.82149200	53.44343200	37.51730100	C	49.82677600	53.32488400	34.92097000
H	38.19844500	50.11835500	36.40196100	O	50.43031900	53.25757900	33.87085300
C	43.15300100	48.32600000	42.97600100	C	49.25872900	51.23881500	36.05278700
C	41.65161500	48.04455300	42.91505800	O	47.90223600	51.59198900	36.21945300
C	40.97925900	48.63366900	41.67065900	H	51.23158100	52.14084200	36.04719500
C	41.26947600	47.88278400	40.39192600	H	49.34759700	50.78632200	35.05980000
O	42.20766000	47.12891800	40.20601700	H	49.54842000	50.49896200	36.80520400
O	40.35300100	48.14688200	39.43839600	H	47.73949000	51.59778000	37.18574500
H	43.66005800	47.86769500	42.12299600	N	48.73231000	54.11440000	35.08983600
H	41.47324000	46.96266100	42.94818800	C	47.94892900	54.69299800	33.99800500
H	41.16331200	48.47154400	43.79909700	C	46.78313500	53.75772600	33.65844400
H	39.89169900	48.68628100	41.79151700	O	46.06348200	53.36899100	34.80435400
H	41.32139700	49.66857300	41.51543500	H	48.22819000	54.01796600	35.95951500
H	40.59737300	47.63199700	38.61602800	H	48.60892400	54.80831300	33.13858900
C	47.52197900	51.20006700	43.95317000	H	46.07853200	54.27286800	33.00037700
C	47.34183900	51.10335200	42.42058800	H	47.17334100	52.87457900	33.14097700
O	47.20609700	52.09132800	41.72879300	H	46.61221400	52.73036300	35.29388800
C	48.98985400	50.99760400	44.31860100	C	53.17046300	51.34362300	28.66622700
H	47.19526900	52.19551200	44.24843200	C	52.06163000	51.76857900	27.67059200
H	49.12808200	51.11479700	45.39071100	O	51.34574600	52.72683600	27.88676400
H	49.33230800	50.00436700	44.03464400	C	53.02392000	49.89778100	29.14163800
H	49.60764800	51.73313100	43.80923200	C	51.64366600	49.62610700	29.72912900
N	47.32901400	49.84836500	41.89733800	H	54.13707900	51.48698400	28.17985100
C	47.36511200	49.46696000	40.46362900	H	53.20702800	49.20560900	28.31593600
C	46.96088500	50.65025900	39.58737900	H	53.78773600	49.70932700	29.89979700
O	47.78464900	51.15519900	38.83806300	H	50.88251400	49.68017400	28.95367100
C	46.49889400	48.21806300	40.28697300	H	51.61331300	48.63169500	30.16962000
C	46.58933900	47.56678200	38.90226400	N	51.96117100	51.06654200	26.50247500
C	48.02398200	47.17970500	38.54761200	C	50.85931200	51.25119400	25.54578300
C	45.69671700	46.32439000	38.88335700	C	49.73130700	50.27910600	25.92852900
H	47.49802400	49.07726000	42.52647900	O	49.89994800	49.35014700	26.68871900
H	48.40823000	49.24290300	40.20765200	C	51.33719400	51.04751400	24.10579400
H	46.81667400	47.48136000	41.03063700	C	51.79286800	49.61992200	23.82125500
H	45.45584600	48.46490400	40.49583400	H	52.40968900	50.16470900	26.45659900

H	50.50920400	52.27897400	25.69417500	N	43.20200900	46.23555200	30.82779400
H	50.51763600	51.30509100	23.43075400	C	42.59683800	45.16869100	31.60592700
H	52.15838700	51.74048100	23.91404300	C	43.71880600	44.17740800	31.94909000
H	52.69523500	49.37859100	24.37674200	O	44.59641400	43.94646600	31.13285800
H	51.01921500	48.90576800	24.09386600	C	41.48208200	44.46623000	30.82731800
N	48.54406800	50.55065200	25.34547600	C	40.31125000	45.39268800	30.47536800
C	47.33668300	49.80713200	25.62810500	C	39.29451000	44.62120600	29.63630700
C	46.29708400	50.66626300	26.36470200	C	39.64412400	45.96368900	31.72599400
C	44.94003700	49.96685000	26.38143600	H	43.81405700	45.92021900	30.08786700
C	46.75719200	50.96727500	27.78792400	H	42.20118200	45.63491400	32.50971400
H	48.45923100	51.36809300	24.76284900	H	41.91067800	44.05536500	29.91058100
H	47.63077300	48.95669200	26.24574900	H	41.11542400	43.62900100	31.42612700
H	46.19576300	51.61462300	25.81938500	H	40.69442500	46.22924200	29.88189600
H	45.01881700	49.00969100	26.88997100	H	39.76015400	44.21655600	28.74095500
H	44.21072100	50.57622600	26.91130100	H	38.87828800	43.79462000	30.20876600
H	44.58225800	49.78646300	25.36927900	H	38.47819000	45.27205300	29.33275800
H	47.72551700	51.46245700	27.78481100	H	39.37942600	45.16924600	32.42210200
H	46.03515800	51.60996500	28.28730000	H	40.30223100	46.66843600	32.22709700
H	46.84537600	50.04269300	28.35301500	H	38.73483000	46.49444200	31.45311400
C	43.56029200	53.60976600	24.06910700	N	43.69551400	43.61810000	33.16527600
C	42.50615000	53.67150700	25.15268000	C	44.76613400	42.72339900	33.59800000
O	42.26117400	54.71672200	25.75207900	C	44.62791700	42.69347200	35.11454900
H	44.39718100	53.00581800	24.41459800	C	43.12187900	42.84843600	35.31244900
H	43.90743600	54.61418000	23.84824400	C	42.73697100	43.85838000	34.23119100
N	41.84619200	52.52924400	25.40039700	H	45.72748200	43.10108800	33.24664100
C	40.86989400	52.33908000	26.46797800	H	45.01482600	41.77613200	35.54963600
C	41.63916000	52.28081900	27.82038900	H	45.15245500	43.53820600	35.56099500
O	42.78355000	52.72685100	27.90206200	H	42.62549500	41.89513200	35.12735400
C	40.04131100	51.09109500	26.19937800	H	42.86352900	43.19176200	36.31120400
H	42.16025300	51.68655200	24.94255100	H	41.71125300	43.72007300	33.88367900
H	40.23762600	53.23504700	26.49456000	H	42.83897700	44.88265700	34.60922600
H	40.60941900	50.19131400	26.42808000	C	47.86100900	44.55309600	30.49698800
H	39.13352400	51.09144700	26.79645500	C	47.26745600	45.92580200	30.81456100
H	39.74318700	51.06596100	25.15372900	C	47.75029000	46.40420600	32.15099600
N	40.96651000	51.82386600	28.87253000	C	48.92482600	47.14188700	32.25991100
C	41.58975000	51.44969600	30.14997500	C	47.05507700	46.08361400	33.30985600
C	42.16623700	50.03663500	29.89263400	C	49.38828700	47.55785400	33.49706600
O	41.55906400	49.25777900	29.17878200	C	47.52087800	46.49063100	34.54846500
C	40.49491100	51.45267900	31.22347000	C	48.68641400	47.23340800	34.64556400
C	40.98968000	50.83288100	32.52302100	H	47.52918900	43.82422700	31.23098100
C	40.01071000	52.88226200	31.45920600	H	47.55607000	46.63723800	30.03770700
H	40.10923400	51.31585800	28.70231500	H	46.18088800	45.83354200	30.82470000
H	42.38510500	52.15768200	30.38868800	H	49.48234400	47.38588400	31.36580300
H	39.66319800	50.84456700	30.84682700	H	46.13703500	45.51905600	33.23346100
H	41.83839900	51.38779800	32.90626700	H	50.29794900	48.13628100	33.56489600
H	40.19471800	50.85973700	33.26427700	H	46.96861200	46.23271700	35.44152200
H	41.29382700	49.80008100	32.37471000	H	49.04501600	47.56203900	35.60878700
H	39.60959300	53.31948000	30.54752900	C	44.45691100	51.85310000	32.84541900
H	39.22579900	52.89159500	32.20900100	N	37.43631500	42.62353600	36.17232900
H	40.83013500	53.50233200	31.81677500	O	43.76518300	52.98666400	32.46560400
N	43.38069800	49.80802100	30.39913100	S	39.37120800	44.63103800	36.10769200
C	43.97236300	48.49204600	30.32013800	C	44.21072100	51.19879500	34.05191100
C	43.16847400	47.52103900	31.20498200	N	47.03424100	49.67670300	31.32938000
O	42.52577400	47.92399600	32.15804400	O	37.10539200	45.91850900	35.48148100
H	43.79769400	50.44661200	31.07087800	C	44.92148900	50.03248900	34.36340100
H	43.93957200	48.14769000	29.28341500	O	36.56746400	40.75650600	37.09521600
H	45.00382300	48.54523000	30.66779100	C	45.85759500	49.53628600	33.45777300

O 38.09149700 48.49497100 35.61667200
C 46.11868900 50.20001400 32.24798900
O 40.94853400 46.86374000 37.14750700
C 45.39719300 51.36288700 31.93543800
C 44.77374400 49.36806000 35.71776500
C 43.37320000 49.23029900 36.30279200
C 43.32750000 49.22599600 37.80757500
C 42.28873000 49.09513900 35.52425700
C 40.85045100 49.00109700 35.96813500
C 40.34976800 47.55168700 36.01841900
C 38.83507000 47.40626900 36.17955500
C 38.26046500 46.11091500 35.84326600
C 38.28072400 43.38578200 35.29298300
C 37.42701100 41.27895600 36.38122100
C 38.50393400 40.44519600 35.70212300
C 38.00515300 48.51941200 34.18642400
H 45.38059300 49.94613400 36.43009300
H 43.80539200 48.32812600 38.21599700
H 40.23810000 49.56465800 35.26148300
H 37.66632900 43.95375000 34.59165200
H 39.50296200 40.73253300 36.05060000
H 39.00078800 48.52358900 33.72597600
H 45.25363800 48.38030200 35.67874600
H 42.31411600 49.25388200 38.20497500
H 40.68337300 49.45076100 36.95012200
H 38.94262000 42.71699600 34.74360900
H 38.33157000 39.39560400 35.94592000
H 37.43672700 47.65984400 33.82695400
H 43.87424600 50.08035800 38.21611700
H 38.49093400 40.55802900 34.61181600
H 37.48414400 49.44217500 33.92325300
H 43.44152500 53.41705900 33.27639000
H 36.75919400 43.13786800 36.73306200
H 41.91398600 46.88170600 37.02256000
H 47.50225200 50.37558700 30.76328300
H 47.71153400 49.04313900 31.74258000
H 43.48088800 51.58736700 34.75319700
H 46.41977800 48.64104300 33.70134900
H 45.59908400 51.91624000 31.02140800
H 42.43766300 49.05657800 34.44729400
H 40.69958800 47.03029700 35.11472900
H 38.20209700 47.56818400 37.52737800
H 33.18024900 50.31596500 41.36346000
H 33.05161900 48.78215400 40.49350400
H 31.90848700 48.55855600 34.88111000
H 29.69407000 48.00249000 31.02070600
H 31.23099000 45.47542500 38.52918800
H 42.78147600 41.15305800 43.03336600
H 43.69867100 35.64132300 33.89508300
H 33.16579300 39.20743900 37.82759300
H 37.13774200 32.53934600 35.20890800
H 38.40716200 32.61614100 36.43720000
H 38.55888200 58.39249600 33.15753800
H 40.31116700 58.29119100 32.96243700
H 36.24197000 55.89406200 28.16040500
H 36.95404500 56.53673000 29.64021900
H 36.76034000 54.18652100 32.05745100

H 37.29183500 55.32543600 33.28855600
H 35.58633600 55.37322800 40.46232900
H 34.01157100 56.10142800 40.10236900
H 43.59373500 47.92948200 43.89819000
H 43.34338600 49.40648300 42.95189900
H 46.89704500 50.45280300 44.44503700
H 46.15493100 52.94519000 39.02434600
H 50.04040400 52.98774400 37.07847000
H 47.58233300 55.66790200 34.32666100
H 53.09313900 52.02809600 29.51005900
H 46.91626600 49.43629700 24.68656500
H 43.15614200 53.15889200 23.16663800
H 44.61154900 41.73119100 33.16069300
H 48.94814700 44.59252700 30.50819500
H 47.53104500 44.21892100 29.51727800
H 30.64653400 50.70600400 29.92299500
H 52.01182900 49.50433800 22.76263900
H 51.40990300 50.35662000 30.50054200
H 43.00800600 55.33676700 27.10684900

Coordinates of DH3-IM₁ system

C 43.01389000 55.32858100 27.12201700
C 51.38883600 50.43889400 30.52198500
C 52.00162200 49.48517900 22.77064000
C 30.64570400 50.70537900 29.92165100
N 47.55004000 44.22148500 29.51023800
C 48.94789900 44.58634400 30.53131000
N 44.61007100 41.73001100 33.16385700
H 43.15256900 53.16281700 23.16630400
H 46.93031300 49.40863200 24.69163300
H 53.11211700 52.04529300 29.49733300
H 47.58901500 55.67179700 34.32199500
H 50.07255800 53.00994500 37.07052600
H 46.15999200 52.93659700 39.04086100
C 46.97785900 50.40323000 44.46309000
C 43.37018400 49.40153200 42.95975300
O 43.55932600 47.91705800 43.90835800
C 33.99090700 56.08596300 40.07860100
C 35.56341300 55.37353600 40.48228500
C 37.28844400 55.33121000 33.27458100
H 36.76683600 54.16473600 32.06509000
H 36.95103100 56.52383500 29.64138000
H 36.24284400 55.89981000 28.15169300
H 40.30817600 58.29709700 32.96455600
H 38.55704700 58.39219100 33.17201800
H 38.40830100 32.61540600 36.43358100
H 37.14380300 32.54971300 35.19959100
H 33.16348400 39.20164900 37.83591900
N 43.70044500 35.65119500 33.88929500
C 42.79723000 41.14851900 43.03274000
C 31.16519400 45.05585400 38.40707000
H 29.69494200 48.00224600 31.02173200
H 31.89160100 48.63311000 34.86790900
H 32.94754600 49.02845900 40.04222100
H 33.07746100 50.14929300 41.40681000
C 38.01940500 47.58366900 37.89089700
C 40.88680100 46.86030300 35.13465500

O	42.59422400	48.94709200	34.31151000	H	47.50900200	43.82609300	31.22327600
C	45.63268400	51.94446500	30.91827900	H	48.64083200	47.22821800	34.65348000
C	46.53272200	48.70847900	33.62104800	H	47.47210800	46.49259500	34.53998400
C	43.54005800	51.60130900	34.66396400	H	49.35967600	47.55027200	33.51471100
H	47.79597200	49.10814000	31.65177700	H	47.02009600	46.09058700	33.29474900
H	47.57268700	50.43487700	30.66815700	H	48.91056300	47.13778700	32.27120800
H	42.07477800	46.95562400	37.07397100	C	47.73333900	46.40745400	32.14578400
H	36.74101200	43.27826800	36.61968800	C	47.26845400	45.92921800	30.80294100
H	43.45155500	53.41363900	33.18484800	O	47.86100900	44.55317200	30.49702300
H	37.26580600	49.46258700	34.29275500	C	42.84330800	44.88715300	34.60644200
H	38.48843800	40.53044500	34.73658200	C	41.71232300	43.72570700	33.88596100
H	43.81602100	50.23904500	38.06161300	C	42.86456700	43.20363200	36.31052400
N	37.22403300	47.67766400	34.15347100	H	42.62499700	41.90256400	35.13221800
C	38.21156500	39.44196500	36.11306200	H	45.15486700	43.54377100	35.55804200
C	39.02037400	42.67944300	34.80215500	H	45.01545800	41.78166600	35.55218800
O	40.74226900	49.46453200	36.70413400	H	45.72760900	43.09927000	33.24480700
C	42.32669800	49.28960100	38.04701800	H	42.73901400	43.86267700	34.23018200
C	45.37512100	48.44076000	35.61052200	H	43.12338100	42.85552600	35.31364300
C	38.72550500	48.57508600	33.76984800	H	44.62895500	42.69818000	35.11483500
H	39.41704000	40.74765200	36.22360300	H	44.76613500	42.72340500	33.59800400
H	37.83519400	43.98647900	34.55698800	N	43.69585600	43.61796400	33.16324700
H	40.35315300	49.37985700	34.99812900	C	38.72870800	46.48850500	31.52660700
H	43.88366500	48.49031100	38.16268700	C	40.30913900	46.67445800	32.27082900
H	45.44549300	50.01473100	36.35533600	O	39.40466100	45.16753300	32.47856800
H	37.83843000	48.54033000	34.41427000	C	38.44392600	45.29203500	29.39898100
H	38.43161400	40.47254700	35.82982500	H	38.85597400	43.80915900	30.26017000
H	37.34326200	41.37269200	36.39803600	H	39.71499500	44.23825700	28.78071600
H	38.37093000	43.39737200	35.30282200	H	40.66929500	46.24372300	29.91945000
N	38.35937100	46.08720900	35.98473500	H	41.11263000	43.63152300	31.43658700
C	39.00831700	47.31711700	36.10054300	H	41.88442500	44.06884700	29.91174100
C	40.50019300	47.46771300	35.96610000	N	42.20855700	45.63732400	32.51182700
O	40.95973200	48.91968300	35.78111700	C	43.81869300	45.91572100	30.08881600
C	42.40720700	49.03478200	35.37919100	C	39.64843500	45.96547100	31.77919800
C	43.35378300	49.32247700	37.68621500	O	39.26416000	44.63839400	29.68575700
C	43.45645900	49.24851000	36.18688300	C	40.29510100	45.40343200	30.51359600
H	44.86812400	49.41503400	35.63663800	H	41.47078400	44.47283100	30.83842900
H	45.44922100	51.39703800	31.83945600	H	44.59375000	43.94256600	31.12819800
H	41.10681700	46.90802900	37.17212700	H	43.71749800	44.17488300	31.94631500
H	46.19340100	50.24953400	32.15604300	H	42.59684600	45.16868700	31.60593100
H	38.21785500	48.46411000	35.79686000	H	43.20191500	46.23302400	30.82404300
H	45.95311100	49.59127200	33.37396900	N	45.00056000	48.54562900	30.67694600
H	36.41966600	40.90756300	37.07406400	C	43.95002100	48.14882200	29.28257000
N	45.01194500	50.07517200	34.28003700	C	43.80267300	50.45257200	31.05716300
C	37.14364300	45.86885900	35.79707000	O	42.51164200	47.92487300	32.14283000
C	47.11227500	49.73357100	31.23730100	C	43.16230000	47.51919900	31.19692900
O	44.27702600	51.22523700	33.96338500	C	43.97231600	48.49203300	30.32010600
H	39.48439800	44.57941200	36.17647500	C	43.37946400	49.80730600	30.39684400
H	43.79052900	52.99699200	32.37307800	H	40.82974800	53.51003300	31.80852200
H	37.41703100	42.70112000	36.12655300	H	39.22704500	52.89868500	32.20673900
N	44.50480200	51.87602400	32.75237200	H	39.60644700	53.32145600	30.54290900
C	48.98873500	47.55344400	35.62189500	H	41.28231200	49.80410400	32.38079100
C	46.90677500	46.23605000	35.42520900	H	40.19888200	50.88214300	33.26845200
C	50.27154600	48.12369300	33.59549300	H	41.84700800	51.38822100	32.90045000
C	46.09986800	45.53173600	33.20561600	H	39.66276600	50.84878700	30.84865400
H	49.48244000	47.37730700	31.38489300	N	42.38667000	52.15657500	30.38672600
H	46.18151400	45.84115600	30.79707700	C	40.10830600	51.31684800	28.70299500
H	47.57151800	46.63824700	30.02934100	C	40.01025000	52.88768400	31.45505000

C	40.99015100	50.84105200	32.52375900	H	46.61170900	52.76081700	35.33512500
C	40.49504700	51.45747300	31.22306500	H	47.16349400	52.86553000	33.17314000
C	41.55339800	49.25570900	29.18344000	H	46.07346400	54.26573900	33.01574700
H	42.16356300	50.03507900	29.89384700	C	48.60006300	54.79815800	33.13057600
H	41.58972400	51.44966700	30.14991100	C	48.25034700	54.04584300	35.96618800
H	40.96682500	51.82319200	28.87198200	C	46.06189900	53.38905500	34.83337400
H	39.73955000	51.07047500	25.15227000	C	46.77826800	53.75748700	33.67885100
H	39.13346800	51.09146400	26.79648100	C	47.94893500	54.69299400	33.99800800
H	40.60789300	50.19167300	26.42236800	H	48.74199000	54.12185500	35.08731900
H	40.23845000	53.23556600	26.49749800	H	47.75029800	51.66168800	37.26726500
H	42.15582900	51.68890100	24.93793200	H	49.52755800	50.52454600	36.85732100
H	40.03989800	51.09244100	26.19736000	H	49.28522400	50.78531100	35.11299800
H	42.78672500	52.71828100	27.89949100	H	51.22263300	52.11783500	36.03086300
H	41.64041700	52.27669200	27.81921300	H	47.88899300	51.64168000	36.29669900
C	40.86988600	52.33908800	26.46797500	H	49.23264500	51.25700800	36.09970200
C	41.84497300	52.53077800	25.39949500	H	50.39922300	53.21010300	33.85182300
C	43.91023700	54.61371700	23.85058500	H	49.81785800	53.30828800	34.91205300
C	44.39600200	53.00214100	24.41098900	H	50.19702600	52.45998100	36.13907300
N	42.26971500	54.71533700	25.75966500	C	40.31166600	51.77241800	37.39277700
C	42.50904100	53.67156200	25.15558900	C	40.15002000	50.64708100	39.63651700
N	43.56029500	53.60976000	24.06910400	C	42.45291100	53.17423600	37.23839400
H	46.80473400	50.11773000	28.33923900	C	44.12265100	53.98399500	39.52475900
H	45.99246400	51.68032800	28.21607400	C	44.24145100	52.75575000	40.78862800
H	47.69034800	51.52262800	27.74197700	C	45.04367000	52.15227200	37.90710500
H	44.58151800	49.77079500	25.33584000	C	45.02590500	50.60650400	40.21457500
H	44.19345500	50.59253900	26.85734700	C	41.00502100	51.86989800	38.12247400
H	45.00903800	49.03033100	26.87723500	O	40.96526200	51.26904900	39.32824400
C	46.18465300	51.61302100	25.75251400	H	42.02350300	51.53678300	40.04814600
C	47.62603100	48.97522900	26.27265200	H	42.16855100	52.57766900	38.07876800
C	48.46329400	51.35409800	24.74263500	H	42.79276300	52.36260900	39.28035400
C	46.72313400	51.02520400	27.74619400	H	44.10990900	52.90951200	39.71751400
C	44.92987800	49.97539400	26.34664600	H	45.28722700	52.28013900	38.96828600
C	46.28349200	50.68128800	26.32635500	H	45.67321000	51.00560400	39.55185300
C	47.33668000	49.80714000	25.62813100	H	44.61921000	46.63018800	39.23011900
C	48.54445500	50.54844600	25.34192700	H	45.99939300	45.58042800	39.51439000
H	51.00014800	48.89940200	24.10094000	C	45.53177800	45.97894000	37.86686800
H	52.67914600	49.35936100	24.38732100	C	47.96740900	46.52703400	37.66192200
H	52.16275300	51.72414100	23.91298300	C	48.40070700	46.54173300	39.36631900
H	50.51911800	51.30002900	23.42998100	C	48.62287700	47.99288800	38.37984600
H	50.51417400	52.28127400	25.68973600	O	46.23026300	48.31285300	38.16400900
H	52.39656800	50.15653600	26.46780600	O	45.44461500	48.48204000	40.51597700
H	51.78052900	49.60620100	23.82821200	H	46.80083200	47.48728400	41.03616200
H	51.33595900	51.03845500	24.10677300	H	48.40135300	49.23064200	40.19109400
C	49.89166800	49.36921800	26.71191500	H	47.60788900	49.08781200	42.51766700
C	49.72808900	50.28583300	25.93575000	H	45.61539200	46.37321900	38.87685000
C	50.85931200	51.25119500	25.54578100	H	47.97647800	47.13786400	38.56092500
C	51.96069600	51.06511700	26.50322000	H	46.55584000	47.57944600	38.90880900
C	51.54743200	48.70308300	30.22556400	C	46.48348100	48.22781200	40.29618700
N	50.84093000	49.74490600	28.98973900	C	47.81790400	51.21972000	38.91833700
H	53.74819600	49.71636200	29.92817400	O	46.96883900	50.66657800	39.60369200
H	53.14839600	49.19949100	28.35535100	C	47.36511300	49.46697400	40.46362600
H	54.13944700	51.45255800	28.17570800	H	47.36635700	49.84710800	41.89798400
H	51.60199600	49.68729100	29.76500900	H	49.55129500	51.89954300	43.73622000
H	52.98709400	49.91118700	29.16889600	H	49.42413100	50.15372400	43.96103400
H	51.36768600	52.74713200	27.87140500	H	49.18195800	51.23977800	45.33067800
H	52.06962600	51.77656800	27.66502100	N	47.12755100	52.16481700	44.26726200
H	53.17046200	51.34362300	28.66622700	C	49.01391800	51.11522300	44.26364800

C	47.05563300	52.07449800	41.75183300	H	37.19276600	57.38367200	28.12171200
O	47.29416200	51.09559100	42.42881700	H	43.24662500	55.30411500	28.14984100
C	47.52197600	51.20006400	43.95317100	H	42.18951500	56.03242900	28.88985800
C	40.63535000	47.64497300	38.57923600	N	40.84891900	55.43991200	28.47825600
C	41.35754400	49.72426800	41.48957300	C	39.62324100	56.24724600	28.88963800
C	39.91142400	48.75513700	41.73988200	C	38.37037600	55.58704700	28.31244100
H	41.15066700	48.51459100	43.75775500	O	37.11204100	56.39803700	28.57292200
H	41.44048200	47.00400700	42.90580500	C	43.86229100	54.04968700	35.18511800
H	43.66868100	47.85853000	42.13384000	C	41.57860300	53.06293400	34.86971300
H	40.34087700	48.12303600	39.41489400	H	44.12087900	56.47813100	35.24370700
H	42.30554200	47.29339800	40.13565100	H	39.63287000	54.53565500	34.68385200
H	41.30535300	47.95572200	40.34509600	H	42.15751100	57.95164300	35.04648300
H	40.99929400	48.69202000	41.62882700	H	38.66221500	56.71331100	35.00080700
H	41.64556100	48.08173000	42.88010400	H	39.68157900	58.11041500	35.36915700
H	43.15291700	48.32595500	42.97593000	H	39.29990400	56.89777000	32.59001100
H	38.33600500	50.11838000	36.48253400	N	42.98851900	54.67617600	35.06670500
H	38.86776100	53.49656700	37.47964000	C	41.72154300	54.13500200	34.90158500
N	36.04896100	50.27483400	37.11281400	C	43.13736300	56.05347200	35.11143500
C	37.13152300	54.91515600	38.47261200	C	40.61799700	54.96478500	34.79465400
C	34.29034600	51.72651000	38.05991900	C	42.03395100	56.87912800	34.99998400
C	33.75354700	54.56336000	38.12744400	H	40.75968800	56.34472300	34.84691100
C	33.86061800	53.68025600	39.62932500	H	39.56784200	57.24885900	34.70859000
N	35.36037500	56.29161400	38.98135300	H	39.42307900	57.74192500	33.26702300
C	38.59972300	51.04874100	36.68837500	H	33.33735600	35.96369500	35.28321300
N	37.58424300	51.78405000	37.23537700	H	32.09197100	33.81776700	35.99568800
H	37.86667900	53.10007900	37.62140300	H	35.76996700	35.80747100	35.87815100
H	36.28387300	51.29333100	37.41075300	H	36.82193800	33.68145300	38.02141700
H	36.87202100	53.90299400	38.17871600	H	36.18026300	32.12728900	37.46763300
H	35.29995500	52.11812900	37.95848400	H	37.75717700	34.11404500	35.75160800
H	35.56519800	53.43612900	38.36226900	C	33.73810400	35.15652700	35.74726300
H	34.44932900	54.29661900	38.93689500	C	33.13787600	34.00913900	36.12876800
H	34.86997100	55.58602600	39.66102900	O	33.98052800	33.17537000	36.67602700
C	37.11832000	51.30237400	32.27883600	H	35.05665000	35.03537700	36.08095000
C	35.65943300	52.17882200	31.79747400	H	35.19330100	33.79801800	36.65340300
O	35.52909800	50.58197900	32.52146000	N	36.43522900	33.13938100	37.15284500
C	34.11153600	53.13402800	33.56718700	C	37.50698900	33.10202100	36.06397300
O	34.50996700	52.93542300	35.27892100	C	35.26541500	37.49519900	41.06137000
H	33.96503000	51.55404400	34.33160100	O	35.29484700	35.86200800	40.39483500
H	36.36520100	51.40763400	34.66632300	C	34.07682200	36.30310800	41.58997400
H	36.80315700	53.75456300	35.09749900	H	33.44425300	35.09991100	38.79472300
H	37.94521300	53.04458900	33.96306600	H	32.10713700	36.19347000	38.43649900
N	35.59932100	54.85165000	33.19835600	H	32.28636300	35.52298400	40.05190200
C	36.08563400	51.51655800	32.54683300	H	33.04938300	37.88687400	39.97697200
C	34.55858900	52.46567500	34.29898600	H	35.26926900	38.33894200	38.80453700
O	36.00318400	52.14205700	33.93790500	N	35.05517500	36.80233300	37.95958200
H	36.90814600	53.37109100	34.07965600	C	32.93044500	37.67555000	36.95224000
H	36.61905500	54.49335000	33.09101100	C	35.26532000	39.46582800	36.55609000
H	43.20169900	54.26916200	28.34459500	O	34.64366200	36.66357100	40.73503900
H	44.18402500	55.66224300	28.33246700	C	32.83237100	35.90546100	39.19272200
H	42.35813200	55.93105600	29.96334500	C	33.70401400	37.08798800	39.60768500
C	42.23509200	57.08984900	28.62327300	C	34.52495600	37.63052500	38.43212200
C	40.84677600	55.36163900	27.39002200	H	33.67304000	38.34296900	37.38797400
O	40.76480600	54.43700900	28.89605100	H	34.51590400	38.83383300	36.28132400
C	39.54773400	56.30226500	29.97660100	H	35.71047900	38.22305500	30.97821000
C	39.70350600	57.26516400	28.50604300	H	34.47044600	37.08751200	31.55557500
H	38.49826300	55.46803200	27.23395700	H	33.82451900	39.70619500	31.08586900
H	38.25630400	54.59014200	28.74561200	H	33.11525200	38.80688000	32.44073100

H	35.54410800	40.64488600	32.55496700	C	41.96354600	41.92646800	41.28692800
H	34.09651100	40.70779600	33.57629900	N	41.23649300	41.89714200	38.01528000
H	36.30939600	39.35172400	34.46076600	O	40.29667500	41.11667400	39.33018100
N	35.00629500	38.00730300	31.79104700	S	40.02319700	43.80125700	38.32645900
C	34.04486800	39.17601800	32.00962700	C	43.25551900	42.18082600	39.44133700
C	34.76898300	40.04500500	33.03512200	N	42.16443900	42.06287200	39.95972700
O	33.48930400	37.71318000	34.61959700	O	40.87618700	41.99720000	39.03616500
H	34.38030200	38.46147100	35.00016800	C	40.03490600	43.17126400	39.12296100
H	35.40898200	39.00999200	33.95000900	O	35.83896100	44.52130100	42.25755700
H	35.73388000	37.89371100	33.04470600	C	37.38229600	43.65170000	42.47475300
N	34.64341700	35.10935300	32.64699300	O	36.97268200	46.60855500	41.85568600
C	35.74600000	34.28544300	33.75164600	C	38.00275300	45.90038800	43.10717700
C	35.71837300	33.84097600	32.03684700	O	38.94265000	46.62306000	40.56917300
O	36.67349600	35.99684400	31.38755600	C	39.69065200	45.35737600	41.54081000
C	38.46026000	35.34084300	33.55773700	C	38.25505500	44.95962400	39.02867500
C	35.63113900	34.66565900	32.73942500	C	36.87387000	44.45163100	41.92956000
C	37.22282200	36.94295800	34.42970000	C	37.63045300	45.77101600	42.09393400
C	36.58250400	36.90608000	33.38597200	C	38.76287200	45.67337600	41.06446100
H	36.72501900	35.69198500	32.43700600	C	39.17546400	42.63302000	41.13216100
H	38.05048500	35.10981700	32.66270400	C	39.21215000	43.36763200	40.15380100
H	39.27272300	31.72114200	31.88687900	C	38.30060700	44.60227900	40.05891600
H	39.25186700	32.29155200	33.55997800	C	36.96957100	44.21149500	40.50620100
H	40.77765200	31.78440900	32.81346700	C	32.91392100	41.03411700	40.09023100
H	40.64780500	33.70165600	31.21355100	C	33.41644400	41.29051300	41.75926100
H	40.55081600	34.36325300	34.08100200	C	33.88585700	39.81882000	40.91350000
H	39.82665500	32.28113400	32.63499400	C	37.08437800	41.64181400	41.04782300
H	38.17162900	34.04578800	30.69015600	H	36.24038900	40.14870800	41.41125500
H	38.67461200	34.31875500	31.76065300	H	35.86678700	41.60149900	42.33046100
H	40.05798800	33.70300800	32.13499500	H	35.31556600	41.16252700	39.35661500
N	40.80987200	34.48120800	33.11350600	H	34.48665100	43.51574100	41.12707900
C	42.93687800	37.82940700	35.93916600	H	33.61636500	42.54987300	38.52764200
C	43.16056400	39.19967600	34.85195400	H	33.72623200	40.88668500	40.79714700
C	44.32363100	37.87536900	34.84855200	H	36.12582300	41.22766900	41.34202300
C	40.39133400	37.32039000	33.19693400	H	35.02403500	41.55285900	40.33890100
H	40.84222700	38.85325100	33.93842800	H	36.21158100	43.87046900	38.42892500
H	40.56309800	37.43794900	34.95072800	H	36.05782200	43.75360700	39.63849200
H	42.80142100	37.71803400	32.88620300	H	34.79979300	43.07115400	40.17789700
H	42.26829900	35.52310400	34.93502500	H	33.72357900	43.26826500	39.22755500
H	43.26895100	38.12118300	34.94469500	H	30.80983900	43.83447700	35.61454000
H	40.96909800	37.77435800	33.99854300	H	31.44951000	45.21941700	34.73607100
H	42.44673200	37.40758600	33.87434500	H	30.39543700	45.47170100	36.12042300
C	42.31610000	35.32223400	31.66463700	H	34.40620800	44.01711600	36.73311300
C	41.92353200	35.20137700	32.80534300	H	33.80707200	44.32627600	35.11055500
C	42.64000100	35.88800000	33.97600100	H	33.19291000	42.94578900	36.01409800
C	41.72022100	44.49562100	44.35046500	H	32.77659700	45.88319100	36.74362300
C	41.46427200	42.75726700	44.49910500	H	31.55193400	43.37922300	37.98039600
C	40.86319000	43.61897400	43.08193900	H	31.19280900	44.84679800	35.72431900
C	44.26379700	44.24838200	41.59434500	H	33.52236200	43.98017900	36.10087000
C	43.45785300	45.38610400	42.67624200	H	32.40366700	44.85789500	36.65579800
H	42.55371500	44.58875100	41.39214000	H	33.32401400	45.41988600	39.74805000
H	43.80069100	43.24664800	43.84118700	H	33.06772900	44.42205100	39.07249800
H	43.95758600	41.80689000	41.84573500	H	31.95527300	44.39049200	38.05377700
H	41.00088200	41.90456000	41.60451000	H	29.67186800	49.52870100	29.03674200
H	41.68051000	43.55968800	43.79724200	H	31.32638600	49.12691000	29.50557900
H	43.34114800	44.45442100	42.12997600	H	28.98709600	49.58397300	31.43096000
H	43.00973800	43.31156600	43.08534000	H	31.18532400	50.12899800	32.41309400
H	43.00085800	41.96993500	42.34373800	H	30.42187100	49.64550100	29.81365300

H 29.90300300 49.06895600 31.12408200
H 30.89557000 49.19068000 32.18549400
H 34.88034400 48.90187300 35.18302300
H 35.23967500 47.19714200 35.46971700
H 33.83167500 47.94751700 36.23143100
H 35.23638600 46.71753700 32.99501600
H 34.90458800 48.41184400 32.63095000
H 33.83742400 47.14522300 32.00948600
H 33.13614100 46.56061200 34.28571600
H 32.87585600 49.53883100 33.70886800
H 34.43843900 47.91733500 35.32744200
H 34.44553600 47.45055300 32.85725500
H 33.58945700 47.53915400 34.11657600
H 31.16973700 46.99341500 32.62251500
H 31.45947700 48.14938900 32.84855900
H 32.46007900 48.55405000 33.93697000
H 36.05599200 46.05947000 37.63274500
H 37.65587000 49.34012500 39.75552300
H 34.35690900 46.69287400 39.45364600
H 34.57755900 48.21512600 41.80377300
H 35.53326000 49.67669800 41.60136700
H 33.90220300 50.51718100 39.87607000
H 37.17171300 47.67495500 38.48083300
H 36.11822800 46.86789000 38.34820300
H 35.20882700 47.24169600 39.25381000
H 36.93149800 48.58754400 39.49208200
H 35.68434800 48.32233700 39.99290200
H 34.87823400 48.97649400 41.07208200
H 33.62305700 49.71502500 40.56400400

Coordinates of DH3-TS2_b system

C 33.62301700 49.71498900 40.56399800
C 33.80029000 48.56965900 39.56122900
C 35.22443400 48.16008500 39.35826600
C 36.41276600 48.72839500 39.72862000
N 35.56498400 47.03798200 38.61018100
C 36.89314300 46.93182600 38.52498400
N 37.43228100 47.94766500 39.20335100
H 33.98769300 49.43174700 41.55701600
H 33.22147200 47.69280200 39.87883900
H 33.38371200 48.86341500 38.58816300
H 34.90344100 46.31967000 38.25457700
H 36.61801000 49.62739400 40.28538900
H 37.40577300 46.16185900 37.97671600
C 32.46000800 48.55401600 33.93699200
C 31.55336200 48.17419600 32.75746500
O 31.46774200 47.04029400 32.33536500
C 33.58397000 47.53847700 34.12165800
C 34.59376200 47.64300000 32.98393200
C 34.24924800 47.72025500 35.48269300
H 32.86230600 49.55849000 33.78326800
H 33.12671900 46.54976500 34.07048800
H 34.09482100 47.50046500 32.02861900
H 35.08035300 48.61652900 32.98506600
H 35.35894100 46.87826400 33.08727400
H 33.53649500 47.52671600 36.28193000
H 35.08174800 47.03168100 35.59564000

H 34.62258100 48.73836500 35.58831700
N 30.83223400 49.19936700 32.23968100
C 29.90299900 49.06898100 31.12403600
C 30.33590000 49.92401500 29.94051500
H 30.94360500 50.12430300 32.62453900
H 28.90116900 49.35909600 31.45638800
H 31.32677600 49.62871600 29.60427600
H 29.63713600 49.79689400 29.11874900
C 33.32621500 43.20864200 36.48069700
C 34.06113800 43.86654500 37.63052700
O 33.85977100 45.03180800 37.98111900
C 33.21160100 44.08017400 35.22857700
C 34.53288100 44.09310900 34.46457600
C 32.08247200 43.58714300 34.32719700
H 33.79019500 42.25046700 36.24158900
H 32.97402500 45.09304100 35.56369100
H 34.86203200 43.07475900 34.26147200
H 34.41004300 44.60249800 33.51239000
H 35.30565400 44.60739900 35.02928100
H 31.13667400 43.56884100 34.86410900
H 31.96959700 44.24616200 33.46946800
H 32.29071500 42.58196700 33.96506400
N 34.85425600 43.02536100 38.29567700
C 35.41932500 43.24195500 39.61103000
C 36.83741600 43.78064400 39.45427600
O 37.51676900 43.44495700 38.49715800
C 35.44368300 41.85374300 40.29859100
C 36.10732000 41.84910200 41.67100900
C 34.01841800 41.31526700 40.41685300
H 35.20678800 42.19168500 37.82003300
H 34.77966600 43.94281100 40.15510000
H 36.01972700 41.19770300 39.63639200
H 35.54404300 42.45849400 42.37519900
H 36.12099900 40.83140900 42.05482400
H 37.13651000 42.19413300 41.62292100
H 34.03662600 40.31552700 40.84223700
H 33.42552500 41.95390100 41.06914400
H 33.53149000 41.26723400 39.44657300
N 37.32318100 44.63547400 40.37431600
C 38.77096900 44.85384100 40.40811600
C 39.45191000 43.48505200 40.31170800
O 39.28503100 42.66349000 41.20491900
C 39.01359900 45.49302500 41.77446500
C 37.68975000 46.17315000 42.11002200
C 36.65553900 45.21040200 41.52797800
H 39.08865100 45.49792400 39.58195800
H 39.21565800 44.70429500 42.50040100
H 39.85520400 46.17850000 41.75062300
H 37.55798800 46.30902700 43.18116700
H 37.62744700 47.14835200 41.62892300
H 36.41148400 44.43844500 42.26154800
H 35.73448900 45.71605300 41.22548000
N 40.21112000 43.26520700 39.24039500
C 40.87620600 41.99718700 39.03614000
C 42.18587200 41.95855500 39.94027400
O 43.27651100 42.02511500 39.41118700
H 40.26086200 43.95129100 38.50095900

H	40.20909000	41.18175500	39.32503500	H	36.30705700	39.35465100	34.46305800
H	41.18801400	41.90831200	37.99975500	H	34.07686800	40.69417700	33.58837700
N	41.98516400	41.86366000	41.27090800	H	35.52729300	40.65849600	32.56669700
C	43.00086000	41.96993500	42.34374700	H	33.11430800	38.80071400	32.43770300
C	42.79622300	43.21930800	43.20424700	H	33.82068100	39.71228300	31.08979500
C	42.82817200	44.47671800	42.34198900	H	34.47879000	37.09316100	31.54985300
C	41.50064000	43.13229700	44.00905400	H	35.71182200	38.23660100	30.97261000
H	41.02162500	41.85288100	41.58602600	N	34.49911900	38.83306900	36.26937700
H	43.97148600	42.00022200	41.84608200	C	33.67302800	38.34298000	37.38795800
H	43.63614000	43.25537800	43.90745700	C	34.55909200	37.73031400	38.46557800
H	41.97938900	44.50585100	41.66355500	C	33.77210800	37.26333500	39.69465600
H	42.79935600	45.36662400	42.96322300	C	32.88177200	36.06575300	39.37253300
H	43.73311300	44.50656700	41.74178800	C	34.74487700	36.89980600	40.81506100
H	40.63877900	43.05446400	43.35084000	H	35.22692600	39.49307600	36.53131600
H	41.51221800	42.26282600	44.66279400	H	32.97374700	37.61551400	36.97898300
H	41.38213500	44.02106800	44.62476800	H	35.10165000	36.88121600	38.04621600
C	42.64000100	35.88799800	33.97600500	H	35.29075900	38.48193700	38.77301400
C	41.91431300	35.21255400	32.80450800	H	33.13665000	38.08949000	40.03649000
O	42.29483000	35.34835400	31.66133900	H	32.38260000	35.71662200	40.27329800
C	42.49087000	37.41136700	33.86343900	H	32.11707200	36.32547500	38.64546800
C	41.02357200	37.81994700	33.97960900	H	33.47339100	35.24544400	38.97314300
C	43.32867500	38.10899800	34.93196000	H	34.20340100	36.59879000	41.70852400
H	42.25159300	35.53973800	34.93457700	H	35.37859900	36.07223800	40.50526100
H	42.85709400	37.70456500	32.87428400	H	35.38217300	37.74495900	41.06786300
H	40.60736800	37.50850100	34.93592200	C	37.50699100	33.10201900	36.06397100
H	40.92831200	38.90128400	33.90291300	C	36.49516600	33.19580500	37.20595400
H	40.43510100	37.36985300	33.18344500	C	35.23304700	33.84022100	36.74020100
H	44.37659700	37.83467000	34.83980500	C	35.07347400	35.05865600	36.13452200
H	43.24919800	39.18932100	34.83319900	N	34.02347400	33.21686000	36.82496700
H	42.98673900	37.83187000	35.92722500	C	33.16022300	34.03106500	36.28074200
N	40.80752600	34.48239100	33.11458200	N	33.74389700	35.16694000	35.84274900
C	40.05799300	33.70301100	32.13498900	H	37.74819400	34.09774400	35.69695400
C	38.67280100	34.31473300	31.76061100	H	36.25200500	32.20056800	37.57830400
O	38.16641800	34.03426100	30.69377200	H	36.92993100	33.77358300	38.02729400
C	39.82992600	32.28037000	32.63407600	H	35.77630000	35.82784300	35.88870300
H	40.55893200	34.35036100	34.08305100	H	32.11081800	33.83411200	36.18992400
H	40.64770300	33.70401000	31.21341700	H	33.32896400	35.95256300	35.35510500
H	40.78192900	31.78629000	32.81455100	C	39.42300700	57.74197600	33.26698300
H	39.25266700	32.28881500	33.55757800	C	39.62263700	57.23381700	34.69676400
H	39.27932900	31.71907800	31.88448900	C	40.82633300	56.33897600	34.78577600
N	38.05135200	35.11111900	32.65989200	C	42.09816800	56.87960800	34.93478800
C	36.72501300	35.69197100	32.43700600	C	40.69653600	54.95998400	34.69308300
C	36.58819100	36.91184600	33.37989800	C	43.21002000	56.06030600	35.00518400
O	37.22984600	36.95168700	34.42269700	C	41.80849800	54.13756200	34.75846400
C	35.63037700	34.67222900	32.75929800	C	43.07208000	54.68403600	34.92196500
H	38.46660200	35.34825100	33.55084500	H	39.28299300	56.90453000	32.58491500
H	36.66630300	35.98795000	31.38559100	H	39.75057100	58.08879000	35.36312100
H	35.71086600	33.83800300	32.06733300	H	38.73253800	56.68601500	35.01298400
H	35.74989500	34.30528000	33.77597300	H	42.21403300	57.95131900	35.01103600
H	34.64357100	35.11814800	32.66709400	H	39.71317400	54.52646600	34.58324800
N	35.74206300	37.90180100	33.03770400	H	44.19136500	56.49138400	35.13494000
C	35.40898300	39.00999300	33.95001500	H	41.67492900	53.06612200	34.69403700
C	34.38028200	38.44454500	34.99213000	H	43.95095200	54.05996200	35.00870300
O	33.51084800	37.67442400	34.60872300	C	37.11203400	56.39803200	28.57292900
C	34.75937000	40.04534400	33.04221900	C	38.36900400	55.57509900	28.34586300
C	34.04272300	39.17749900	32.01048300	C	39.62543700	56.26857000	28.87382900
C	35.01054700	38.01499800	31.78634000	C	40.85079300	55.44730700	28.48973600

C 42.19236700 56.07687100 28.83902400
N 43.24042400 55.33773000 28.09695100
H 37.18718600 57.35733300 28.06731500
H 38.26107900 54.60339400 28.83407600
H 38.48695300 55.39741800 27.27431900
H 39.69631100 57.26548700 28.43682700
H 39.56194500 56.37989700 29.95720700
H 40.78302900 54.46927000 28.96569000
H 40.83033100 55.30772400 27.40788400
H 42.21206900 57.12327500 28.52929200
H 42.39254700 56.02267600 29.91047500
H 44.17894000 55.70565200 28.25208900
H 43.20429900 54.30790800 28.31474700
C 36.61903400 54.49340400 33.09104500
C 36.89496400 53.41781700 34.13434600
C 36.02336700 52.16388700 34.00197200
C 34.55865500 52.46567200 34.29895200
C 36.17250200 51.50121000 32.63451000
H 35.58434600 54.82061600 33.13500600
H 37.94292800 53.11256200 34.06965100
H 36.74255200 53.83583100 35.13243100
H 36.37576500 51.45998700 34.76443100
H 33.98470400 51.54169200 34.33328200
H 34.46234400 52.96010000 35.26307700
H 34.12598800 53.10327900 33.53221500
H 35.61281900 50.56967100 32.60489500
H 35.78810300 52.14405100 31.84692100
H 37.21578000 51.27382700 32.42635400
C 34.86998600 55.58600600 39.66099700
C 34.43216000 54.33139500 38.88490900
C 35.53295100 53.40337700 38.38917500
C 35.22618300 52.08596400 38.01367000
C 36.86610600 53.80661100 38.24461400
C 36.19469600 51.20611500 37.52527700
C 37.84723900 52.94353400 37.75685500
C 37.52315300 51.62984100 37.39800000
O 38.52758600 50.83371800 36.91318700
H 35.45427800 56.26836400 39.03397300
H 33.75004700 53.74723700 39.51650500
H 33.82484000 54.65063200 38.02462800
H 34.19830000 51.73809600 38.09187900
H 37.15873000 54.81476700 38.52100700
H 35.92436400 50.19151600 37.24666800
H 38.87214700 53.28741600 37.65960300
H 38.27267900 49.88730000 36.84197200
C 43.15300600 48.32600400 42.97600900
C 41.61851100 48.29359500 42.96544000
C 40.95145600 48.82393600 41.68269700
C 41.09116000 47.94748200 40.44797100
O 42.04509100 47.18011900 40.29718200
O 40.16029300 48.09914200 39.51925800
H 43.55141800 47.68603200 42.18644400
H 41.27466300 47.26800200 43.15761700
H 41.24412200 48.89976300 43.79987100
H 39.88512800 49.01320700 41.85798000
H 41.39088900 49.79846300 41.42037700
H 40.58857800 47.33555400 38.49293000

C 47.52197200 51.20006900 43.95316100
C 46.86261000 50.67764300 42.66173900
O 45.67408800 50.83722900 42.44373100
C 48.24068400 52.51745700 43.67087600
H 46.72559400 51.35575500 44.67915400
H 48.68350100 52.90473000 44.58505600
H 49.03149100 52.38297800 42.93535700
H 47.53786000 53.25460100 43.28975600
N 47.69408600 50.07172600 41.77998900
C 47.36510900 49.46695400 40.46360900
C 46.89928800 50.55934800 39.49823400
O 47.63834200 50.90988900 38.58150800
C 46.40164500 48.28905100 40.61890200
C 46.28715600 47.41751400 39.36172100
C 47.63208600 46.83599600 38.92633900
C 45.30239600 46.28067200 39.63514800
H 48.66138300 49.99628400 42.05108800
H 48.32050000 49.10974500 40.07353700
H 46.76401800 47.67167800 41.44499700
H 45.41250600 48.65643500 40.89297800
H 45.90766200 48.03882200 38.54488900
H 48.29368100 47.60522400 38.53569500
H 48.12266000 46.33650600 39.75909100
H 47.47723600 46.10507800 38.13642000
H 45.15231600 45.67737300 38.74251900
H 45.69535900 45.62985900 40.41294900
H 44.33512500 46.65320500 39.96416000
N 45.70114600 51.09891700 39.70926200
C 45.28731900 52.28018400 38.96833200
C 44.08073800 52.95560700 39.62372400
C 42.78108500 52.38261100 39.16692400
C 42.23751400 52.42996500 37.90948500
N 41.93849400 51.70943000 40.00001300
C 40.91528900 51.36184800 39.26852600
N 41.04631300 51.77102900 37.98884300
H 45.23855800 50.90782600 40.59884700
H 45.05756200 52.00363100 37.93331200
H 44.14711800 52.85509100 40.70760100
H 44.10340500 54.01896700 39.37386200
H 42.59201800 52.87946600 37.00647500
H 40.06410800 50.81356800 39.61708400
H 40.38120400 51.59637300 37.24934400
C 50.19703700 52.45996700 36.13908300
C 49.85843900 53.39524300 34.96292400
O 50.54988300 53.46617500 33.96953400
C 49.32631000 51.20753300 35.90760400
O 47.94594100 51.49101600 35.99329000
H 51.24991300 52.19653600 36.09208000
H 49.51101000 50.82995300 34.89669900
H 49.59621800 50.42980400 36.62787100
H 47.69966400 51.38410700 36.93326100
N 48.69224500 54.08223300 35.09934200
C 47.94892200 54.69300100 33.99799900
C 46.84150600 53.73946500 33.53579900
O 46.07186900 53.26928300 34.61732800
H 48.12866600 53.86530300 35.90894000
H 48.65243700 54.88645200 33.18848900

H	46.15802400	54.26660900	32.86442100	O	41.65489800	49.32372200	29.04255600
H	47.28850300	52.89709200	32.99671800	C	40.50649100	51.40314000	31.23419900
H	46.60497700	52.60747400	35.09190500	C	41.03703900	50.80049600	32.52933300
C	53.17042800	51.34356700	28.66627900	C	39.97061000	52.81308800	31.48139000
C	52.10060800	51.80339100	27.64313200	H	40.09487400	51.34347800	28.71203200
O	51.45224300	52.81760900	27.81202600	H	42.37652100	52.16259300	30.40390200
C	52.85409800	49.96818700	29.25628300	H	39.69343300	50.76734600	30.86276700
C	51.45332600	49.91435000	29.85560300	H	41.88140800	51.37718700	32.89063600
H	54.14184100	51.33017100	28.16945900	H	40.25579100	50.81944800	33.28608100
H	52.94464800	49.19645100	28.48816000	H	41.35733200	49.77145400	32.38925300
H	53.59268900	49.74887700	30.03069800	H	39.55737100	53.24468900	30.57230500
H	50.70395400	50.00078700	29.07166200	H	39.18341700	52.78718500	32.22863000
H	51.29905100	48.96859200	30.37069600	H	40.76519700	53.46010600	31.84756000
N	51.95197700	51.05311300	26.51107300	N	43.37903500	49.80705100	30.42106500
C	50.85931900	51.25133500	25.54551600	C	43.97230100	48.49232300	30.31950900
C	49.73461700	50.26904700	25.90857100	C	43.17208300	47.51172400	31.19947700
O	49.91490100	49.31102300	26.62924600	O	42.53330900	47.91714700	32.15495000
C	51.34703700	51.06288700	24.10615000	H	43.71833700	50.39152600	31.17420800
C	51.84527400	49.64948400	23.82307300	H	43.93637000	48.16653000	29.27784100
H	52.34058200	50.12221300	26.50975200	H	45.00441900	48.55000300	30.66730200
H	50.50931400	52.27788200	25.70120900	N	43.19531400	46.22959800	30.81563700
H	50.52113100	51.29743500	23.43029000	C	42.59695100	45.16880400	31.60605100
H	52.14855900	51.77919200	23.91732300	C	43.72246800	44.17540000	31.94524700
H	52.75562800	49.43903100	24.37796400	O	44.60566200	43.96064400	31.12899200
H	51.09452100	48.91237500	24.09844600	C	41.46328300	44.47655600	30.84654500
N	48.53787000	50.56473500	25.35759400	C	40.28415100	45.40824000	30.53646200
C	47.33650500	49.80702100	25.62873300	C	39.23799000	44.64134800	29.72958500
C	46.31265200	50.62269600	26.43388900	C	39.65901800	45.97913700	31.80932700
C	44.96149500	49.91189400	26.44937100	H	43.82746300	45.90445900	30.09637700
C	46.80887800	50.85820200	27.85760700	H	42.21784800	45.63761000	32.51579600
H	48.44451200	51.40369700	24.80776300	H	41.86742100	44.07696000	29.91395100
H	47.64480100	48.92548200	26.19376700	H	41.11020300	43.63208600	31.44282100
H	46.19064200	51.59616600	25.93956500	H	40.65084400	46.24357000	29.93073900
H	45.05850800	48.93360800	26.91252800	H	39.67340300	44.23547200	28.81970300
H	44.23723200	50.49062000	27.01899600	H	38.83774900	43.81588500	30.31485100
H	44.58405900	49.77236200	25.43791700	H	38.41426700	45.29475100	29.45238100
H	47.76645500	51.37383100	27.85276700	H	39.42813000	45.18501100	32.51708300
H	46.09022100	51.45925300	28.41093200	H	40.32710400	46.69000500	32.28784300
H	46.93520500	49.90794800	28.37076700	H	38.73456700	46.49959400	31.56885700
C	43.56042500	53.60970400	24.06920900	N	43.68551800	43.59872600	33.14987300
C	42.50056100	53.66972200	25.14732900	C	44.76603900	42.72302600	33.59809500
O	42.24012500	54.71910900	25.73440900	C	44.47156200	42.46891000	35.07136700
H	44.40089600	53.01489900	24.42172800	C	42.95617300	42.62994800	35.15527100
H	43.89982500	54.61553300	23.84282300	C	42.68426600	43.77650100	34.18484700
N	41.85284000	52.52392400	25.40643800	H	45.72720300	43.20887000	33.42205400
C	40.86983200	52.33905400	26.46804100	H	44.80568300	41.48639300	35.39449200
C	41.62977900	52.29589800	27.82828000	H	44.96000200	43.22041400	35.68891600
O	42.77314700	52.74304700	27.91091500	H	42.46184800	41.72194400	34.80727600
C	40.05394300	51.08008000	26.21037100	H	42.61430500	42.85540900	36.16200100
H	42.17686900	51.67812400	24.96138600	H	41.67352000	43.74049600	33.77761600
H	40.23071700	53.23026900	26.48044500	H	42.82492300	44.73964400	34.68882700
H	40.62361400	50.18969100	26.47044200	C	47.86104200	44.55324100	30.49697700
H	39.13524200	51.08795300	26.79057700	C	48.17666900	45.78175300	31.35397700
H	39.77537200	51.02984400	25.16029400	C	47.42793900	45.73494900	32.65504100
N	40.95325900	51.84871700	28.88466100	C	47.98972900	45.18288200	33.79959600
C	41.58977700	51.44960500	30.14980500	C	46.13438300	46.23423300	32.72838000
C	42.19936500	50.06048700	29.84586000	C	47.28065800	45.14791300	34.98833500

C 45.42033500 46.20276300 33.91188600
C 45.99665100 45.66433400 35.05032200
H 46.78602500 44.42298200 30.40200500
H 49.25195800 45.82472400 31.54231400
H 47.88831300 46.68197700 30.80632300
H 48.99319300 44.78341400 33.76255100
H 45.69114600 46.66868800 31.84673100
H 47.73464500 44.71782700 35.86964700
H 44.42654900 46.62471300 33.94922700
H 45.45030100 45.65239700 35.98313000
C 44.69432500 51.45376100 32.91325600
N 37.41861100 42.60687700 35.76363900
O 43.97894100 52.52798900 32.40422800
S 39.62341200 44.30022100 35.96371200
C 44.39127900 50.89739900 34.15481500
N 47.45180000 49.27867500 31.76845000
O 37.25577800 45.54499000 35.80837400
C 45.14253300 49.81461800 34.62793500
O 36.27046500 41.02417000 36.89379600
C 46.17665300 49.30543600 33.84367700
O 38.24623000 48.14800500 36.09322500
C 46.46444000 49.84683800 32.58021900
O 41.01813000 46.70188300 37.68470200
C 45.71035300 50.93235400 32.11192900
C 44.90978200 49.25379800 36.01695200
C 43.46876600 49.06675700 36.47813000
C 43.27063600 49.15153900 37.96841700
C 42.47536800 48.79942200 35.61732900
C 41.00995800 48.66033800 35.94636000
C 40.50328200 47.23217800 36.08399700
C 39.09857500 47.01902800 36.01946000
C 38.48087900 45.76378400 35.90679000
C 38.52294300 43.15723500 35.02633900
C 37.28772200 41.35748500 36.26598400
C 38.39859800 40.36108600 36.00360700
C 37.68524800 48.46101600 34.80987600
H 45.40812800 49.92206500 36.73375300
H 43.68371100 48.27427500 38.47872200
H 40.43721900 49.11798900 35.13152600
H 38.12765700 43.72279600 34.18012900
H 39.32460900 40.67856400 36.49682700
H 38.47732500 48.69203700 34.08678300
H 45.44832700 48.29993100 36.10416500
H 42.22267800 49.21426500 38.26093300
H 40.73431800 49.21077800 36.84932600
H 39.16498000 42.36005100 34.65239900
H 38.09815400 39.39007100 36.40016600
H 37.09321400 47.61848900 34.45224400
H 43.78839900 50.01734600 38.39116200
H 38.61817600 40.24770300 34.93560400
H 37.04675500 49.33785200 34.94292800
H 43.71291200 53.07269400 33.16419300
H 36.75945200 43.29989400 36.10269200
H 41.98082900 46.76502900 37.83876300
H 47.91308300 49.93197600 31.14494100
H 48.13498400 48.73266500 32.27929100
H 43.58329500 51.30079700 34.75540100

H 46.78226400 48.48656300 34.21856500
H 45.93262000 51.39592400 31.15389800
H 42.71480900 48.70957200 34.55959300
H 41.09968500 46.47967000 35.57417000
H 38.45764000 48.09365900 39.35276100
H 32.56533000 49.97680600 40.65340300
H 34.16777800 50.60801500 40.24079600
H 31.82685800 48.57317500 34.82825700
H 29.89698300 48.01102600 30.85558900
H 32.32020500 43.00882400 36.86370000
H 42.93349200 41.06703600 42.95549700
H 43.69413700 35.62101700 33.89918900
H 33.11065900 39.18971800 37.79431500
H 37.09408800 32.51814400 35.24391700
H 38.42281800 32.62188900 36.40546500
H 38.54879800 58.38569200 33.21030800
H 40.29217100 58.30861500 32.94024100
H 36.23965600 55.87656100 28.18798300
H 36.96056300 56.58223000 29.63425700
H 36.82908900 54.13472100 32.08654600
H 37.25070900 55.35984900 33.27620300
H 35.48134700 55.32238900 40.53105000
H 33.99097200 56.13311300 40.01454800
H 43.53950100 47.97851200 43.94110500
H 43.52497200 49.34563300 42.81681600
H 48.22156000 50.45790000 44.34007900
H 46.13625900 52.97520700 38.93778000
H 49.95717000 52.91365000 37.09957400
H 47.52214400 55.63202400 34.35851800
H 53.18089200 52.09827900 29.45145300
H 46.89481000 49.48566500 24.67890900
H 43.16380400 53.14951600 23.16807600
H 44.74191900 41.79769700 33.01289500
H 48.26556500 43.65623100 30.96055100
H 48.29940700 44.65868000 29.50782300
H 30.35888600 50.97721900 30.21482700
H 52.06560000 49.53867200 22.76424300
H 51.31317600 50.72700600 30.56512400
H 42.98697800 55.33880100 27.07179300

Coordinates of DH3-IM2(b2) system

C 42.99546300 55.33729900 27.08637800
C 51.32487100 50.61950600 30.53407800
C 52.04410700 49.52291400 22.76490500
C 30.43732200 50.92023600 30.14273300
N 48.30384000 44.64702700 29.50865800
C 48.26075000 43.66003600 30.97176300
N 44.70821600 41.77833100 33.04718900
H 43.16105300 53.15235500 23.16786000
H 46.90266800 49.46496800 24.68180200
H 53.15394900 52.07927500 29.46927000
H 47.54571000 55.64673000 34.34725000
H 49.96245500 52.92006100 37.09775500
H 46.11654900 52.99875900 38.97288300
C 48.23215000 50.46357000 44.33182900
C 43.52753500 49.33247800 42.75322800
O 43.53765400 48.03928000 43.96207200

C	34.01071900	56.12304000	40.07332500	H	41.26139600	45.63549400	38.24436600
C	35.57921200	55.40438300	40.47608200	H	46.28874100	50.02970700	32.39605900
C	37.24641100	55.36029100	33.28887100	H	38.22248800	48.20683700	35.79876600
H	36.83380300	54.14903900	32.08255000	H	46.04450500	49.44189500	33.64642200
H	36.95784700	56.56443300	29.63682300	H	36.20768700	41.07684800	36.90097800
H	36.24062300	55.88331700	28.17683700	N	45.06271100	49.94094700	34.50189000
H	40.29492100	58.30353000	32.93873000	C	37.30318100	45.69364800	35.42903700
H	38.54784500	58.38155400	33.18351500	C	47.22994400	49.47524200	31.51884100
H	38.42310000	32.62321500	36.40642500	O	44.31078500	51.05558900	34.10765200
H	37.09427700	32.51600300	35.24535000	H	39.54340400	44.35745100	35.88434600
H	33.10697600	39.18795800	37.79273400	H	43.85455600	52.75675500	32.43176800
N	43.69232400	35.61543600	33.89385900	H	37.33264500	42.63903600	35.72583500
C	42.97996200	41.03666100	42.91319500	N	44.56664900	51.65523500	32.87452300
C	32.23469000	43.17097400	36.93081700	C	45.42616500	45.75494900	35.96036500
H	29.84746200	48.00322200	30.89478800	C	44.41222500	46.67918500	33.90142800
H	31.86490400	48.52110300	34.85337500	C	47.71397100	44.82585000	35.88099100
H	34.20027500	50.63113000	40.40007100	C	45.68863000	46.67649900	31.80305200
H	32.56214400	49.97870600	40.56439300	H	48.98357400	44.84203900	33.77773500
C	38.59693100	48.04541300	39.47102500	H	47.89690900	46.68410300	30.78058000
C	41.10916800	46.52513900	36.10213800	H	49.25204100	45.83068800	31.53597000
O	42.47418400	49.13991000	34.59795600	H	46.78594300	44.42529500	30.39890200
C	45.73468300	51.65495600	31.06574900	H	45.97749000	45.74499700	35.03092700
C	46.64957800	48.59767200	33.96062700	H	45.40619700	46.25607200	33.87730600
C	43.55433900	51.45915900	34.77240400	H	47.26327300	45.23066000	34.98636800
H	47.92273300	48.89914200	31.98269900	H	46.12710500	46.26248800	32.69712200
H	47.68399600	50.14942600	30.91213000	H	47.97873600	45.23918700	33.80070900
H	40.66583600	46.38571700	38.47707900	C	47.42208200	45.76446200	32.64111400
H	36.60426300	43.29548700	35.98181900	C	48.17760700	45.78974000	31.34266200
H	43.57060500	53.24940200	33.22056700	O	47.86101700	44.55329600	30.49698600
H	37.18363300	49.41941500	34.53288400	C	42.84391100	44.79159800	34.66673900
H	38.64761700	40.26096900	35.10437600	C	41.68745800	43.75205900	33.80716600
H	44.52072000	48.32685700	38.19906100	C	42.68972400	42.97226700	36.21393100
N	37.33228100	47.72829500	33.97529000	H	42.49056300	41.78180100	34.91335800
C	38.14537500	39.51776300	36.63481500	H	45.01832700	43.30102500	35.66039800
C	39.08720300	42.38406000	34.64187700	H	44.84770100	41.55659000	35.44026200
O	41.04311600	48.87213000	37.32597300	H	45.72938500	43.18594900	33.37743200
C	43.29350700	49.54081100	38.50417400	H	42.70375800	43.81045500	34.19996300
C	45.53674400	48.43390600	35.93465700	H	42.99840100	42.70158100	35.20753000
C	38.74130100	48.83156300	33.87665400	H	44.51025100	42.52771700	35.08757000
H	39.30350000	40.87220000	36.63033300	H	44.76606200	42.72305300	33.59810500
H	38.04146600	43.72375100	34.12177900	N	43.68826800	43.60328400	33.15292400
H	40.34975100	49.49283100	35.84139400	C	38.72062400	46.47235900	31.54382800
H	42.82006100	47.87523200	38.14676800	C	40.30264000	46.65595500	32.28954800
H	45.36670500	50.02645900	36.60372100	O	39.40297600	45.14499400	32.48627800
H	37.85056300	48.55996900	34.45457600	C	38.43242900	45.28228700	29.41496800
H	38.40552400	40.46200000	36.15479900	H	38.86011200	43.79433500	30.26068100
H	37.23864500	41.41375700	36.30460500	H	39.70927200	44.24482700	28.78268400
H	38.43199500	43.18381900	34.98643700	H	40.65727700	46.24268300	29.93280600
N	38.49643600	45.81430500	35.68415900	H	41.11776900	43.62507900	31.43480600
C	39.12590300	47.14670800	35.83975300	H	41.88120900	44.07482500	29.91036900
C	40.44052800	47.37395900	36.01368300	N	42.21295500	45.63754500	32.51371900
O	41.03244400	48.73411800	36.23560300	C	43.86040600	45.90060000	30.12453100
C	42.41680200	48.95409300	35.66702600	C	39.64200200	45.95038300	31.79325600
C	43.52893200	48.66318400	37.88842600	O	39.25901500	44.63277400	29.69297000
C	43.53025800	48.98896100	36.41175800	C	40.28841100	45.39766100	30.52297800
H	44.91025300	49.33476500	35.87822700	H	41.46957800	44.47180100	30.84069300
H	45.53697100	51.14806600	32.00723200	H	44.59767600	43.95174000	31.12430100

H	43.72169300	44.17488500	31.94636100	H	52.15279900	51.76268200	23.91593800
H	42.59690500	45.16879300	31.60596900	H	50.51981700	51.29949900	23.43045200
H	43.20002000	46.22827800	30.81727900	H	50.51065600	52.27878100	25.69838300
N	44.99630100	48.54889200	30.68904900	H	52.36042500	50.13358100	26.49506900
C	43.96003600	48.15947100	29.27932600	H	51.82425000	49.63645600	23.82355300
C	43.75850700	50.41793000	31.12132100	H	51.34315800	51.05593300	24.10620100
O	42.46164800	47.92601200	32.10213500	C	49.90702300	49.32981000	26.65692000
C	43.14525700	47.51603300	31.18080200	C	49.73264300	50.27411300	25.91711600
C	43.97233000	48.49219400	30.31998600	C	50.85935200	51.25124700	25.54576700
C	43.38093900	49.80845300	30.40381100	C	51.95518700	51.05709900	26.50820900
H	40.79203200	53.47812200	31.83219200	C	51.38082900	48.86604400	30.31036500
H	39.20321100	52.82863800	32.22662000	N	50.75263800	49.89518500	29.02489400
H	39.57318100	53.27276800	30.56570500	H	53.64378700	49.73607200	29.99727500
H	41.33497500	49.78273100	32.38211000	H	53.02683700	49.19375800	28.43899700
H	40.23743600	50.83343800	33.28216900	H	54.14277700	51.37625100	28.17182700
H	41.86766700	51.38265800	32.89446500	H	51.50068800	49.82540100	29.81168300
H	39.68179200	50.79732200	30.85835200	H	52.90191900	49.94456700	29.22297500
N	42.38031000	52.16021600	30.39799600	H	51.42136000	52.79300100	27.83338900
C	40.10143500	51.33114200	28.70794600	H	52.08950200	51.79404900	27.65098800
C	39.98620500	52.84047100	31.47454000	H	53.17047600	51.34362500	28.66624800
C	41.02104400	50.81314000	32.52784600	H	46.60136900	52.63956500	35.14921300
C	40.50229300	51.42273500	31.23137000	H	47.23964200	52.89371000	33.04060000
C	41.60591300	49.29324900	29.10194000	H	46.12577100	54.27752500	32.91382500
H	42.18287400	50.04892000	29.86403800	C	48.64133600	54.85794600	33.17279000
H	41.58977800	51.44967500	30.14988700	C	48.14390300	53.88901800	35.91663100
H	40.95803200	51.83959700	28.88018700	C	46.06777200	53.30759500	34.68365200
H	39.76297500	51.04387300	25.15743100	C	46.81709800	53.75014300	33.57681900
H	39.13432000	51.08962200	26.79262900	C	47.94892800	54.69301200	33.99800600
H	40.61778900	50.19015400	26.45404900	H	48.70081300	54.09018600	35.09833700
H	40.23344800	53.23221200	26.48571800	H	47.69396700	51.39010000	36.94351000
H	42.17071600	51.68122100	24.95425100	H	49.58495400	50.43648300	36.64098800
H	40.04891300	51.08440000	26.20596900	H	49.50025200	50.82665400	34.90734400
H	42.77699500	52.73695500	27.90754600	H	51.24825300	52.19047200	36.08989800
H	41.63328700	52.29018000	27.82536400	H	47.94002900	51.50331300	36.00334800
C	40.86983200	52.33905400	26.46797100	H	49.31870100	51.21112100	35.91631700
C	41.85033100	52.52585200	25.40411200	H	50.54134000	53.44388200	33.95779700
C	43.90223200	54.61507500	23.84440200	H	49.85829900	53.38922300	34.95817400
C	44.39992400	53.01205500	24.41923200	H	50.19704300	52.45999200	36.13907300
N	42.24853400	54.71796500	25.74181100	C	40.34607900	51.59863800	37.17990600
C	42.50294600	53.67032400	25.14960600	C	40.32792200	50.28753400	39.32423100
N	43.56041600	53.60970800	24.06920600	C	42.36195400	53.19135200	37.10594300
H	46.89752600	49.96205300	28.36424600	C	44.02531900	53.97385000	39.33524300
H	46.07000000	51.52272500	28.36149000	C	44.08474000	52.81171900	40.67413100
H	47.75218800	51.40784700	27.82571100	C	45.09439800	52.00589100	37.92466800
H	44.58290300	49.78350200	25.40911100	C	45.22648300	50.89228900	40.58315800
H	44.22679600	50.53136300	26.97485300	C	41.04872200	51.69468000	37.89737000
H	45.03986500	48.96841200	26.90278600	O	41.06783400	51.01615200	39.06376300
C	46.19541600	51.60627800	25.89090200	H	42.09380300	51.34416900	39.80088600
C	47.63931900	48.93828800	26.21526300	H	42.13946100	52.51462900	37.90357500
C	48.45097700	51.38713700	24.78468300	H	42.78006200	52.28515600	39.09285500
C	46.78899000	50.90274300	27.82995700	H	44.03926200	52.91206100	39.58913200
C	44.95226700	49.93866900	26.42128400	H	45.28724900	52.28013800	38.96825000
C	46.30721500	50.64219200	26.40573200	H	45.70379300	51.09959100	39.70577900
C	47.33656800	49.80706700	25.62797500	H	44.45679200	46.58674000	39.94176700
C	48.54035500	50.55849000	25.35055700	H	45.61306300	45.64544700	40.87595200
H	51.06415700	48.90871200	24.09831400	C	45.44613700	45.36071100	39.14721600
H	52.73145500	49.41413000	24.37898300	C	47.91729000	45.59733400	39.11089100

C	48.10294800	46.15469400	40.77138000	H	33.97692400	51.54600000	34.31638300
C	48.71227600	47.12976700	39.42901300	H	36.37353000	51.43774000	34.71523600
O	46.43304100	47.57132000	38.65135600	H	36.74992600	53.81229000	35.12440900
O	45.36501300	48.66369200	40.66263200	H	37.94260600	53.09664100	34.04757300
H	46.57470500	47.89515700	41.67675800	N	35.58321600	54.81645000	33.13631200
H	48.31177900	49.09671800	40.06597900	C	36.14127000	51.53171000	32.58755100
H	48.68393800	50.04004400	42.02375200	C	34.55856400	52.46579400	34.29897100
H	45.44227900	46.12901000	39.91658200	O	36.01607100	52.16076400	33.97328400
H	47.90493000	46.47616800	39.75104900	H	36.89640000	53.40610300	34.12066900
H	46.54120900	47.16080400	39.66200700	H	36.61907800	54.49334500	33.09106000
C	46.39275900	48.30069200	40.67848500	H	43.20411200	54.29811200	28.32358400
C	47.64087600	50.90468100	38.57891900	H	44.18081400	55.69480900	28.27572300
O	46.89676900	50.55359300	39.49241000	H	42.38287300	55.99628500	29.92634300
C	47.36509400	49.46693500	40.46365100	C	42.21897700	57.11484200	28.55727700
H	47.71349100	50.10359500	41.76152700	C	40.83536200	55.32435600	27.40188200
H	47.50842900	53.26383000	43.31980500	O	40.77809800	54.45978500	28.94479200
H	49.01657400	52.42058600	42.95882400	C	39.55775300	56.35711600	29.96320500
H	48.65477600	52.91339000	44.61456300	C	39.69857400	57.26623300	28.45742500
N	46.72076300	51.33237500	44.67842600	H	38.49043900	55.41950100	27.26117500
C	48.22123800	52.53237000	43.69324300	H	38.26011200	54.59893100	28.80640400
C	45.68302500	50.82762500	42.43880600	H	37.18863600	57.36572800	28.08383000
O	46.87360100	50.68462100	42.65318400	H	43.24268800	55.32938700	28.11235300
C	47.52197800	51.20007700	43.95316000	H	42.19180100	56.06485900	28.85404900
C	41.90143700	45.78873100	38.97666400	N	40.85045900	55.44564900	28.48603900
C	41.43044600	49.66019600	41.29598100	C	39.62491600	56.26268400	28.87842400
C	39.89939700	48.96375000	41.80238600	C	38.36959100	55.57892800	28.33524100
H	41.24452100	48.96792500	43.74958300	O	37.11203400	56.39803400	28.57292800
H	41.26991000	47.29108200	43.23424900	C	43.93439400	54.10445700	35.11006800
H	43.54723300	47.63680000	42.22759700	C	41.67082300	53.10960900	34.70869400
H	40.15037300	47.78483700	39.56034700	H	44.16131100	56.53429500	35.28764900
H	42.02843300	46.94393500	40.45351900	H	39.70932500	54.56613600	34.55841800
H	41.06395500	47.73307900	40.48673200	H	42.18329200	57.99016600	35.12672800
H	40.95946900	48.72782400	41.63973300	H	38.71301300	56.72580100	35.02865000
H	41.61792700	48.29784000	42.96445900	H	39.72485300	58.13812100	35.35883800
H	43.15295900	48.32603200	42.97615300	H	39.29470700	56.88834000	32.60296200
H	38.17608800	49.92004200	36.70428700	N	43.05654600	54.72773700	35.00641700
H	38.81509400	53.27711800	37.63574000	C	41.79952200	54.18043500	34.79318600
N	35.85077900	50.20629100	37.16372300	C	43.18625900	56.10269400	35.11914600
C	37.12210700	54.77334100	38.59477600	C	40.68730600	55.00032800	34.70738500
C	34.14575900	51.71968700	38.11233200	C	42.07389900	56.91966900	35.02820900
C	33.68673400	54.50434000	38.22017600	H	40.80969300	56.37786900	34.82892200
C	33.83919900	53.69497600	39.75923000	H	39.60577200	57.26832900	34.71057000
N	35.35553000	56.24516000	38.93277600	H	39.42300800	57.74197100	33.26698900
C	38.44358800	50.85774300	36.80114000	H	33.32377500	35.94640600	35.35249600
N	37.45304900	51.63770400	37.33943800	H	32.11098900	33.82422800	36.18387400
H	37.79091800	52.93330300	37.74218200	H	35.77131700	35.82903300	35.88995500
H	36.12775500	51.20868800	37.47869700	H	36.92975100	33.77815900	38.02565300
H	36.82217200	53.77737400	38.28525700	H	36.25355900	32.20313900	37.58099200
H	35.17247600	52.06827000	38.02267300	H	37.74762900	34.09706600	35.69468600
H	35.49265000	53.36906000	38.44282200	C	33.74063400	35.16238600	35.84053400
H	34.40850800	54.26991700	39.01637000	C	33.15964900	34.02419800	36.27650800
H	34.87000600	55.58598300	39.66097500	O	34.02451300	33.21227500	36.82120200
C	37.18110900	51.31464200	32.35228200	H	35.07023500	35.05771300	36.13415200
C	35.73824600	52.19214800	31.82439800	H	35.23238400	33.83921300	36.73898400
O	35.58392300	50.59924800	32.54528100	N	36.49543200	33.19768800	37.20604700
C	34.12014900	53.12728900	33.55622300	C	37.50699100	33.10201900	36.06397100
O	34.47968300	52.93466500	35.27731800	C	35.37495300	37.76151100	41.07254400

O	35.39127800	36.08859200	40.51092900	H	42.25363000	35.53775800	34.93463400
C	34.20619700	36.60335400	41.70949900	H	43.35020000	38.10252400	34.93306700
H	33.49907300	35.24013000	38.97411400	H	41.03515200	37.82875800	34.00060900
H	32.13324300	36.30595300	38.63955600	H	42.49918800	37.41262300	33.87006000
H	32.39873700	35.70239600	40.26926500	C	42.27440500	35.37252900	31.65894600
H	33.12978700	38.08176300	40.03279200	C	41.90642900	35.22155900	32.80432800
H	35.28686200	38.49224800	38.77725500	C	42.64000100	35.88799800	33.97600500
N	35.11080300	36.89102600	38.04797100	C	41.32575000	43.83704800	44.73770900
C	32.97679600	37.61153600	36.98082800	C	41.53034800	42.08585100	44.68886800
C	35.21958800	39.49701800	36.53019500	C	40.60636400	42.90242100	43.42798800
O	34.74764100	36.90953600	40.81783900	C	43.62091500	44.56486500	41.86165400
C	32.89781500	36.05512500	39.36990700	C	42.65172900	45.32075400	43.12141800
C	33.77492800	37.26190200	39.69385900	H	41.87132700	44.47846500	41.78639800
C	34.56131900	37.73584300	38.46691600	H	43.59984900	43.20470200	43.96067000
H	33.67300400	38.34295400	37.38797200	H	43.96269100	42.06233300	41.83687100
H	34.49670200	38.83345400	36.26831800	H	41.01646000	41.85435600	41.59163000
H	35.71118100	38.23769800	30.97167500	H	41.47385200	42.98473700	44.07850600
H	34.47740800	37.09541700	31.54942600	H	42.72190000	44.46126500	42.46193400
H	33.82171600	39.71546800	31.09016100	H	42.75411200	43.16600700	43.26459100
H	33.11448200	38.80361600	32.43733500	H	43.00085900	41.96993700	42.34374700
H	35.52868500	40.65967800	32.56786900	C	41.97827700	41.87592800	41.27477100
H	34.07748300	40.69537300	33.58931100	N	41.19378400	41.94497200	37.99815200
H	36.30781300	39.35306500	34.46451300	O	40.20128900	41.18023900	39.29749800
N	35.01009000	38.01674100	31.78571000	S	40.53702100	44.08480200	38.75746800
C	34.04323000	39.17993900	32.01052000	C	43.27666400	41.93931200	39.41569100
C	34.76025500	40.04680500	33.04305500	N	42.18199500	41.92384300	39.94059600
O	33.51096200	37.67375000	34.60711500	O	40.87622700	41.99717900	39.03613000
H	34.37933700	38.44400500	34.99101500	C	40.21399200	43.25966900	39.28176000
H	35.40898200	39.00997300	33.95001600	O	35.72376000	45.66309900	41.31584500
H	35.74195700	37.90286200	33.03675200	C	36.36979100	44.34784000	42.32554800
N	34.64316200	35.11899700	32.66711300	O	37.65752100	47.04126100	41.75162900
C	35.74919000	34.30628800	33.77656300	C	37.52930300	46.19363000	43.29818100
C	35.71027500	33.83836000	32.06818400	O	39.85195800	46.00208000	41.93464500
O	36.66659900	35.98732600	31.38537500	C	39.13889100	44.52186200	42.60863900
C	38.46671600	35.34634800	33.55161300	C	39.08912100	45.46835500	39.73226800
C	35.62985400	34.67289500	32.75975400	C	36.63306300	45.13368300	41.61425200
C	37.23000800	36.95426800	34.42145600	C	37.67943300	46.06172200	42.22906800
C	36.58847300	36.91235600	33.37899800	C	38.98728700	45.34524200	41.90945200
H	36.72501500	35.69197400	32.43699900	C	39.16189200	42.50849900	41.13238600
H	38.05117300	35.11090600	32.66038900	C	39.41421100	43.40592700	40.33351400
H	39.28069100	31.71913700	31.88042200	C	38.75520700	44.77780900	40.51053700
H	39.25297700	32.28569800	33.55455800	C	37.30408900	44.58299500	40.45069700
H	40.78282400	31.78550300	32.81116100	C	33.47037300	41.31872100	39.39509000
H	40.64750900	33.70624700	31.21322400	C	33.37497600	41.96711800	41.03353100
H	40.56829700	34.33584400	34.08546400	C	33.97060600	40.32982600	40.76567800
H	39.83062000	32.27939500	32.63127400	C	37.08530200	42.13635900	41.60062300
H	38.16625600	34.03517900	30.69379600	H	36.04974500	40.77460100	41.98076700
H	38.67279700	34.31472400	31.76073900	H	35.49274500	42.39584500	42.35911700
H	40.05799100	33.70300900	32.13499200	H	35.96310400	41.22517200	39.58100500
N	40.80700400	34.48082500	33.11634700	H	34.74641100	43.96292300	40.18391800
C	43.01533700	37.82516500	35.93061100	H	35.09628200	42.24112500	37.82854800
C	43.27681900	39.18358800	34.83766000	H	33.96113500	41.33962300	40.36450000
C	44.39553600	37.82208400	34.83117200	H	36.05106100	41.80594300	41.63489200
C	40.43671300	37.38237200	33.20972500	H	35.39281900	41.86703400	40.26192100
H	40.94528100	38.91080800	33.92585900	H	37.43904700	43.59899100	38.44746700
H	40.62698400	37.51814000	34.96068200	H	36.79528300	43.82890200	39.46284700
H	42.85804300	37.70663300	32.87844900	H	35.37954600	43.27535500	39.61486100

H	34.79734500	43.09406300	38.30104100	N	37.44085900	47.93630600	39.16573100
H	32.13185700	42.71393800	34.02062800	H	34.11526500	49.68500200	41.54231500
H	31.83943300	44.38748600	33.53542000	H	33.37997200	47.56839400	40.36913900
H	31.02791300	43.72908200	34.95068300	H	33.26774300	48.43410100	38.85518200
H	35.22227400	44.66166900	34.99800100	H	34.89911400	46.19473400	38.45765700
H	34.29772800	44.62455900	33.50122100	H	36.64848100	49.63830300	40.23291300
H	34.72877300	43.11197800	34.28914100	H	37.38887400	46.10501200	38.00898500
H	32.92843100	45.20988400	35.58988500	C	32.45970500	48.55418400	33.93671000
H	33.65351400	42.34504500	36.27903100	C	31.54125800	48.16458800	32.77076900
H	31.95892000	43.72358900	34.38852900	O	31.42819000	47.02263600	32.37775500
H	34.42802800	44.14382600	34.46713900	C	33.61302400	47.56751600	34.10539100
H	33.12366300	44.18597700	35.26001200	C	34.57308200	47.64626400	32.92335100
H	33.88827900	45.14052700	37.98227600	C	34.33798600	47.81563500	35.42560600
H	34.02720000	43.96248000	37.64483000	H	32.83800500	49.56818600	33.78307700
H	33.23736600	43.32493400	36.51911100	H	33.17662600	46.56876300	34.11383900
H	29.65640200	49.73402800	29.09477600	H	34.05064200	47.40842500	32.00029000
H	31.34012800	49.50839500	29.57726100	H	34.99976600	48.64350600	32.83443700
H	28.91746600	49.41574300	31.45070900	H	35.38659000	46.93689100	33.05211600
H	30.99980100	50.13298600	32.57483300	H	33.66468900	47.65794900	36.26633100
H	30.36569400	49.85976600	29.90764300	H	35.18022900	47.13739700	35.53180300
H	29.90298400	49.06898300	31.12404500	H	34.70991900	48.83897400	35.46628100
H	30.84490500	49.19898700	32.22882300	N	30.84111800	49.19455500	32.23320800
H	34.74618700	48.86404700	35.39081700	C	29.90314900	49.06892000	31.12424200
H	35.26423600	47.17494400	35.41134400	C	30.35506400	49.88736800	29.92215200
H	33.76413200	47.64162500	36.20920700	H	30.98072800	50.12487600	32.59534600
H	35.35000500	46.95828000	32.90740600	H	28.91186700	49.39455800	31.45533600
H	34.98779000	48.67916700	32.76130800	H	31.33547200	49.55688900	29.58803000
H	33.98393500	47.48687400	31.92701800	H	29.64921700	49.76422600	29.10583700
H	33.21129300	46.58064700	34.06495500	C	33.24380100	43.25403700	36.54992900
H	32.81480300	49.57837000	33.79685300	C	34.00369300	43.85948500	37.70938400
H	34.40122900	47.83141300	35.34770900	O	33.82241300	45.01783200	38.09945300
H	34.54664300	47.68717700	32.83522800	C	33.18199200	44.14771800	35.30882600
H	33.63362800	47.58475000	34.05222900	C	34.51644700	44.12367100	34.56796400
H	31.38729400	47.01885800	32.41331200	C	32.05178200	43.70526700	34.38273600
H	31.52426100	48.16584000	32.78456800	H	33.66248400	42.27803500	36.29989700
H	32.45998900	48.55404000	33.93694400	H	32.97432400	45.16381500	35.65516100
H	37.52327700	46.12877100	38.14279900	H	34.82291700	43.09643900	34.37472200
H	36.73559200	49.69088400	40.28072600	H	34.42421400	44.63099900	33.61136300
H	34.99265200	46.37880000	38.29090300	H	35.29260400	44.62260000	35.14187500
H	33.59686200	49.09868800	38.49056200	H	31.09862900	43.70301900	34.90684000
H	33.27983900	47.79329900	39.61157500	H	31.96753100	44.38335900	33.53661500
H	33.87879300	49.31913700	41.55211100	H	32.23740100	42.70192400	34.00391100
H	37.54369500	47.96277600	39.27652500	N	34.79304000	42.99124000	38.34075000
H	36.99725200	46.94313800	38.61265000	C	35.37760600	43.18071700	39.65212500
H	35.66717900	47.08573300	38.64101200	C	36.78579100	43.74114000	39.48090100
H	36.52635700	48.78317000	39.73893700	O	37.44117300	43.45467500	38.49316700
H	35.33175100	48.23825500	39.34400700	C	35.41846200	41.77874600	40.30865000
H	33.90385800	48.68342700	39.46055500	C	36.09819400	41.75025400	41.67260400
H	33.62307900	49.71493500	40.56403500	C	33.99639800	41.23344300	40.43428600
Coordinates of DH3-TS3_b system				H	35.14761000	42.17569400	37.83495600
C	33.62308400	49.71492500	40.56402700	H	34.74009100	43.86286600	40.22248600
C	33.81984300	48.40033800	39.80361200	H	35.98863800	41.13923000	39.62585600
C	35.24669400	48.07151600	39.49445100	H	35.54341200	42.34769500	42.39358800
C	36.43474300	48.70489900	39.74023600	H	36.11605800	40.72613700	42.03868800
N	35.57402300	46.92912600	38.77103100	H	37.12668800	42.09600700	41.61672900
C	36.89026300	46.87043900	38.57466400	H	34.02289900	40.22642900	40.84131800
				H	33.40972100	41.85807500	41.10554700

H	33.49742000	41.20166700	39.46954800	H	40.78207900	31.78663500	32.81540500
N	37.28453200	44.57075400	40.41866300	H	39.25317300	32.28961500	33.55889400
C	38.73206300	44.79223400	40.43510100	H	39.27906000	31.71893700	31.88608200
C	39.41137500	43.42394100	40.30245600	N	38.05116100	35.11090900	32.66024600
O	39.22442500	42.56456600	41.15568300	C	36.72499500	35.69197800	32.43699300
C	38.98895500	45.42268900	41.80275900	C	36.58714400	36.91105100	33.38085200
C	37.66538300	46.09584900	42.15428400	O	37.22663900	36.94880200	34.42523100
C	36.63680300	45.11243700	41.59872500	C	35.63000600	34.67188300	32.75685900
H	39.03688000	45.44179100	39.60810300	H	38.46589600	35.34831700	33.55130700
H	39.19747600	44.62920200	42.52165200	H	36.66725300	35.98911500	31.38585000
H	39.83020100	46.10842400	41.77536300	H	35.71078200	33.83883500	32.06351100
H	37.54877500	46.24401100	43.22542800	H	35.74874000	34.30316000	33.77297500
H	37.58204100	47.06414200	41.66021400	H	34.64339800	35.11824500	32.66472000
H	36.43937400	44.32741700	42.33280100	N	35.74271600	37.90196000	33.03783500
H	35.69321300	45.59517700	41.33175200	C	35.40899900	39.00996300	33.95003500
N	40.15608600	43.23704200	39.21662800	C	34.38107600	38.44350300	34.99242000
C	40.87624800	41.99717900	39.03616000	O	33.51442700	37.66984800	34.60982900
C	42.15490100	42.14002800	39.95942100	C	34.75890400	40.04548600	33.04268400
O	43.16459500	42.64073500	39.49438000	C	34.04394200	39.17760200	32.00980100
H	40.45147300	44.01291000	38.62151500	C	35.01359600	38.01677200	31.78516400
H	40.25210300	41.15847600	39.34453300	H	36.30693900	39.35548300	34.46309300
H	41.19883300	41.91216900	38.00232200	H	34.07555800	40.69348100	33.58878500
N	42.01861800	41.77445900	41.24988600	H	35.52658100	40.65971100	32.56840900
C	43.00085300	41.96993500	42.34372600	H	33.11576000	38.79904400	32.43601700
C	42.60925400	43.10911900	43.28852900	H	33.82176700	39.71283600	31.08943900
C	42.57166700	44.43724100	42.53995900	H	34.48355700	37.09471500	31.54572200
C	41.27704400	42.82432600	43.97996600	H	35.71619900	38.24111400	30.97337100
H	41.09105600	41.50188300	41.54884800	N	34.49773700	38.83463300	36.26922600
H	43.95629300	42.18633100	41.86331700	C	33.67303000	38.34295100	37.38796400
H	43.39246400	43.16073200	44.05348900	C	34.55917100	37.72207700	38.46098100
H	41.79577600	44.42938500	41.77914700	C	33.77190200	37.24138300	39.68468700
H	42.37248800	45.25488500	43.22686400	C	32.89135000	36.03928100	39.35296600
H	43.52112700	44.62639500	42.04711700	C	34.74388700	36.87783300	40.80583600
H	40.46858400	42.76076600	43.25539700	H	35.21970700	39.50219600	36.52939000
H	41.32252300	41.88620500	44.52889900	H	32.97062600	37.61911700	36.97764700
H	41.04415900	43.61949200	44.68460800	H	35.10378600	36.87809100	38.03409300
C	42.64000200	35.88799700	33.97600400	H	35.28899800	38.47228400	38.77610200
C	41.92151000	35.20320600	32.80537700	H	33.12892600	38.06031100	40.02968900
O	42.31341400	35.32428900	31.66459500	H	32.38874500	35.68398400	40.24940800
C	42.48779500	37.41022600	33.85087500	H	32.12959100	36.29657000	38.62201500
C	41.01889600	37.81673500	33.95358400	H	33.49047000	35.22400700	38.95460300
C	43.31665600	38.11855400	34.91946400	H	34.20191500	36.56695400	41.69562000
H	42.24694100	35.54581700	34.93495900	H	35.38454900	36.05693100	40.49256900
H	42.86033000	37.69696900	32.86231200	H	35.37432500	37.72592800	41.06616000
H	40.59556300	37.51033000	34.90852900	C	37.50698800	33.10202100	36.06397000
H	40.92241700	38.89734000	33.86891000	C	36.49173200	33.18992100	37.20329200
H	40.43754000	37.36071300	33.15566400	C	35.23007900	33.83401100	36.73581700
H	44.36563300	37.84494200	34.83740000	C	35.07107000	35.05301300	36.13112200
H	43.23637800	39.19782300	34.80966000	N	34.02068500	33.20995500	36.81763600
H	42.96727900	37.84909700	35.91446700	C	33.15808900	34.02437700	36.27256200
N	40.80740700	34.48354500	33.11365800	N	33.74207000	35.16096800	35.83702200
C	40.05799500	33.70301300	32.13499600	H	37.74711500	34.09942300	35.70082500
C	38.67269900	34.31455700	31.76085400	H	36.24904700	32.19296500	37.57133000
O	38.16611700	34.03386800	30.69425100	H	36.92303400	33.76538100	38.02816200
C	39.82999600	32.28061400	32.63511600	H	35.77399000	35.82254700	35.88664000
H	40.55072400	34.36171400	34.08133000	H	32.10898800	33.82691400	36.17951200
H	40.64796300	33.70312800	31.21365300	H	33.32808500	35.94760000	35.35015600

C	39.42300900	57.74197100	33.26698900	H	35.85077300	56.07311000	39.65439800
C	39.55827200	57.31411300	34.73038700	H	33.63288700	54.32221900	38.41439900
C	40.69912000	56.35812300	34.95350500	H	34.67949400	55.40483000	37.51986900
C	42.01451800	56.78485900	34.80288400	H	34.13865500	52.09981600	37.81261200
C	40.46942500	55.04269800	35.33552500	H	37.40217200	54.81207200	38.45772400
C	43.06985800	55.92435000	35.04260800	H	35.74198000	50.26353800	37.41040500
C	41.52444000	54.17858900	35.57943100	H	38.99848100	52.98694500	38.06118600
C	42.83111100	54.61824300	35.44144600	H	38.09887300	49.68617000	37.18770400
H	39.25768100	56.87154500	32.63351300	C	43.15296800	48.32603300	42.97616300
H	39.71784700	58.20541600	35.34233600	C	41.61865100	48.35189200	42.86424000
H	38.62633600	56.84724600	35.05565000	C	41.03761800	48.93947800	41.56447500
H	42.21207100	57.80815600	34.51654800	C	41.06574000	48.05940000	40.32308600
H	39.45415500	54.69554000	35.46475200	O	41.69194600	47.00260800	40.28567900
H	44.08692000	56.27077200	34.93519800	O	40.36298700	48.55700300	39.30573100
H	41.32052500	53.16482200	35.89303700	H	43.58213000	47.67736400	42.20645000
H	43.66777700	53.97173000	35.66723100	H	41.22789600	47.33662100	43.00597700
C	37.11205100	56.39801800	28.57293900	H	41.21907100	48.95203900	43.69088700
C	38.36769000	55.57210500	28.35019200	H	39.99403200	49.24389700	41.71958900
C	39.62424100	56.26409500	28.87960100	H	41.56103600	49.87003000	41.30219900
C	40.84816500	55.43984600	28.49767900	H	41.91437900	45.80147500	38.93865900
C	42.19063700	56.06438600	28.85220100	C	47.52197800	51.20007700	43.95316000
N	43.23738500	55.32946900	28.10401500	C	46.87213500	50.65830600	42.66826500
H	37.19048900	57.35649400	28.06617400	O	45.66614200	50.72439000	42.49403900
H	38.25692900	54.60171500	28.84028200	C	48.08961400	52.59478800	43.69711900
H	38.48761200	55.39202000	27.27923200	H	46.74116900	51.24812800	44.71048400
H	39.69761900	57.26056200	28.44185200	H	48.52254900	52.99468800	44.61045300
H	39.55930500	56.37604500	29.96279000	H	48.86310500	52.56830100	42.93202600
H	40.77551500	54.46139900	28.97197000	H	47.30063600	53.26646700	43.36740200
H	40.83024800	55.30208800	27.41548000	N	47.71570600	50.15182300	41.73658200
H	42.21245100	57.11331100	28.55114200	C	47.36509500	49.46693900	40.46365000
H	42.39043400	56.00006600	29.92313500	C	46.81906400	50.47486900	39.45198000
H	44.17626300	55.69511500	28.26196500	O	47.41503500	50.63782500	38.39049300
H	43.19948800	54.29724800	28.31380000	C	46.45509100	48.26441500	40.75018400
C	36.61903900	54.49340900	33.09100500	C	46.55609500	47.12211800	39.72995200
C	36.87236900	53.50534500	34.22391400	C	47.95050200	46.49816600	39.69624600
C	36.05575800	52.20925600	34.14411100	C	45.52950800	46.04976000	40.09555300
C	34.55872500	52.46567800	34.29896500	H	48.69673900	50.14959800	41.96587000
C	36.33842200	51.43421900	32.85953300	H	48.31483400	49.11866600	40.05349600
H	35.57656500	54.79826700	33.06641600	H	46.73350700	47.87033900	41.73133800
H	37.93321300	53.24078000	34.23366400	H	45.42080100	48.60212100	40.82227600
H	36.64994100	53.98851200	35.17867700	H	46.33133700	47.50991900	38.73186500
H	36.37366600	51.59295900	34.99377400	H	48.69013700	47.18178700	39.28694800
H	34.02550600	51.52176300	34.39200200	H	48.26226700	46.20265300	40.69603400
H	34.36632200	53.05502100	35.19233500	H	47.94028500	45.61086200	39.06813300
H	34.16197700	52.99577000	33.43666700	H	45.51978100	45.25461100	39.35444900
H	35.82190600	50.47795600	32.87758500	H	45.78044700	45.61076700	41.05919200
H	35.99152500	51.98416700	31.98845600	H	44.52862400	46.46824200	40.16236500
H	37.40259900	51.23739900	32.75123800	N	45.72881900	51.15975200	39.78344100
C	34.87000900	55.58597800	39.66097300	C	45.28724800	52.28013500	38.96825000
C	34.64806000	54.73750300	38.39399500	C	44.16825500	53.06687700	39.63652500
C	35.63470400	53.60179300	38.18695900	C	42.81722500	52.44115400	39.51729500
C	35.20475000	52.30484500	37.88052400	C	42.25090800	51.73519500	38.48808800
C	37.02012300	53.81824800	38.24035000	N	41.89831700	52.60120800	40.51241200
C	36.10615300	51.25981800	37.64531500	C	40.81271000	52.00696200	40.09994700
C	37.93187000	52.79254800	38.01692500	N	40.97012000	51.46086900	38.87536400
C	37.48192900	51.49727400	37.72591800	H	45.33342100	51.03859800	40.71705000
O	38.43685200	50.53049200	37.56065800	H	44.96157000	51.90793600	37.99181200

H	44.38413200	53.20419200	40.69756000	H	46.09571900	51.30115100	28.50012400
H	44.12969700	54.06040300	39.17866700	H	46.98100500	49.77830100	28.37366600
H	42.63763700	51.39495000	37.55056500	C	43.56064200	53.60899000	24.06956800
H	39.89466400	51.96153600	40.65097100	C	42.50128800	53.66975700	25.14857200
H	40.28432200	50.92360000	38.36269700	O	42.24220300	54.71942200	25.73595500
C	50.19704400	52.45999000	36.13907400	H	44.39697900	53.00556100	24.41708500
C	49.85703900	53.37804700	34.94899200	H	43.90708700	54.61376500	23.84923100
O	50.53482000	53.41602300	33.94442900	N	41.85195900	52.52470800	25.40603400
C	49.35063500	51.19272200	35.90037200	C	40.86954100	52.33964800	26.46762400
O	47.96537400	51.47154300	35.90704100	C	41.63062200	52.29902600	27.82888700
H	51.25443100	52.21235800	36.10991700	O	42.77865900	52.73594900	27.90753100
H	49.59613600	50.79189200	34.91100100	C	40.06036900	51.07490300	26.21639800
H	49.58789700	50.43670200	36.65357700	H	42.17726100	51.67828100	24.96308600
H	47.63393800	51.24922000	36.79621500	H	40.22693200	53.22821400	26.47832300
N	48.70717500	54.08808100	35.09130300	H	40.63191300	50.19027400	26.49193100
C	47.94892700	54.69301300	33.99800500	H	39.13737600	51.08553200	26.78974600
C	46.76194100	53.78884300	33.63828200	H	39.79015000	51.01187700	25.16484400
O	46.06012300	53.36584800	34.78242500	N	40.95162500	51.86669300	28.89007400
H	48.15462100	53.90415800	35.91637400	C	41.58979400	51.44945700	30.15007700
H	48.62151600	54.80740800	33.14833600	C	42.22122100	50.07626400	29.81820600
H	46.05161000	54.34025700	33.01646700	O	41.72035100	49.37451800	28.95637700
H	47.12563900	52.92073500	33.07824800	C	40.49851600	51.38173000	31.22823500
H	46.58847000	52.66356900	35.19905500	C	40.99748700	50.73943100	32.51690600
C	53.17047000	51.34363800	28.66626500	C	39.98330700	52.79309200	31.51253300
C	52.15133300	51.84050400	27.60919900	H	40.08422000	51.37629600	28.72027100
O	51.59618600	52.91707000	27.71115600	H	42.36484100	52.16879100	30.42156000
C	52.64810400	50.11284900	29.41008700	H	39.68035400	50.76843900	30.83077800
C	51.32060300	50.39022800	30.10557600	H	41.80182600	51.32910400	32.94128600
H	54.11198700	51.11357800	28.16550900	H	40.18609400	50.70091900	33.24015100
H	52.51966500	49.28076500	28.71348100	H	41.35432400	49.72636600	32.35234900
H	53.39219400	49.81304400	30.15136300	H	39.57702000	53.25692400	30.61604100
H	50.55394200	50.63079200	29.37183500	H	39.19834700	52.76149100	32.26198800
H	50.99778800	49.51485600	30.66516300	H	40.79075600	53.41386300	31.89554200
N	51.93199100	51.03313100	26.52997000	N	43.37385700	49.80414700	30.43617000
C	50.85933500	51.25119700	25.54572900	C	43.97246400	48.49213500	30.31992000
C	49.74606800	50.24051700	25.85734000	C	43.16882900	47.50813600	31.19196000
O	49.95328200	49.21443200	26.46951000	O	42.51611300	47.91219000	32.13754000
C	51.37495300	51.10374700	24.10995700	H	43.67335000	50.35267900	31.23699700
C	51.95704600	49.72393700	23.82300600	H	43.93211700	48.17807900	29.27494100
H	52.24624600	50.07504700	26.58065200	H	45.00606500	48.55256000	30.66368200
H	50.49798000	52.27096700	25.71744200	N	43.19742400	46.22446000	30.81023800
H	50.54367600	51.29812900	23.42763900	C	42.59690200	45.16881600	31.60598900
H	52.13716800	51.86573100	23.93807900	C	43.72203600	44.17559300	31.94638900
H	52.87248900	49.56648500	24.38692800	O	44.60004200	43.95202100	31.12559400
H	51.24867700	48.94236300	24.08719900	C	41.46672900	44.46972600	30.84713900
N	48.52849600	50.59161500	25.39218500	C	40.28955600	45.39832300	30.52223900
C	47.33645100	49.80747900	25.62790400	C	39.25752100	44.63162400	29.69697200
C	46.30907900	50.56544700	26.48215600	C	39.64422300	45.96237700	31.78752700
C	44.97427400	49.82458600	26.48342200	H	43.83927900	45.89605600	30.10108500
C	46.82132600	50.74761200	27.90802600	H	42.21678400	45.64154000	32.51305300
H	48.41933600	51.47440400	24.91897300	H	41.87615700	44.06219100	29.92011800
H	47.65852300	48.89903800	26.14025700	H	41.11082900	43.63067400	31.44939800
H	46.15905700	51.55715600	26.03396200	H	40.66317200	46.23652500	29.92475000
H	45.09812700	48.83108200	26.90590900	H	39.70642400	44.23365300	28.79007800
H	44.24251900	50.36305000	27.08190800	H	38.85383700	43.80051900	30.27187000
H	44.58912600	49.71662300	25.47109300	H	38.43417300	45.28293600	29.41348700
H	47.76442500	51.28954200	27.91205800	H	39.39237400	45.16251600	32.48159800

H	40.30876400	46.66177600	32.28718800	H	43.47293300	47.53405100	38.39705900
H	38.72960600	46.49414800	31.53394900	H	40.28230200	49.37314700	36.55456900
N	43.68931500	43.60450800	33.15309900	H	38.18853800	43.72675500	34.23226900
C	44.76605700	42.72304900	33.59809300	H	39.29813200	40.67221900	36.58131100
C	44.51138600	42.53309500	35.08882600	H	38.80505500	48.75353200	34.37905500
C	42.99956100	42.70771400	35.21009200	H	45.47407900	48.40896100	36.12411800
C	42.70255300	43.81117200	34.19826300	H	42.87365100	49.13366700	38.83365500
H	45.73023900	43.18307500	33.37479300	H	40.78943100	48.40605500	38.21001100
H	44.85123500	41.56258100	35.44237900	H	39.19529500	42.34302800	34.71042000
H	45.02065200	43.30948300	35.65671200	H	38.06701800	39.38842500	36.46647900
H	42.49029200	41.78660600	34.92242200	H	37.38627800	47.65683900	34.37611800
H	42.68648300	42.99019300	36.21174000	H	44.60464100	48.87909300	38.64623700
H	41.68651500	43.74694400	33.80752900	H	38.62829600	40.22935500	35.00721500
H	42.83520700	44.79321800	34.66430100	H	37.22018600	49.33172200	34.97851000
C	47.86100200	44.55331100	30.49700200	H	43.35929900	53.29288000	33.65927500
C	48.15703000	45.80666200	31.32552200	H	36.75903000	43.29861000	36.09631500
C	47.42676200	45.77140500	32.63823600	H	42.64752100	44.48815700	38.57834000
C	48.01039300	45.24087500	33.78223100	H	47.36470300	50.24779700	31.07475300
C	46.13025900	46.26095700	32.72439900	H	47.62036800	48.95242100	32.08231100
C	47.31968400	45.21876600	34.98212400	H	43.41803000	51.47212700	35.14249900
C	45.43347600	46.23964600	33.91902300	H	46.45666700	48.61421400	34.10638300
C	46.03159200	45.72371900	35.05664200	H	45.42457400	51.76104800	31.35208200
H	46.78801700	44.39918300	30.41359500	H	42.36121500	49.16698700	35.06376400
H	49.23331300	45.88054900	31.49850500	H	41.16082000	46.44925700	36.35022300
H	47.84072300	46.68754500	30.76076500	H	38.44695800	48.16605600	39.16351300
H	49.01700300	44.85019200	33.73530300	H	32.55796100	49.89623300	40.72927800
H	45.66887900	46.67866400	31.84370400	H	34.03266400	50.56122700	40.00229900
H	47.79180300	44.81014800	35.86414700	H	31.84102800	48.55474900	34.83839400
H	44.43635500	46.65292500	33.96540700	H	29.86495400	48.00649300	30.87667200
H	45.49835500	45.72294100	35.99668800	H	32.22613100	43.10000800	36.92273300
C	44.34752300	51.71647800	33.21481700	H	43.06919100	41.02561400	42.88743300
N	37.42598400	42.60228600	35.78217300	H	43.69505600	35.62276800	33.90659700
O	43.63203200	52.83705700	32.84346100	H	33.11410900	39.18953000	37.79909100
S	39.66374800	44.25130500	36.05215100	H	37.09747900	32.52009700	35.24086600
C	44.14807400	51.08093700	34.44134400	H	38.42288100	32.62252000	36.40626600
N	46.91820200	49.55137200	31.66240500	H	38.58306700	58.42185100	33.14911100
O	37.33326000	45.51930700	35.79953300	H	40.32478800	58.24576800	32.92747500
C	44.91127000	49.95177500	34.76763000	H	36.23940900	55.87791700	28.18668900
O	36.23667300	41.03957700	36.89708500	H	36.95852400	56.58375400	29.63368900
C	45.84131100	49.46924700	33.84631500	H	36.87964700	54.06497300	32.12672500
O	38.19377800	48.06269300	36.24875800	H	37.22588500	55.38418900	33.23790100
C	46.02429400	50.08892200	32.60335700	H	34.81249400	54.96624000	40.56228400
O	41.99797500	45.12723200	38.23148900	H	34.10913600	56.36977900	39.73373500
C	45.26364400	51.22286700	32.28359900	H	43.45757400	47.94125300	43.95504500
C	44.85524600	49.31776400	36.14030000	H	43.57980100	49.32929400	42.86160600
C	43.52302400	48.96719600	36.78088700	H	48.30919400	50.52343700	44.28880200
C	43.62691000	48.60632400	38.24354400	H	46.15050000	52.93508200	38.79558000
C	42.35681500	48.91685100	36.12610400	H	49.93615900	52.92078600	37.09082400
C	41.00357700	48.55981500	36.67254000	H	47.59788400	55.67255900	34.33285000
C	40.46720600	47.28660500	36.39750100	H	53.32197400	52.16882500	29.36029200
C	39.11525500	46.99018800	36.27255700	H	46.89057800	49.53304800	24.66495300
C	38.54232200	45.70810600	36.02311500	H	43.15964100	53.15775400	23.16582700
C	38.55691400	43.14567800	35.07971900	H	44.70527700	41.77637300	33.05065600
C	37.27303900	41.35968800	36.29300500	H	48.28849500	43.67566000	30.97665000
C	38.38327900	40.35379000	36.06845000	H	48.28936000	44.64701800	29.50231800
C	37.88774600	48.46885600	34.90694200	H	30.40967900	50.94470800	30.17529300
H	45.38811000	49.98680200	36.83254400	H	52.19319200	49.63298800	22.76570500

H 51.41471700 51.22831600 30.79232800
H 42.98440800 55.33782800 27.07902400

Coordinates of DH3-IM3_b system

C 42.99133000 55.32184700 27.09578000
C 51.30339300 50.78292100 30.57521400
C 52.07229100 49.53889100 22.76732300
C 30.58735100 50.76810900 29.97487700
N 48.28980900 44.64804300 29.50249000
C 48.27431900 43.66437700 30.96840600
N 44.72065100 41.79061100 33.02554400
H 43.15689900 53.15839700 23.16668700
H 46.90148200 49.47568400 24.67840400
H 53.19427000 52.10730100 29.44242300
H 47.53293000 55.63860100 34.35399000
H 49.96817900 52.92211900 37.09823500
H 46.13915200 52.97127900 38.94514900
C 48.23289500 50.46816300 44.33868100
C 43.68547300 49.25959300 42.75554000
O 43.49417000 47.98023300 43.95889200
C 33.98834800 56.05661100 40.10558000
C 35.63519500 55.49807700 40.44025000
C 37.27692700 55.34123200 33.26992500
H 36.78749600 54.14682200 32.07438600
H 36.95638800 56.57985400 29.63408400
H 36.23969600 55.88060900 28.18245200
H 40.29439300 58.30655800 32.94274600
H 38.55133500 58.38941600 33.21310500
H 38.41912900 32.62015200 36.41296300
H 37.12631200 32.54656300 35.20921300
H 33.12854100 39.18749400 37.82089900
N 43.69727200 35.63417000 33.89832200
C 42.99298100 41.04058700 42.91733000
C 31.55958700 43.04944500 37.37280200
H 29.74123500 47.99782100 30.99047000
H 31.87205900 48.70185100 34.84709300
H 33.18863500 49.98932900 39.59788200
H 32.91872700 49.99550000 41.35200000
C 37.20504700 47.75338800 37.34312900
C 40.94952600 46.48897700 34.93297500
O 42.80214900 48.46463900 34.46484300
C 45.88854500 51.49112800 31.06715700
C 46.77388100 48.56774400 34.10952000
C 43.56134200 51.35521100 34.68537700
H 48.10479100 48.82293300 32.15565600
H 47.86963000 50.02550000 31.02814500
H 41.09707400 46.51892900 37.42202600
H 36.53337700 43.42305400 35.66436800
H 43.62699800 53.11736300 33.10071200
H 37.01407100 49.45431100 34.90283300
H 38.56624200 40.31095300 35.11475700
H 43.68314300 50.06211000 38.27943400
N 37.05078000 47.76566500 34.30576500
C 37.89757400 39.63120800 36.61402100
C 39.02931400 42.36538900 34.48799600
O 40.15108100 47.44673000 39.03440700
C 42.15487100 49.19161500 38.07677500

C 45.51271700 48.42151100 36.04300200
C 38.45132700 48.85488100 34.02279100
H 39.05688000 40.98412400 36.67495100
H 38.07381800 43.74423200 33.91454400
H 40.64790800 49.09063600 36.52448800
H 43.63762100 48.31013900 38.37273000
H 45.35921300 50.04864700 36.64311200
H 37.64582600 48.58325000 34.71228200
H 38.21312100 40.55333800 36.12399600
H 37.05382200 41.52658400 36.11931700
H 38.39570900 43.19527500 34.80223100
N 38.37639900 45.80364800 35.72785000
C 39.04663100 47.01767900 35.76610700
C 40.43561900 47.26840700 35.49356800
O 41.14279900 48.36175700 35.88283900
C 42.53392900 48.63320400 35.50675400
C 43.22030600 49.17353700 37.84025100
C 43.48196100 49.06792000 36.36068000
H 44.91546700 49.33795400 35.93099600
H 45.67714400 51.02216500 32.02474600
H 40.81375400 46.07839400 38.24851600
H 46.43670000 49.93472200 32.47901200
H 38.22117800 48.17403700 35.97041900
H 46.16334700 49.38700700 33.74333100
H 35.97556900 41.24170200 36.66348000
N 45.13499300 49.88999600 34.53831100
C 37.12230700 45.62400300 35.70940700
C 47.41526400 49.36941100 31.65372800
O 44.36873200 50.96615400 34.07404500
H 39.47179300 44.31571800 35.78996600
H 43.93959200 52.60666100 32.33487800
H 37.21866400 42.70214100 35.46840000
N 44.66096200 51.53280800 32.83502100
C 45.49125700 45.68408900 35.98767600
C 44.45119800 46.64497800 33.96208800
C 47.77676900 44.74685900 35.85836500
C 45.69765000 46.68538300 31.84703900
H 49.01654000 44.80634600 33.74007800
H 47.87833100 46.68606400 30.78023200
H 49.25484400 45.84615900 31.51255600
H 46.78579800 44.41651700 30.41325800
H 46.03149500 45.69163800 35.05139800
H 45.44548100 46.22616100 33.91633900
H 47.31484600 45.17495100 34.98002200
H 46.14903000 46.25474500 32.72664600
H 48.01355300 45.20638700 33.78506500
C 47.44195500 45.75534700 32.64401300
C 48.17796600 45.79411400 31.33553300
O 47.86103600 44.55329800 30.49698400
C 42.85824900 44.77480800 34.69268200
C 41.68613200 43.76875200 33.81549400
C 42.66169000 42.91644700 36.19750900
H 42.47138100 41.76372400 34.86475000
H 45.00188000 43.24726200 35.67739300
H 44.82358700 41.51044700 35.41008600
H 45.72970700 43.19541600 33.39926100
H 42.70380100 43.80546100 34.20525800

H	42.98241500	42.67145900	35.18834500	C	44.39818400	53.00690200	24.41436400
H	44.49434800	42.49231100	35.07961100	N	42.25214900	54.71677800	25.74615700
H	44.76604800	42.72303500	33.59809000	C	42.50503000	53.66924500	25.15227800
N	43.68856200	43.60613100	33.15760500	N	43.56039300	53.60972100	24.06923300
C	38.74957300	46.53522300	31.48413500	H	46.91739700	49.93556100	28.36735400
C	40.33837300	46.74232800	32.20551300	H	46.06884700	51.48497900	28.38438000
O	39.43158300	45.25121900	32.48146000	H	47.74916800	51.39771100	27.83787400
C	38.43780800	45.26763400	29.40247700	H	44.58396000	49.76193000	25.42338900
H	38.83946100	43.81511500	30.31905100	H	44.22851300	50.49217300	26.99713500
H	39.69203600	44.17507000	28.81790500	H	45.05564900	48.93780500	26.90715600
H	40.67831200	46.21178300	29.86895700	C	46.18264000	51.59497700	25.91344800
H	41.09952800	43.64256900	31.46229400	C	47.64372600	48.93142600	26.20273100
H	41.87970300	44.04178300	29.93144400	C	48.44427400	51.40387800	24.80665300
N	42.21442100	45.64323700	32.51121000	C	46.79277100	50.87971600	27.84269000
C	43.83633700	45.89504600	30.09817800	C	44.95702700	49.91157500	26.43501100
C	39.67012600	46.01849900	31.74742500	C	46.30552500	50.62723800	26.41884200
O	39.25274800	44.61627900	29.70942400	C	47.33658100	49.80701900	25.62792700
C	40.29934100	45.40040000	30.49939000	C	48.53754900	50.56564100	25.35763000
H	41.46701100	44.46821600	30.84846700	H	51.10058000	48.91186400	24.10072900
H	44.60074100	43.95350800	31.13122900	H	52.76005200	49.44271400	24.38242600
H	43.72134100	44.17657900	31.95039400	H	52.14873400	51.78069400	23.91818400
H	42.59685700	45.16872400	31.60604300	H	50.52264500	51.29513700	23.43015200
H	43.19823400	46.22404300	30.81037500	H	50.51064800	52.27822100	25.70141000
N	45.00351500	48.55438900	30.67013600	H	52.32326700	50.11274100	26.52310200
C	43.94155100	48.17140400	29.27646800	H	51.85016100	49.65030400	23.82572100
C	43.69212600	50.37490200	31.19647100	H	51.34853900	51.06286500	24.10683600
O	42.52665200	47.91147700	32.14258000	C	49.91496700	49.31025400	26.62714300
C	43.17225400	47.50677700	31.19237400	C	49.73425100	50.26908300	25.90748800
C	43.97242800	48.49235900	30.31994400	C	50.85933300	51.25123800	25.54579100
C	43.37205600	49.80293000	30.42532700	C	51.95017000	51.05005100	26.51294300
H	40.74582200	53.43584400	31.85802600	C	51.25418800	49.02349000	30.39638900
H	39.17179600	52.74486200	32.23855600	N	50.67908400	50.05576000	29.08845300
H	39.53690900	53.21859900	30.58469700	H	53.56278600	49.75664800	30.04872100
H	41.36583700	49.74548300	32.38036700	H	52.90284800	49.19950300	28.51279600
H	40.25213900	50.76799500	33.28011300	H	54.14188800	51.30615800	28.17063200
H	41.87019500	51.35112700	32.89736100	H	51.42699600	49.96138800	29.87288600
H	39.69871800	50.74121900	30.85180800	H	52.82805700	49.98147200	29.27221300
N	42.37182400	52.16382000	30.41494600	H	51.47859800	52.83719500	27.79370400
C	40.08445500	51.36996900	28.71987600	H	52.10994500	51.81043500	27.63663900
C	39.95648100	52.78374800	31.48948600	H	53.17049200	51.34363000	28.66625500
C	41.03437800	50.76997600	32.52450300	H	46.60431500	52.61660000	35.11781000
C	40.50515400	51.38025700	31.23217900	H	47.26625800	52.89561200	33.01521500
C	41.68862000	49.35509200	28.98498300	H	46.14159100	54.26998400	32.88941800
H	42.20989700	50.06956000	29.82340500	C	48.64665200	54.87365600	33.18064100
H	41.58984600	51.44962800	30.14969400	C	48.13664900	53.87763400	35.91282700
H	40.95012600	51.86350200	28.88965200	C	46.07210400	53.28318200	34.64912200
H	39.78321400	51.02056300	25.16175400	C	46.83049100	53.74297700	33.55527800
H	39.13662400	51.08599000	26.78950100	C	47.94893600	54.69300700	33.99801100
H	40.62826800	50.18981600	26.48076400	H	48.69685000	54.08609300	35.09859800
H	40.22873600	53.22875200	26.48169800	H	47.71146600	51.41716800	36.97816000
H	42.17267500	51.68015400	24.95777300	H	49.59298100	50.43478400	36.64291200
H	40.05743900	51.07713300	26.21263800	H	49.48181700	50.83002800	34.91219800
H	42.78001700	52.72628500	27.90620500	H	51.24770700	52.18883700	36.08565200
H	41.63080400	52.29349900	27.82828200	H	47.93920900	51.50394100	36.03141000
C	40.86979600	52.33904900	26.46805600	H	49.31606900	51.21205400	35.92457600
C	41.85158700	52.52549700	25.40585600	H	50.54188200	53.44822600	33.96015500
C	43.90558200	54.61485500	23.84860800	H	49.85667200	53.38930900	34.95868400

H	50.19704800	52.46000300	36.13905900	N	36.05023500	50.31769000	37.00308700
C	40.43295500	51.73570600	37.12166100	C	37.18389500	54.85802200	38.60815900
C	40.08992100	50.76508000	39.42214000	C	34.32533600	51.70240200	38.07495700
C	42.61904400	53.07190600	37.02160600	C	33.69680300	54.35136500	38.34059500
C	44.11914500	54.01930700	39.42623200	C	34.04312700	53.60875300	39.88097900
C	44.13664300	52.80766800	40.71713000	N	35.25419700	56.25943000	38.88650300
C	45.05352800	52.01757300	37.93067000	C	38.62108700	51.06040000	36.63459600
C	45.20931500	50.86699400	40.55896600	N	37.61674000	51.78432900	37.23193300
C	41.07871400	51.86456300	37.88814600	H	37.90950700	53.07761600	37.67582100
O	40.93631900	51.35109400	39.12660500	H	36.30947300	51.30421600	37.37617000
H	41.94565900	51.65299200	39.90020600	H	36.91787300	53.86157900	38.26985900
H	42.25904700	52.54474100	37.87921300	H	35.33325900	52.09919600	37.97776500
H	42.78754800	52.40474000	39.13608100	H	35.60961900	53.39391200	38.44287800
H	44.08284900	52.94827000	39.63700400	H	34.49625800	54.21245000	39.08260700
H	45.28722200	52.28010300	38.96825300	H	34.87000500	55.58598800	39.66097500
H	45.69848000	51.08856200	39.69362600	C	37.16836300	51.25937100	32.37115100
H	44.29490800	46.72059400	39.96598600	C	35.72914500	52.12992100	31.82235600
H	45.64273200	45.64870400	40.33574400	O	35.57024700	50.55501400	32.58897200
C	45.04920700	45.76995900	38.68589200	C	34.11727800	53.11018400	33.54269400
C	47.38069100	46.17784500	38.03642100	O	34.48541700	52.95969100	35.26550400
C	48.06375000	46.34349000	39.65198500	H	33.97493700	51.54806300	34.34265600
C	48.22818500	47.65106100	38.46933900	H	36.37157500	51.44121800	34.72336000
O	45.84666200	48.11481200	38.54255900	H	36.77574800	53.79478400	35.11364300
O	45.41550100	48.66446900	40.91992400	H	37.94433200	53.07580400	34.01337300
H	46.77004200	47.65167300	41.40888200	N	35.59409600	54.84339000	33.17423500
H	48.31819800	49.10453200	40.07259700	C	36.13030400	51.48771100	32.60220800
H	48.66976100	50.01296400	42.04130400	C	34.55858800	52.46579800	34.29893300
H	45.24138500	46.33576200	39.59431600	O	36.01332700	52.15190800	33.97210600
H	47.56346900	46.87831800	38.84736600	H	36.90229600	53.39331400	34.10501400
H	46.23775600	47.46455900	39.33089400	H	36.61901900	54.49338900	33.09111900
C	46.39353300	48.29618900	40.61028100	H	43.20302000	54.28340800	28.33369700
C	47.68027400	50.97114100	38.63682200	H	44.17870000	55.68050200	28.28278700
O	46.91396200	50.57696000	39.51153700	H	42.38575200	55.98935000	29.93596900
C	47.36508900	49.46696200	40.46367500	C	42.21699000	57.10135800	28.56230600
H	47.69720500	50.06318600	41.78356900	C	40.83353800	55.29784800	27.42088300
H	47.50817500	53.25183500	43.28077100	O	40.77209500	54.45235000	28.97448900
H	49.01026900	52.39737700	42.92105600	C	39.55696500	56.36648700	29.96773200
H	48.66584800	52.92172600	44.57057000	C	39.70174700	57.25577700	28.45041200
N	46.72760000	51.34860000	44.68282100	H	38.48920000	55.39592600	27.27773700
C	48.22232100	52.52504800	43.66078600	H	38.25380800	54.59866000	28.83437700
C	45.67013500	50.79900800	42.45266800	H	37.19284000	57.35847800	28.07034600
O	46.86284800	50.66248500	42.66648300	H	43.24017000	55.31511100	28.12196500
C	47.52197700	51.20006400	43.95314000	H	42.19111900	56.05268700	28.86398500
C	41.55978400	46.18790500	38.87882300	N	40.84816300	55.43211600	28.50352900
C	41.64355100	49.96953000	41.32484900	C	39.62462600	56.25793800	28.88430700
C	40.03740700	49.43363200	41.79177400	C	38.36735700	55.57124500	28.34922300
H	41.38894900	49.28308000	43.76699100	O	37.11203200	56.39803500	28.57292800
H	41.12211000	47.62533700	43.25253600	C	43.94077400	54.03823600	34.96587900
H	43.43223600	47.58178700	42.22975900	C	41.65614800	53.05046300	34.68313700
H	40.04945700	48.18785100	39.70522900	H	44.19062200	56.46799600	35.08318300
H	41.97518100	47.24425000	40.39353100	H	39.69884500	54.51672500	34.59146500
H	41.09467300	48.08760100	40.54360300	H	42.21630300	57.93475500	34.98013400
H	41.06838100	49.09080400	41.66241300	H	38.72846700	56.68085000	35.00867700
H	41.64090000	48.55684200	42.98558300	H	39.75311500	58.07743200	35.36471900
H	43.15298700	48.32604100	42.97622300	H	39.27965000	56.90833600	32.58098900
H	38.41327200	50.10491700	36.58753000	N	43.06247300	54.66445400	34.88755900
H	38.91533700	53.46900300	37.55993000	C	41.79468600	54.12160700	34.74169800

C 43.20610900 56.04050400 34.96642100
C 40.68471500 54.94766300 34.68819700
C 42.09621000 56.86322900 34.90791300
H 40.82088500 56.32638700 34.77527200
H 39.62065900 57.22631200 34.69424000
H 39.42300300 57.74197500 33.26699000
H 33.32311300 35.92391800 35.32807400
H 32.09189000 33.78843300 36.10451700
H 35.76052200 35.78628700 35.88706900
H 36.86366500 33.68373900 38.03525200
H 36.21913500 32.12383100 37.50161700
H 37.74520000 34.11458700 35.74429500
C 33.72943700 35.12732500 35.80485400
C 33.13973800 33.98412000 36.21411100
O 33.99523300 33.16042000 36.75675300
H 35.05448300 35.01402600 36.11347900
H 35.20558700 33.78553000 36.70073700
N 36.46094200 33.13617700 37.17749900
C 37.50698900 33.10202100 36.06397000
C 35.36322800 37.62579100 41.04891200
O 35.40761500 35.97696800 40.42210200
C 34.20902700 36.42588600 41.63364100
H 33.53760100 35.14971900 38.86770600
H 32.16591000 36.20814400 38.53451900
H 32.40917300 35.56727400 40.15322200
H 33.11673400 37.95119400 40.00829300
H 35.28812000 38.42897300 38.78344700
N 35.11192900 36.86408100 37.98068300
C 32.95759400 37.63344500 36.97392400
C 35.16472800 39.56396700 36.50438000
O 34.74983900 36.77526000 40.75754700
C 32.92024300 35.94798000 39.27211500
C 33.77707900 37.15573900 39.64260200
C 34.56235200 37.68809000 38.43866000
H 33.67298800 38.34293200 37.38799400
H 34.48716800 38.84327600 36.26559000
H 35.72953500 38.25344100 30.97426200
H 34.49724800 37.10018200 31.53363600
H 33.82650900 39.71591900 31.08756500
H 33.12195600 38.79631100 32.43098000
H 35.52919900 40.66218400 32.57278800
H 34.07639900 40.69389600 33.58881200
H 36.30591300 39.35469700 34.46489400
N 35.02327900 38.02242200 31.78112600
C 34.04939100 39.17939000 32.00705200
C 34.76047900 40.04651500 33.04324100
O 33.53162600 37.64625000 34.61130800
H 34.38195200 38.43882500 34.99173300
H 35.40899900 39.00996100 33.95000500
H 35.74528800 37.90320100 33.03723700
N 34.64187500 35.11972100 32.65321400
C 35.74225300 34.29462000 33.75873700
C 35.70923200 33.84303600 32.04571000
O 36.67390400 35.99412800 31.38688500
C 38.45724200 35.33400700 33.56072000
C 35.62747000 34.67102400 32.74500800
C 37.21029200 36.93681400 34.43612500

C 36.58182200 36.90691000 33.38531400
H 36.72500600 35.69198300 32.43698800
H 38.04939200 35.10806300 32.66358700
H 39.27251600 31.72124600 31.88666000
H 39.24879400 32.29270100 33.55932500
H 40.77580500 31.78462800 32.81586200
H 40.64831900 33.70127900 31.21390400
H 40.55150800 34.36169600 34.08150400
H 39.82528400 32.28155400 32.63540600
H 38.17428300 34.05116500 30.68736600
H 38.67523600 34.32002300 31.75982900
H 40.05799200 33.70300900 32.13499900
N 40.80925500 34.48141300 33.11387200
C 42.96503400 37.83634000 35.92628400
C 43.21019500 39.19662200 34.83153500
C 44.35385900 37.85549900 34.83729900
C 40.41637900 37.34682400 33.18380800
H 40.89273200 38.88173300 33.90677100
H 40.58787300 37.48332200 34.93673000
H 42.83397900 37.70731100 32.87379700
H 42.25644500 35.53537700 34.93496800
H 43.30281700 38.11739500 34.93065100
H 41.00025800 37.80136700 33.98085200
H 42.47203300 37.40966500 33.86318900
C 42.31222400 35.32615200 31.66410400
C 41.92160100 35.20370800 32.80531200
C 42.64000300 35.88799800 33.97600300
C 41.25211300 43.80999200 44.70868200
C 41.43545500 42.05963800 44.60776100
C 40.55691700 42.93071700 43.34851500
C 43.59512700 44.58636700 41.87608200
C 42.55905000 45.31965800 43.10121400
H 41.84755400 44.45404700 41.74074900
H 43.53557200 43.22535000 43.97259500
H 43.96423400 42.08548800 41.84531900
H 41.02601700 41.76762100 41.58327800
H 41.40696900 42.97789500 44.02541700
H 42.67704000 44.46278000 42.44384900
H 42.71139800 43.16912800 43.25263600
H 43.00091100 41.96994900 42.34382500
C 41.98654500 41.84718000 41.26968200
N 41.20474300 41.89174500 38.00551500
O 40.24859800 41.15668300 39.34155300
S 40.21441000 43.93747600 38.46948000
C 43.25852800 42.24290200 39.43408000
N 42.17659200 42.04126500 39.94734500
O 40.87614700 41.99715400 39.03604100
C 40.13308400 43.22724000 39.18595300
O 35.50547300 45.35135700 41.30271600
C 36.47397800 44.26009600 42.32389400
O 37.29172500 47.00290300 41.26114400
C 37.38416300 46.41543200 42.93248500
O 39.61925700 46.24411800 41.44613000
C 39.10741100 44.80177000 42.33636300
C 38.76919600 45.32531500 39.36182000
C 36.51542800 44.99673900 41.51522200
C 37.47129700 46.12713300 41.88744200

C 38.82637700 45.51168100 41.55640600
C 39.21758800 42.62109600 41.15361100
C 39.33921200 43.42337700 40.23524100
C 38.55892900 44.74102900 40.26262300
C 37.13089200 44.42472800 40.33293400
C 33.38026400 40.93444200 39.58920500
C 33.39640200 41.59260400 41.22569700
C 34.02022000 39.97237900 40.92134000
C 37.14199500 41.89529000 41.46866600
H 36.20259900 40.49184800 41.94868200
H 35.62139200 42.09837600 42.36246700
H 35.86979200 40.94404000 39.54387000
H 34.65278400 43.61304600 40.37369100
H 34.89893400 42.21170000 37.77778900
H 33.94655100 40.97736000 40.51591400
H 36.13090400 41.51792900 41.59556400
H 35.34395600 41.54987600 40.28947600
H 37.28538100 43.17405700 38.48841100
H 36.63596700 43.53140600 39.45680800
H 35.23445500 42.97739200 39.70179500
H 34.51877300 42.88671800 38.44529300
H 31.70799500 42.64729900 34.41464400
H 31.53089000 44.34512300 33.96090900
H 30.56257000 43.68052300 35.27135200
H 34.76020800 44.45207300 35.73385900
H 33.98371100 44.45356200 34.15648900
H 34.29421000 42.92205300 34.96874700
H 32.45223100 45.05421300 36.13972700
H 32.90891900 42.09654100 36.71901400
H 31.54138900 43.65158600 34.79866500
H 34.00631200 43.96021100 35.12430800
H 32.63618300 44.03207400 35.79231500
H 33.07818400 44.57032200 38.84434200
H 33.42309800 43.59023000 38.16846900
H 32.58966400 43.09748500 37.01191700
H 29.67247300 49.57671000 29.04800500
H 31.33797500 49.23174200 29.52270800
H 28.96305300 49.53638900 31.43439600
H 31.13058800 50.14264700 32.45912700
H 30.40960200 49.70317800 29.83559500
H 29.90299300 49.06898000 31.12405400
H 30.87882500 49.20192400 32.19887200
H 34.68183100 48.73454000 35.45787100
H 35.08057900 47.01539400 35.56386100
H 33.60748800 47.63322300 36.32453800
H 35.19676700 46.59721900 33.14880900
H 34.97908000 48.31984500 32.82931400
H 33.90473200 47.13458000 32.07494100
H 32.97020000 46.51704200 34.25156300
H 32.94044700 49.50212300 33.68307100
H 34.26671700 47.72765100 35.46312900
H 34.45677400 47.37575400 32.97976800
H 33.50435800 47.46562400 34.16828200
H 31.22052600 47.00338400 32.56213000
H 31.47154900 48.15917100 32.83087900
H 32.45997900 48.55404000 33.93693600
H 36.04639300 45.55861300 37.42854000

H 36.33897500 49.39295000 39.15316500
H 34.10805800 45.76575300 39.11384400
H 32.98003200 47.64343500 40.48581500
H 34.28447200 47.93887300 41.62180500
H 34.53551200 50.30451700 40.70334600
H 36.49756400 47.53397600 38.07025400
H 35.81367000 46.39074900 38.07879000
H 34.84819500 46.49765600 38.99475000
H 35.94902000 48.40114100 38.99889200
H 34.89066900 47.75882500 39.58280800
H 33.91147200 48.20624100 40.62382100
H 33.62307900 49.71493300 40.56403600

Coordinates of DH3-TS4_b system

C 33.62308000 49.71493100 40.56403700
C 34.98280500 49.05173600 40.88586800
C 35.68780100 48.33961700 39.76368500
C 36.90836200 48.57544300 39.17481600
N 35.21989900 47.17510100 39.15872900
C 36.12531700 46.75113000 38.25881900
N 37.16616700 47.57745000 38.25266600
H 33.74230600 50.48530600 39.79721600
H 35.67385300 49.81744800 41.25537500
H 34.84246200 48.34450600 41.71495800
H 34.35863700 46.65397900 39.36477900
H 37.61661900 49.36793700 39.35389100
H 36.01907000 45.87963200 37.63387800
C 32.45991400 48.55411400 33.93693600
C 31.47923900 48.14855000 32.83175800
O 31.23242100 46.99070700 32.56511500
C 33.63880500 47.59723300 34.07365700
C 34.47219600 47.55941900 32.79747900
C 34.48997500 48.00868400 35.27001500
H 32.82053900 49.56978800 33.75184600
H 33.23407100 46.59948500 34.24009400
H 33.86642600 47.22239800 31.95988100
H 34.87323800 48.54471300 32.56525200
H 35.30323300 46.87037500 32.92368100
H 33.91133800 47.96875500 36.19186400
H 35.34595500 47.34915100 35.36616800
H 34.85583600 49.02565600 35.13874400
N 30.88298100 49.18969900 32.19676600
C 29.90300200 49.06896800 31.12407700
C 30.40913400 49.71056500 29.83903700
H 31.13401800 50.12965600 32.46071900
H 28.96610000 49.53827000 31.44088400
H 31.33490000 49.23750300 29.52087400
H 29.66972800 49.59347500 29.05202500
C 32.25184800 44.00130500 37.51381800
C 33.32241300 44.26721700 38.54764100
O 33.29033000 45.25193100 39.28765300
C 32.47988500 44.72013400 36.17540100
C 33.77712200 44.23607600 35.53310100
C 31.29140900 44.47286400 35.24923500
H 32.17950400 42.92757900 37.33292500
H 32.55448000 45.79439100 36.37290900
H 33.82242600 43.14829000 35.54309100

H	33.84380800	44.57059200	34.50101400	C	41.92506300	35.19938200	32.80547900
H	34.63055500	44.63728400	36.07592100	O	42.32080000	35.31678300	31.66546300
H	30.36128900	44.76773100	35.72973700	C	42.46858400	37.40871000	33.85824300
H	31.39004400	45.04591400	34.32984500	C	40.99538700	37.79590800	33.97242000
H	31.22467600	43.41787500	34.99209900	C	43.29632900	38.12162700	34.92472500
N	34.27511200	43.33223800	38.65185500	H	42.25519200	35.53725900	34.93513100
C	35.11858500	43.20209900	39.82052800	H	42.83127500	37.70428800	32.86848300
C	36.54257500	43.67492700	39.53661400	H	40.58244900	37.47835000	34.92824100
O	37.14192600	43.32302500	38.53157700	H	40.88240600	38.87551300	33.89480100
C	35.16471600	41.71336000	40.23220100	H	40.41458300	37.33695000	33.17579100
C	36.00274700	41.50502500	41.48988500	H	44.34793700	37.86088900	34.83426300
C	33.74943200	41.18751600	40.46277100	H	43.20231900	39.20043400	34.82141100
H	34.41474400	42.63523900	37.92665200	H	42.95708200	37.84354600	35.92071300
H	34.65529700	43.79451900	40.61294400	N	40.81103000	34.48027900	33.11336000
H	35.62343700	41.16884400	39.40011000	C	40.05799100	33.70300900	32.13499900
H	35.56250100	42.03624400	42.33173200	C	38.67880400	34.32636000	31.75613900
H	36.02846700	40.44703000	41.74033500	O	38.18452100	34.06816600	30.67802500
H	37.02758300	41.83985800	41.35494100	C	39.81706000	32.28425600	32.63908500
H	33.78989200	40.14788900	40.77590300	H	40.54805800	34.36749600	34.08040600
H	33.25547300	41.76127200	41.24475800	H	40.64993000	33.69594400	31.21504700
H	33.14777700	41.25072000	39.55987300	H	40.76466800	31.78337500	32.82396800
N	37.12678700	44.47192500	40.44658100	H	39.23777100	32.30092700	33.56114100
C	38.56694200	44.70413500	40.35798800	H	39.26398100	31.72412400	31.89043700
C	39.29164900	43.35877000	40.25887500	N	38.04889600	35.10708500	32.66330000
O	39.14196900	42.50503600	41.12291100	C	36.72500800	35.69198400	32.43698800
C	38.90190200	45.39749500	41.68017700	C	36.58164300	36.90682900	33.38610200
C	37.60335700	46.10839100	42.04194400	O	37.20566100	36.93177000	34.43943600
C	36.55402400	45.07659900	41.63482500	C	35.62655100	34.67360700	32.75107500
H	38.79257500	45.31942200	39.48164400	H	38.45077400	35.32340100	33.56547200
H	39.12413700	44.63583200	42.42953400	H	36.67313500	35.99229200	31.38661900
H	39.75322700	46.06504000	41.59447500	H	35.70415800	33.84256500	32.05491300
H	37.54319100	46.36332800	43.09755600	H	35.74317000	34.30128900	33.76618400
H	37.49562500	47.01832300	41.44962400	H	34.64172100	35.12429700	32.66122000
H	36.43109000	44.32913400	42.42590900	N	35.75155600	37.90771600	33.03488500
H	35.58585100	45.52973500	41.41459300	C	35.40899800	39.00995800	33.95000500
N	40.09741600	43.20409000	39.20699500	C	34.39356700	38.42565400	34.99548500
C	40.87614200	41.99717000	39.03603100	O	33.59167000	37.57940500	34.62835600
C	42.17269100	42.07388800	39.94902100	C	34.75032000	40.04367600	33.04775600
O	43.24450100	42.33861900	39.44246000	C	34.03972900	39.17137400	32.01565300
H	40.23717200	43.97320300	38.56391000	C	35.02387800	38.02450800	31.78171400
H	40.27397800	41.13622400	39.33419200	H	36.30516900	39.36239000	34.46444400
H	41.20424500	41.91138900	38.00344000	H	34.06829300	40.68867600	33.59835100
N	41.98938100	41.84440800	41.26650200	H	35.51380200	40.66166100	32.57190600
C	43.00091400	41.96994700	42.34383100	H	33.11880400	38.77862300	32.44491600
C	42.68220800	43.13616400	43.28428400	H	33.80516600	39.70658500	31.09833900
C	42.63877200	44.45149000	42.51252200	H	34.50593800	37.09820800	31.53268800
C	41.37383100	42.89985100	44.03736700	H	35.72500100	38.26548800	30.97323100
H	41.03566700	41.70396700	41.57760300	N	34.46139800	38.87020400	36.25944700
H	43.95969800	42.12463500	41.84721600	C	33.67298800	38.34293300	37.38799400
H	43.49767700	43.18343000	44.01466700	C	34.59880300	37.76664100	38.45363900
H	41.83141400	44.44248800	41.78457600	C	33.84505300	37.22134500	39.67183500
H	42.48090600	45.28624800	43.18965700	C	33.05515900	35.96014200	39.33232600
H	43.56998700	44.61299400	41.97655500	C	34.83726300	36.92388600	40.79484300
H	40.53161200	42.85058600	43.35097700	H	35.04271600	39.67465500	36.47683100
H	41.41579400	41.96861300	44.59784600	H	33.00651300	37.58080900	36.98704300
H	41.19428500	43.71156900	44.73868800	H	35.19564800	36.96508800	38.01516000
C	42.64000300	35.88799800	33.97600300	H	35.27986500	38.55683200	38.78042500

H	33.14230900	37.98855800	40.01893800	C	36.01666900	51.58207900	32.46158100
H	32.57178400	35.56934400	40.22454500	H	35.59358300	54.83713300	33.19054700
H	32.28282600	36.16250600	38.59533000	H	37.94096400	53.02192200	33.93177600
H	33.71368300	35.18977500	38.93882800	H	36.80533000	53.71224100	35.08321500
H	34.31664100	36.56558500	41.67948100	H	36.35725400	51.36682700	34.56764800
H	35.54032400	36.15694000	40.47858500	H	33.95233200	51.56186100	34.30784900
H	35.40008100	37.81530700	41.06532900	H	34.54267200	52.89215300	35.29913800
C	37.50698900	33.10202100	36.06397000	H	34.10054200	53.17101600	33.60970400
C	36.48177200	33.12167600	37.19676300	H	35.44955700	50.65504300	32.40939900
C	35.21401200	33.76063000	36.74006900	H	35.56946800	52.28363600	31.76183200
C	35.04720100	34.98539500	36.14975000	H	37.03696700	51.37399200	32.14485700
N	34.00933300	33.12650000	36.81269400	C	34.87000600	55.58598600	39.66097600
C	33.14151200	33.94157800	36.27663000	C	34.41987300	54.30823500	38.93428200
N	33.71816000	35.08750500	35.85671800	C	35.50973400	53.40756500	38.36911000
H	37.73043500	34.11814200	35.74500100	C	35.17698800	52.13131600	37.88626200
H	36.25517500	32.10608500	37.52162400	C	36.85333600	53.78707300	38.27528500
H	36.89391100	33.67051900	38.04916700	C	36.12855100	51.26739700	37.34464900
H	35.74321900	35.76388700	35.91356900	C	37.82001900	52.94069100	37.72857600
H	32.09399000	33.73754100	36.17956100	C	37.46870900	51.66902300	37.26045600
H	33.30717100	35.87694600	35.37298300	O	38.45598800	50.87573500	36.74044300
C	39.42299200	57.74198400	33.26697800	H	35.40337000	56.26749600	38.98875300
C	39.60590800	57.27482600	34.71275600	H	33.80463600	53.71267000	39.62227100
C	40.79756900	56.36814900	34.83044100	H	33.74041700	54.59417400	38.11768400
C	42.07090000	56.89384000	35.01481600	H	34.14033000	51.80319900	37.92658400
C	40.65498200	54.99156600	34.72129400	H	37.16606300	54.76324000	38.63290200
C	43.17249400	56.06239000	35.10259600	H	35.84213800	50.28065300	36.99290100
C	41.75661700	54.15734000	34.80318000	H	38.85292800	53.26886100	37.66312600
C	43.02258300	54.68866400	35.00101700	H	38.10480900	50.01899200	36.38718200
H	39.27938100	56.88607100	32.60912800	C	43.15298700	48.32604000	42.97622200
H	39.74046400	58.14688400	35.35496400	C	41.64043900	48.53607800	43.04595900
H	38.70730900	56.74695300	35.03843700	C	41.01759100	49.03547100	41.73479700
H	42.19614600	57.96350500	35.10347400	C	41.03628000	48.01588000	40.63222800
H	39.67054400	54.56844300	34.58458000	O	41.89338800	47.14530000	40.50355600
H	44.15508700	56.48169400	35.25862800	O	40.01141000	48.13826000	39.77318200
H	41.60909400	53.08863000	34.72355200	H	43.41214200	47.56616000	42.23899800
H	43.89544200	54.05677400	35.09837200	H	41.14447100	47.60381600	43.34972700
C	37.11203500	56.39803500	28.57293100	H	41.40955800	49.27493600	43.82167600
C	38.36775900	55.57152400	28.35210100	H	39.98264300	49.35810200	41.88442900
C	39.62493800	56.26658600	28.87619100	H	41.56417100	49.92090900	41.36865700
C	40.84967400	55.44275000	28.49543300	H	41.52833200	46.14246500	38.96925000
C	42.19167500	56.07331400	28.84133400	C	47.52197600	51.20006300	43.95313800
N	43.23877600	55.33505300	28.09698500	C	46.86525800	50.67048600	42.66428900
H	37.18880300	57.35367400	28.06064600	O	45.67033400	50.80432500	42.45607500
H	38.25793500	54.60337700	28.84682000	C	48.20963000	52.53465800	43.67350900
H	38.48597300	55.38647700	27.28180400	H	46.72781800	51.33429200	44.68582800
H	39.69630300	57.26132500	28.43427200	H	48.64991800	52.92582200	44.58712600
H	39.56184100	56.38319300	29.95901400	H	48.99840300	52.42190900	42.93223300
H	40.78138200	54.46687500	28.97565800	H	47.48836300	53.25866700	43.30184400
H	40.82869900	55.29874000	27.41415500	N	47.69985800	50.08771100	41.77109600
H	42.20988800	57.11964400	28.53123300	C	47.36509400	49.46696100	40.46367800
H	42.39441400	56.01945400	29.91230800	C	46.88972300	50.54091500	39.48146400
H	44.17723200	55.70380700	28.25031400	O	47.60153000	50.84946400	38.53034800
H	43.20412700	54.30493100	28.31413900	C	46.40084700	48.29308100	40.64547700
C	36.61898400	54.49352000	33.09115100	C	46.23122300	47.42884100	39.38989400
C	36.90598500	53.35172200	34.05656800	C	47.55640800	46.85840400	38.88656400
C	35.98660000	52.13847900	33.88410600	C	45.26511700	46.28689400	39.70583900
C	34.55877400	52.46560800	34.29882400	H	48.67227100	50.03534700	42.02929400

H	48.31697200	49.10186300	40.07248700	C	51.34625800	51.06515800	24.10586700
H	46.78948700	47.66907800	41.45450600	C	51.84613200	49.65281700	23.82015000
H	45.42559700	48.66666400	40.95795900	H	52.35724000	50.13120600	26.49627500
H	45.80758600	48.05225700	38.59695800	H	50.50713400	52.27684200	25.70270300
H	48.19154800	47.63567000	38.46921100	H	50.51928100	51.29926600	23.43119500
H	48.09050200	46.35803400	39.69150700	H	52.14650300	51.78290600	23.91697300
H	47.36849300	46.13086800	38.10092500	H	52.75872000	49.44317900	24.37172000
H	45.06302900	45.69230000	38.81810200	H	51.09753400	48.91421300	24.09729700
H	45.69876400	45.62818400	40.45466700	N	48.53777400	50.56614600	25.36017900
H	44.31976500	46.66105700	40.09176900	C	47.33636800	49.80712100	25.62777900
N	45.70889400	51.10815100	39.72031700	C	46.31479600	50.61592500	26.44273400
C	45.28722000	52.28009500	38.96824000	C	44.96321700	49.90586300	26.45363800
C	44.04274100	52.91930600	39.59088800	C	46.81412500	50.83711900	27.86768600
C	42.75801900	52.32477600	39.11413300	H	48.44354400	51.40886300	24.81625600
C	42.22249200	52.37245800	37.85294400	H	47.64532000	48.92031600	26.18416300
N	41.90167000	51.66003100	39.94193600	H	46.19254100	51.59421800	25.95820400
C	40.87850400	51.32356000	39.20158500	H	45.05997600	48.92350900	26.90817600
N	41.02374100	51.72725300	37.92345100	H	44.23968100	50.47994800	27.02875600
H	45.27607300	50.94410700	40.63067400	H	44.58464200	49.77528400	25.44142500
H	45.09407200	51.99580300	37.92819000	H	47.77173300	51.35265500	27.86607700
H	44.08779900	52.82469700	40.67671300	H	46.09671800	51.43218300	28.42896200
H	44.04425100	53.98281800	39.34028700	H	46.94173000	49.88167500	28.37073600
H	42.59130900	52.81770000	36.95431700	C	43.56054800	53.60964300	24.06932900
H	40.01659400	50.79128000	39.54903500	C	42.49989500	53.66954600	25.14690200
H	40.35930400	51.55735300	37.18037900	O	42.23955700	54.71896400	25.73418700
C	50.19704500	52.46000400	36.13906300	H	44.40107600	53.01550900	24.42283100
C	49.86058400	53.39959700	34.96573300	H	43.89948400	54.61558200	23.84274500
O	50.55808000	53.47927900	33.97753000	N	41.85133100	52.52412700	25.40505300
C	49.35388600	51.19380500	35.88333500	C	40.86982500	52.33894500	26.46799700
O	47.96663700	51.45109100	35.94299200	C	41.63241200	52.29783000	27.82725800
H	51.25503300	52.21536100	36.10645500	O	42.77813000	52.73971000	27.90674300
H	49.56609700	50.82694500	34.87395700	C	40.05722400	51.07696600	26.21436000
H	49.62407400	50.41606200	36.60360000	H	42.17563900	51.67815100	24.96053100
H	47.70060500	51.32999400	36.87455300	H	40.22864000	53.22857600	26.48010200
N	48.69025200	54.07938600	35.09866100	H	40.62819500	50.18939600	26.48128200
C	47.94894400	54.69300700	33.99800200	H	39.13685900	51.08600500	26.79193500
C	46.82694100	53.74745500	33.54847000	H	39.78170500	51.02051000	25.16380400
O	46.07763200	53.26686300	34.63983400	N	40.95504600	51.85786200	28.88593700
H	48.12383800	53.86067900	35.90570400	C	41.58963900	51.44970200	30.14984600
H	48.64997400	54.87407900	33.18369600	C	42.20922900	50.06820700	29.83261600
H	46.13101000	54.28354500	32.89752800	O	41.68396600	49.34566600	29.00367200
H	47.25965700	52.90940200	32.99142500	C	40.49636300	51.38406200	31.22402300
H	46.61469300	52.59053100	35.08829800	C	41.01623100	50.77942800	32.52211000
C	53.17050000	51.34365000	28.66625800	C	39.94767000	52.78860500	31.47230400
C	52.08969100	51.79391800	27.65075100	H	40.09160200	51.36108300	28.71421700
O	51.42353900	52.79436400	27.83258500	H	42.36857300	52.16586700	30.41804400
C	52.90837100	49.94092400	29.21655000	H	39.69270700	50.74359800	30.84024000
C	51.50668800	49.81212100	29.80210100	H	41.84503300	51.36673400	32.89898100
H	54.14345800	51.38332200	28.17361800	H	40.22663200	50.77760600	33.26981100
H	53.03878500	49.19396600	28.42984600	H	41.35545300	49.75690000	32.38050100
H	53.64983800	49.73295900	29.99142900	H	39.53822900	53.22197200	30.56226200
H	50.75942700	49.88266800	29.01467100	H	39.15519500	52.75208800	32.21301100
H	51.39006300	48.84978800	30.29581700	H	40.73455000	53.43974700	31.84771500
N	51.95348900	51.05540000	26.50963800	N	43.37613200	49.80501800	30.42881100
C	50.85940100	51.25123200	25.54582100	C	43.97249600	48.49234200	30.31996600
C	49.73545600	50.26730600	25.90733900	C	43.18400100	47.51062800	31.20861100
O	49.91718700	49.30556200	26.62272800	O	42.55968900	47.91178400	32.17528600

H	43.69732800	50.37258000	31.20412700	C	44.93288600	49.85860200	34.70287400
H	43.92481400	48.16802500	29.27845700	O	35.55290200	41.54421300	36.67004600
H	45.00846200	48.55197000	30.65627100	C	45.96095900	49.33913900	33.91717100
N	43.19710400	46.23002000	30.81811700	O	37.83946300	48.46587700	35.53449600
C	42.59685600	45.16872100	31.60602700	C	46.26503000	49.88950700	32.66256300
C	43.72202400	44.17847200	31.95295800	O	40.79481400	46.00690200	38.32769800
O	44.60488700	43.95872000	31.13787900	C	45.53655800	50.99744100	32.20792400
C	41.47952900	44.46476200	30.83221400	C	44.71532600	49.30248200	36.09489000
C	40.31596900	45.39362100	30.46135300	C	43.29763800	49.06638200	36.58964500
C	39.28622000	44.60840200	29.65107400	C	43.15178700	49.08209900	38.08774900
C	39.66220300	46.00874600	31.69794400	C	42.27609000	48.71988600	35.77930900
H	43.81813800	45.90616300	30.08901800	C	40.90785600	48.44528500	36.23458600
H	42.20620800	45.63761600	32.51050200	C	40.09475400	47.52455700	35.67447800
H	41.90850600	44.03858600	29.92266500	C	38.64181100	47.34871100	35.98068700
H	41.10395000	43.63791200	31.43955100	C	38.06204600	46.06140300	35.61744900
H	40.70420300	46.20745800	29.83993500	C	38.20420400	43.37047900	35.01395800
H	39.74277300	44.17197100	28.76603200	C	36.70414900	41.81556800	36.30689400
H	38.86484400	43.80363500	30.25023300	C	37.87799300	40.93084400	36.66117700
H	38.47478400	45.25817100	29.33217400	C	37.86977600	48.66445700	34.11680700
H	39.40117200	45.23755500	32.42104100	H	45.20682800	49.98508000	36.80281300
H	40.32579700	46.72666300	32.17234700	H	43.53678700	48.15124400	38.52087800
H	38.75196100	46.53353900	31.41621100	H	40.51981300	49.03358600	37.06614800
N	43.68582900	43.60399000	33.15909200	H	38.01705000	43.82994800	34.04208700
C	44.76604900	42.72304000	33.59809200	H	38.56330400	41.48611300	37.31048000
C	44.49003400	42.48442600	35.07749000	H	38.89370700	48.84610400	33.76999200
C	42.97662600	42.65606800	35.18343700	H	45.27909600	48.36259500	36.18481300
C	42.69111400	43.78928700	34.20013400	H	42.11345000	49.16456200	38.40953400
H	45.72804100	43.20039300	33.40451700	H	40.09572800	47.39087500	39.11110100
H	44.82165300	41.50218700	35.40424700	H	38.89662300	42.53823800	34.88534200
H	44.99290000	43.23801700	35.68084000	H	37.50851300	40.05474100	37.19555800
H	42.47195100	41.74507700	34.85885400	H	37.45525900	47.79123300	33.60745200
H	42.65612100	42.89700100	36.19406200	H	43.71684700	49.89827300	38.54722400
H	41.67769500	43.73908500	33.79876500	H	38.43844900	40.59824800	35.77969300
H	42.82706700	44.76139600	34.68840300	H	37.25080700	49.53756600	33.90739900
C	47.86103300	44.55329300	30.49698500	H	43.54602900	53.15333700	33.25729800
C	48.17468200	45.78680900	31.34766400	H	36.17904700	43.55628300	35.43374400
C	47.43736500	45.73721500	32.65511500	H	41.07434100	46.42456500	37.49188000
C	48.01289900	45.19066700	33.79557800	H	47.72585200	49.96517100	31.23936300
C	46.14074500	46.22688700	32.73861600	H	47.90823800	48.73793900	32.35109000
C	47.31507600	45.15364300	34.99082500	H	43.39640600	51.36537300	34.84539500
C	45.43766600	46.19234000	33.92873900	H	46.55315000	48.50901700	34.28781400
C	46.02823900	45.66165000	35.06351600	H	45.77700500	51.47461500	31.26085500
H	46.78619000	44.41662800	30.40890700	H	42.46582600	48.60484700	34.71320800
H	49.25109200	45.83902600	31.52670600	H	40.51226700	46.90950600	34.87538100
H	47.87491200	46.68314400	30.79945800	H	38.04388000	47.44202800	37.37612600
H	49.01859500	44.79789600	33.75010000	H	33.21671900	50.17883400	41.46741800
H	45.68578200	46.65655100	31.86061100	H	32.89576100	48.97842200	40.20447300
H	47.78032500	44.72900500	35.86892700	H	31.89053000	48.56369800	34.87071000
H	44.44094700	46.60677700	33.97331600	H	29.73557100	47.99953400	30.98249000
H	45.49047700	45.65047500	36.00143500	H	31.30985800	44.34993900	37.94240300
C	44.52458600	51.52813600	33.00892600	H	43.01951200	41.02609100	42.89282000
N	36.94951500	42.90607200	35.53079500	H	43.69792200	35.63598700	33.90109400
O	43.83959300	52.61890700	32.50009300	H	33.07632200	39.16025500	37.80284900
S	39.13503000	44.61245200	36.01751700	H	37.11499500	32.54735200	35.21384300
C	44.19912200	50.95757400	34.24018800	H	38.42991000	32.62634200	36.39308000
N	47.24316100	49.31133100	31.84606600	H	38.55623900	58.39286500	33.18376000
O	36.92765400	45.85826500	35.18629100	H	40.30097600	58.28945500	32.93089100

H 36.23896400 55.87522800 28.19137500
H 36.96050900 56.58988000 29.63288800
H 36.78788500 54.19245800 32.06011600
H 37.27405500 55.33585500 33.30521800
H 35.53494200 55.35430700 40.50052700
H 33.99994000 56.12006700 40.05435700
H 43.54208000 48.01082500 43.95130800
H 43.66060400 49.26177000 42.71079400
H 48.24064900 50.47136700 44.33039200
H 46.11430500 53.00092800 38.96182900
H 49.93459300 52.90134300 37.09951300
H 47.53433800 55.63880100 34.35516700
H 53.14934800 52.07600600 29.47220800
H 46.89230900 49.49458200 24.67614300
H 43.16478300 53.14877400 23.16817800
H 44.72593800 41.79324500 33.02107700
H 48.27386500 43.66051000 30.96134600
H 48.29269400 44.65781500 29.50483000
H 30.59210800 50.77356400 29.98628200
H 52.06324700 49.54328200 22.76052400
H 51.32587400 50.60197300 30.52795000
H 42.98347500 55.33626100 27.07206900

Coordinates of DH3-P(b3) system

C 42.99534500 55.33274100 27.09558400
C 51.34620400 50.54591300 30.52306900
C 52.02927700 49.51298800 22.76468900
C 30.43034800 50.93673000 30.17112100
N 48.29068700 44.64857900 29.50312300
C 48.28475000 43.67233500 30.97392800
N 44.70309500 41.78307000 33.03986200
H 43.16174100 53.14663100 23.17067700
H 46.90085700 49.46866900 24.68114700
H 53.13792600 52.06603400 29.48075900
H 47.55115600 55.64771100 34.35113000
H 49.93194000 52.90484300 37.09718700
H 46.14735500 52.95558600 38.87921800
C 48.28205700 50.50336000 44.30918900
C 43.89319100 49.08294500 42.69060900
O 43.56704100 47.76453600 43.82109400
C 33.99244600 56.16698400 39.96092000
C 35.34788700 55.19340100 40.56518500
C 37.28461500 55.32664400 33.30782900
H 36.77383800 54.20424900 32.05451800
H 36.95629800 56.56295200 29.63678500
H 36.24035100 55.88545300 28.17466400
H 40.32038000 58.26801100 32.94928000
H 38.58019600 58.42536300 33.20207000
H 38.41580000 32.61931500 36.42051500
H 37.15096500 32.56638200 35.18618500
H 33.15425300 39.19183100 37.84170600
N 43.69833300 35.64050300 33.89285200
C 43.05870400 41.01814700 42.87516800
C 31.67340300 42.94163400 36.81394700
H 29.85360200 48.00625800 30.87957300
H 31.85116900 48.56183100 34.84520000
H 34.20075800 50.49304900 40.05422500

H 32.64880300 50.13524600 40.82979300
C 38.94402000 47.54730500 36.81175700
C 40.40958300 47.79365800 34.10463400
O 42.72201000 48.76296700 34.49041100
C 45.75797100 51.62322300 31.08905300
C 46.71002800 48.60557500 34.01495400
C 43.56098600 51.42761400 34.77922300
H 47.96619300 48.89283900 32.01880800
H 47.70092200 50.12196000 30.92920400
H 38.58368100 47.24727700 38.83083500
H 36.77843700 43.38126200 35.21720800
H 43.59937000 53.22614600 33.25216100
H 36.84355400 49.31725400 33.86883800
H 39.09604300 40.60791300 36.00981000
H 44.16337000 49.48233200 38.43201500
N 37.81447800 47.92008600 33.35450600
C 37.80346100 39.75081000 36.87908100
C 39.61671800 42.59768800 35.60126700
O 40.00768100 48.72710200 39.33616700
C 42.44392100 49.14005200 38.28795200
C 45.60560100 48.48598100 36.02753400
C 38.61845400 49.47299200 33.74121000
H 38.61369300 41.13972600 37.63544400
H 38.99199800 43.66490700 34.32182100
H 41.02309700 48.29306200 37.05876200
H 43.60639800 47.81996000 38.22725000
H 45.37387700 50.09395900 36.64154900
H 37.79317400 48.80041800 33.99951900
H 38.24653800 40.72956200 36.68876000
H 37.17068200 41.64322800 36.15192300
H 38.86088300 43.34175700 35.35657100
N 38.49360300 46.07568800 35.34700400
C 38.89041900 47.51004300 35.72687700
C 40.24677400 47.86695200 35.17734300
O 41.23279100 48.28421400 35.99302800
C 42.55335500 48.69921600 35.56297900
C 43.43059000 48.85692600 37.91379100
C 43.56417400 48.98931400 36.41230100
H 44.95372100 49.36704100 35.93186400
H 45.56393800 51.12315600 32.03489000
H 39.58766600 47.22106800 38.75996700
H 46.32371500 50.01253500 32.43090100
H 37.84675400 48.42747300 35.37957500
H 46.09340900 49.43766400 33.69103300
H 35.97532400 41.34560200 36.23960600
N 45.10742600 49.93753200 34.53943800
C 37.75491500 45.77024600 34.43469700
C 47.26223700 49.45457400 31.55444900
O 44.33614500 51.03271900 34.13117300
H 39.27892000 44.81790500 36.39434300
H 43.87750400 52.73249100 32.46048000
H 37.54775200 42.79622000 35.52440200
N 44.59045100 51.63111200 32.89816000
C 45.51504400 45.72170000 36.00675100
C 44.45311400 46.66581100 33.98233700
C 47.79797800 44.78407800 35.86155100
C 45.68123000 46.69194600 31.85647600

H	49.01692600	44.82432200	33.73057700	N	42.38106900	52.16235500	30.39011400
H	47.84700600	46.68671600	30.76780900	C	40.09239900	51.33366200	28.71330800
H	49.23778500	45.87240000	31.50122300	C	39.97245400	52.83735900	31.45823800
H	46.78772400	44.40344500	30.41170800	C	41.07223600	50.86861700	32.54883500
H	46.04436600	45.72002300	35.06413900	C	40.51563300	51.42538200	31.24429900
H	45.44707600	46.24531000	33.93046000	C	41.62111500	49.29854600	29.08933500
H	47.32704500	45.20250100	34.98356900	H	42.18695400	50.05210700	29.86120900
H	46.14040900	46.26549600	32.73400400	H	41.58962800	51.44969500	30.14984100
H	48.01425800	45.22402000	33.78177600	H	40.95236700	51.83724900	28.88215800
C	47.43272700	45.76579900	32.64197100	H	39.76010800	51.04876900	25.15460500
C	48.16122300	45.80326000	31.32880900	H	39.13253300	51.09172700	26.79029700
O	47.86103300	44.55329400	30.49698700	H	40.61431300	50.19064100	26.44884900
C	42.82185400	44.78347400	34.68146700	H	40.23488200	53.23314900	26.48616500
C	41.68585200	43.72827400	33.81058300	H	42.16944200	51.68138900	24.95312900
C	42.70407800	42.94750200	36.22587000	H	40.04671500	51.08631200	26.20306300
H	42.49893200	41.76661500	34.91535600	H	42.77478400	52.72838400	27.91193000
H	45.02561300	43.28700700	35.66313300	H	41.62927300	52.28613600	27.82726000
H	44.85617500	41.54334200	35.43073100	C	40.86982700	52.33894700	26.46800100
H	45.72917200	43.18594500	33.37709200	C	41.85223900	52.52549900	25.40614100
H	42.69893700	43.80022800	34.21193300	C	43.89705200	54.61577500	23.83995100
H	43.00411900	42.68690500	35.21343600	C	44.40388400	53.01789300	24.42026400
H	44.51640400	42.51680400	35.08666200	N	42.25411500	54.71647100	25.74689500
H	44.76604900	42.72303900	33.59809300	C	42.50542000	53.66969700	25.15211300
N	43.68832600	43.60927000	33.16766900	N	43.56055100	53.60964100	24.06933400
C	38.84380500	46.66348500	30.99447000	H	46.90246100	49.95401400	28.36453500
C	40.33509700	46.77630600	31.91826900	H	46.07556500	51.51541200	28.36860800
O	39.27010100	45.37293900	32.11474800	H	47.75695600	51.40123800	27.83000600
C	38.67306700	45.21586000	28.99397000	H	44.58252500	49.78854600	25.41232700
H	38.93803100	43.81327100	30.02877600	H	44.22933900	50.53074900	26.98119900
H	39.95142800	44.06479500	28.60730800	H	45.04061500	48.96698600	26.90197700
H	40.87489000	46.14195100	29.63537200	C	46.19787000	51.60710500	25.89808000
H	41.06970200	43.67113800	31.41933400	C	47.63829800	48.93611200	26.21223200
H	41.99941100	43.95439900	29.94779500	C	48.45326100	51.38287700	24.78048000
N	42.17699100	45.63219500	32.50032800	C	46.79341700	50.89680100	27.83392100
C	43.85513000	45.90711200	30.12412400	C	44.95345600	49.93934400	26.42454200
C	39.67320300	46.08820000	31.39982500	C	46.30923200	50.64133400	26.40955700
O	39.43400700	44.56731600	29.42095600	C	47.33637100	49.80712300	25.62778600
C	40.41270200	45.37760700	30.26867500	C	48.54128200	50.55696900	25.35054100
H	41.51501300	44.44815000	30.79339100	H	51.04606200	48.90602300	24.09898100
H	44.60696800	43.96464600	31.14867400	H	52.71734400	49.39861800	24.37780400
H	43.72389700	44.18561300	31.96273000	H	52.15467500	51.75231400	23.91433800
H	42.59685500	45.16871800	31.60602600	H	50.51834000	51.29981500	23.43089800
H	43.21045600	46.23265600	30.83203000	H	50.50990200	52.27894000	25.69568700
N	45.00373300	48.55057700	30.66921500	H	52.38720500	50.15057100	26.47528900
C	43.94021200	48.15862200	29.28027900	H	51.81119800	49.62818900	23.82351100
C	43.74685100	50.41093800	31.13948400	H	51.34048600	51.05120400	24.10617400
O	42.49840000	47.92847900	32.13344500	C	49.90446800	49.33749900	26.66945800
C	43.16306400	47.51900200	31.19774600	C	49.73195800	50.27646900	25.92241100
C	43.97248400	48.49234100	30.31996300	C	50.85940100	51.25123300	25.54582200
C	43.38149700	49.80868700	30.41063700	C	51.95814900	51.06264600	26.50582400
H	40.76721000	53.49862700	31.79757300	C	51.44599900	48.79764600	30.27475900
H	39.19662700	52.82675300	32.21714300	N	50.79040100	49.82871300	29.00447500
H	39.54360800	53.24128200	30.54373700	H	53.68621300	49.72808300	29.97162400
H	41.41259300	49.84367300	32.43041200	H	53.08096200	49.19467400	28.40582300
H	40.30530900	50.89054800	33.31921900	H	54.14038100	51.40818500	28.17023200
H	41.90407400	51.47635000	32.88466100	H	51.54098200	49.76664000	29.78944400
H	39.70497100	50.77158600	30.90007400	H	52.93810800	49.92984800	29.20147300

H	51.38301700	52.76148800	27.86121300	H	48.57508100	52.97204200	44.58777100
H	52.07598300	51.78317400	27.66067200	N	46.73529500	51.28793000	44.70075500
H	53.17050000	51.34364900	28.66625800	C	48.13850100	52.56993100	43.67720400
H	46.61202000	52.62182400	35.12025800	C	45.66725100	50.74941200	42.47740200
H	47.22722300	52.91339500	33.01301700	O	46.86897600	50.65588900	42.67007700
H	46.11452300	54.30105100	32.92373000	C	47.52197500	51.20006200	43.95313900
C	48.64403600	54.85850900	33.17515300	C	39.92591300	46.92602200	39.63442400
C	48.13424200	53.87850600	35.91150300	C	41.86771000	50.46005400	41.72661800
C	46.07194400	53.29735500	34.67464800	C	40.31786700	50.32036200	42.50776500
C	46.81127100	53.76020300	33.56955600	H	41.99739000	49.71022500	44.16598700
C	47.94894300	54.69300700	33.99800200	H	41.12483100	48.24134300	43.73007200
H	48.69477100	54.08133100	35.09643800	H	43.01803500	47.62867000	42.14412100
H	47.68129100	51.30576400	36.84273800	H	40.35452100	49.42524900	39.97501700
H	49.61449500	50.41954400	36.61155200	H	40.59036800	47.58289500	41.24910600
H	49.58121500	50.81903500	34.87858400	H	40.69384200	48.80065700	41.10272200
H	51.25540100	52.21664600	36.10949200	H	41.18493100	49.73109200	42.18033700
H	47.96836600	51.45468400	35.92235600	H	41.82896100	48.99304600	43.35510400
H	49.35571300	51.19287700	35.88260800	H	43.15299800	48.32603500	42.97622900
H	50.55180800	53.46141300	33.96827700	H	38.08200400	50.00414700	36.41144100
H	49.85980700	53.39411600	34.96124600	H	38.85518700	53.31873600	37.42214300
H	50.19704700	52.46000400	36.13906300	N	35.87032200	50.23921900	37.18896000
C	40.30112600	51.34252400	37.60395400	C	37.18175800	54.88474000	38.30657400
C	39.68770500	52.13654300	39.92945500	C	34.18297800	51.82553100	38.03904300
C	42.77692200	51.71035600	37.14860600	C	33.97353800	54.89530900	37.82870800
C	44.16481900	54.06614600	39.29727100	C	33.66150800	53.85827300	39.19909300
C	44.20286600	52.99602800	40.69218700	N	35.57470300	56.27502800	39.18270800
C	45.02960000	51.95206700	37.95641200	C	38.46022400	50.84687700	36.75142500
C	45.29606300	50.99049700	40.67660800	N	37.47994800	51.67292700	37.23696500
C	40.95287000	51.75916600	38.25464700	H	37.83047700	52.98899700	37.56527600
O	40.67086200	52.17288500	39.50707600	H	36.15439400	51.26204700	37.42026700
H	41.73017900	52.61815600	40.12306900	H	36.87230600	53.87229400	38.06391400
H	42.29094100	51.96419000	38.06708100	H	35.20976600	52.16355900	37.91661300
H	42.76183800	52.49680500	39.23792000	H	35.53743000	53.48722300	38.24888600
H	44.11487000	53.01674100	39.60422200	H	34.45052100	54.44670500	38.71366400
H	45.28716800	52.28007100	38.96823000	H	34.87001200	55.58599400	39.66098400
H	45.70606000	51.12630400	39.75127000	C	37.00582300	51.36743400	32.11363800
H	44.37540500	46.62974000	40.11535000	C	35.55959400	52.31811600	31.74756700
H	45.70537900	45.62123600	40.67490700	O	35.40058200	50.68452900	32.36796300
C	45.19214800	45.53757700	38.99540700	C	34.10118400	53.18891700	33.62823400
C	47.55976100	45.89493300	38.42406300	O	34.55564000	52.87166100	35.30778400
C	48.15040900	46.25414700	40.04425600	H	33.94265500	51.56817300	34.29517000
C	48.37707100	47.41732500	38.72938400	H	36.35406700	51.35216400	34.53554200
O	45.99084200	47.86008000	38.61476300	H	36.81963800	53.68860000	35.07071700
O	45.42029700	48.65196500	40.90625900	H	37.93956200	53.00459300	33.89948900
H	46.77379400	47.73377700	41.55693600	N	35.59793000	54.84515700	33.20636400
H	48.31535000	49.10982600	40.06191700	C	35.99163200	51.59548900	32.43505900
H	48.68692900	50.08746500	41.99897600	C	34.55875700	52.46561100	34.29882200
H	45.33929300	46.20996300	39.83690200	O	35.97970900	52.13292900	33.86502300
H	47.69449600	46.68704400	39.15643000	H	36.90815800	53.33864000	34.03964600
H	46.34188500	47.31181000	39.49396800	H	36.61898600	54.49349500	33.09114500
C	46.42034600	48.28175900	40.67955200	H	43.20071900	54.29105600	28.33105700
C	47.52363500	50.77275400	38.47455800	H	44.17923300	55.68668600	28.28723000
O	46.85751400	50.51763200	39.47381700	H	42.37823600	55.98746500	29.93569400
C	47.36510400	49.46697400	40.46368300	C	42.21862200	57.10844100	28.56806400
H	47.70860400	50.10794300	41.75931200	C	40.83498300	55.32210300	27.40697000
H	47.37607900	53.26151300	43.32670500	O	40.77395000	54.45442200	28.94835500
H	48.91868900	52.50371000	42.92131900	C	39.55401900	56.34940500	29.96855900

C	39.69862400	57.26291100	28.46554900	H	34.51060300	37.10258100	31.52397700
H	38.49129400	55.41909200	27.26229300	H	33.82183600	39.71406200	31.08998200
H	38.25617900	54.59682000	28.80617400	H	33.12325400	38.78624500	32.43068100
H	37.19108700	57.36639300	28.08547400	H	35.52011100	40.66510500	32.57670400
H	43.24100600	55.32246700	28.12187800	H	34.06903800	40.68634100	33.59606500
H	42.18957700	56.05805600	28.86313600	H	36.30526500	39.36028100	34.46381300
N	40.84845400	55.44091900	28.49145400	N	35.02994400	38.02658200	31.77858500
C	39.62321500	56.25828700	28.88371200	C	34.04828900	39.17638700	32.00794100
C	38.36839000	55.57711300	28.33641800	C	34.75458300	40.04471500	33.04592300
O	37.11203500	56.39803500	28.57293100	O	33.54318200	37.63166400	34.61288400
C	43.75105800	53.87876200	35.26709100	H	34.38506000	38.43333100	34.99009000
C	41.41886100	52.98099700	35.21222100	H	35.40900400	39.00996500	33.94999200
H	44.12303600	56.27844300	34.98003900	H	35.74871900	37.90462700	33.03650200
H	39.52773200	54.51680500	34.96320200	N	34.63982100	35.12305200	32.64147000
H	42.21775100	57.81727100	34.73414700	C	35.73434800	34.28573600	33.74324100
H	38.66024000	56.72220100	35.00423500	C	35.70565600	33.84886700	32.02638300
H	39.73739100	58.07500300	35.36528100	O	36.68190400	35.99907900	31.38798200
H	39.25090200	56.91260900	32.58227900	C	38.44333100	35.31077700	33.57421800
N	42.90201800	54.53024900	35.11367300	C	35.62399400	34.67115400	32.73242000
C	41.60655200	54.03922200	35.09817800	C	37.19783100	36.92764500	34.44510500
C	43.11473200	55.89206400	34.96756200	C	36.57784700	36.90403700	33.38868900
C	40.53547400	54.90591600	34.95536500	H	36.72503300	35.69194100	32.43697400
C	42.04350900	56.75457900	34.82641200	H	38.04684900	35.10370200	32.66763700
H	40.73860200	56.27362100	34.82859100	H	39.26017200	31.72614600	31.88754400
H	39.58041400	57.22412300	34.69875500	H	39.23715900	32.29959900	33.55944900
H	39.42298800	57.74198800	33.26697700	H	40.76202000	31.78081500	32.81922300
H	33.31291400	35.90023300	35.30433300	H	40.64938900	33.69675400	31.21466900
H	32.07713800	33.75264700	36.04188300	H	40.55590200	34.35577400	34.08237200
H	35.74513800	35.75626700	35.87713900	H	39.81513900	32.28389100	32.63657800
H	36.81359600	33.62238200	38.03544900	H	38.19064800	34.08233900	30.67408400
H	36.19623600	32.07288800	37.44421700	H	38.68046400	34.33037800	31.75648700
H	37.74246900	34.12498100	35.77690400	H	40.05798200	33.70301700	32.13499500
C	33.71562000	35.09685400	35.77225200	N	40.81254300	34.47729900	33.11468900
C	33.12358700	33.94859200	36.16331100	C	42.96712000	37.83611600	35.92849900
O	33.97514400	33.11993200	36.70459800	C	43.19988000	39.19863400	34.83247600
H	35.03788100	34.98165900	36.09162200	C	44.34823800	37.86178100	34.83016200
H	35.18506600	33.74707700	36.66706200	C	40.40118500	37.32793100	33.20763700
N	36.43578400	33.09583900	37.15341300	H	40.86879900	38.86866000	33.92011000
C	37.50699000	33.10201800	36.06396900	H	40.58654500	37.47019500	34.95789100
C	35.29256300	37.56869200	41.05282300	H	42.81434900	37.71067600	32.87683500
O	35.39554100	35.93218800	40.39932000	H	42.26250600	35.52959800	34.93518900
C	34.15745900	36.32893900	41.58909400	H	43.29686100	38.11942600	34.93073700
H	33.56168100	35.07371200	38.82115100	H	40.98823800	37.78962000	33.99788800
H	32.19271600	36.11819200	38.43776800	H	42.46188300	37.40865100	33.86831800
H	32.38401700	35.48101200	40.06492600	C	42.30794300	35.33390300	31.66350600
H	33.07271000	37.86298700	39.96186600	C	41.92042100	35.20459900	32.80498300
H	35.28956000	38.35611900	38.78947800	C	42.64000300	35.88799600	33.97600600
N	35.08923300	36.82300700	37.93495500	C	41.10756400	43.57420300	44.76758600
C	32.93726000	37.65960400	36.96527500	C	41.42060000	41.84778800	44.59690500
C	35.15445700	39.57781300	36.47643800	C	40.48637900	42.70529800	43.36807400
O	34.70946400	36.70741500	40.73236100	C	43.40888900	44.64228300	42.00062700
C	32.92253400	35.86614600	39.20233900	C	42.30031200	45.24278600	43.23741900
C	33.75320900	37.08263400	39.60172500	H	41.67444100	44.38443200	41.83439200
C	34.55153100	37.64062100	38.41759600	H	43.43239000	43.18927700	44.02961000
H	33.67299700	38.34291500	37.38796900	H	43.95383200	42.17832400	41.85585900
H	34.48615900	38.84425400	36.26359500	H	41.05442800	41.62380200	41.56515500
H	35.73746100	38.26674800	30.97546600	H	41.32760000	42.78499700	44.05273500

H 42.49444100 44.42640700 42.54740500 H 28.91526400 49.40587300 31.45420500
H 42.61862500 43.10468000 43.30081900 H 30.98786600 50.11903600 32.59236000
H 43.00090400 41.96994100 42.34382800 H 30.36427800 49.87951200 29.92026400
C 41.99967500 41.82131400 41.25877800 H 29.90301500 49.06896700 31.12408300
N 41.20667100 41.98979500 38.00103700 H 30.84297100 49.18848400 32.23270700
O 40.33938500 41.07982700 39.28892500 H 34.77094000 49.00307000 35.27960500
S 40.07656800 43.91632000 38.64695100 H 35.30821500 47.33587100 35.45528600
C 43.22895000 42.42691600 39.44903800 H 33.82672200 47.87188000 36.24897000
N 42.17148100 42.10194800 39.95096000 H 35.37420400 46.92604500 33.02683700
O 40.87612200 41.99718300 39.03603900 H 34.86137700 48.56521500 32.62376800
C 40.01915900 43.13321200 39.27855400 H 33.94698100 47.18141400 32.01833500
O 35.25066500 45.18198200 41.13079700 H 33.20694800 46.58972000 34.24981600
C 35.95523200 44.02945600 42.29202100 H 32.83121400 49.56902300 33.77092000
O 37.08297100 46.70477500 41.38240900 H 34.43245600 47.97061700 35.35063800
C 36.99641000 46.06381900 43.03126200 H 34.50877200 47.56419000 32.86629800
O 39.34346100 45.84139400 41.75040400 H 33.62805700 47.58660300 34.11211800
C 38.69694300 44.38215800 42.52762700 H 31.40786700 47.01126400 32.40033100
C 38.52846500 45.09155900 39.56447300 H 31.53227800 48.15625300 32.78123900
C 36.18195600 44.74278000 41.49432800 H 32.45990100 48.55410100 33.93692700
C 37.16437300 45.80263500 41.98926100 H 36.43327400 45.42681800 37.89050600
C 38.51695300 45.13614000 41.75942800 H 36.43558600 49.22131100 39.68186100
C 39.06572900 42.25927000 41.12107100 H 34.02665800 45.95899000 38.53446800
C 39.15788100 43.16226000 40.30508000 H 32.86877900 48.75829500 38.77750100
C 38.32008600 44.43481200 40.41558700 H 32.83896800 47.72946000 40.19347600
C 36.90120200 44.08757900 40.41726200 H 34.14804800 49.45750500 41.49000300
C 32.96747800 40.94904900 39.56403500 H 36.88643400 47.33645600 38.74587900
C 33.07521800 41.57607500 41.20743900 H 36.10246800 46.34099000 38.36352400
C 33.51680000 39.90201900 40.87703200 H 34.80388000 46.61357000 38.64498200
C 36.81855100 41.55729900 41.41119400 H 36.04759600 48.28841700 39.29982500
H 35.77120600 40.23631500 41.90940700 H 34.74196200 47.85849800 39.25038400
H 35.32505600 41.88750500 42.30917600 H 33.44632600 48.48079100 39.67100600
H 35.45588900 40.66376200 39.51624500 H 33.62313600 49.71502400 40.56407700
H 34.40086900 43.44000900 40.19249000
H 34.81838100 41.99686100 37.64656100
H 33.54666500 40.91422600 40.48365600
H 35.78124800 41.26142900 41.54565900
H 34.99220400 41.34110400 40.24233700
H 37.17145400 42.86869400 38.56762200
H 36.44600500 43.24506000 39.48244000
H 35.00929000 42.74960100 39.60374000
H 34.40025900 42.65742200 38.29337500
H 32.30118700 42.80206800 33.83845200
H 32.08696900 44.52785400 33.52678800
H 30.97846900 43.68639300 34.60082600
H 35.00412700 44.47072300 35.86628300
H 34.52765200 44.76100600 34.18971300
H 34.70116700 43.10207900 34.77408700
H 32.63526200 45.05283000 35.87741800
H 33.11883400 42.06818200 36.26211700
H 32.01712600 43.75243300 34.28624100
H 34.38478200 44.10805700 35.04628600
H 32.91954900 44.07533800 35.47335100
H 33.06121700 44.45766400 38.49990700
H 33.41666600 43.46415600 37.87148600
H 32.73830500 43.03654500 36.58897800
H 29.65732100 49.76223900 29.10401900
H 31.34120300 49.53761100 29.58734300