

Supplementary Information for:

**Controlling the molecular arrangement of racemates through
weak interactions: the synergy between π -interactions and
halogen bonds**

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Cartesian coordinates of the studied species

A

1 C	37.1981000000000	26.5442000000000	38.1343000000000
2 C	34.8740000000000	26.7576000000000	36.7191000000000
3 F	37.6171000000000	24.4666000000000	37.1471000000000
4 F	38.3622000000000	26.4083000000000	38.7946000000000
5 I	37.0155000000000	29.1923000000000	39.6396000000000
6 C	36.4323000000000	27.6830000000000	38.3081000000000
7 F	34.4550000000000	28.8353000000000	37.7063000000000
8 F	33.7099000000000	26.8936000000000	36.0586000000000
9 I	35.0566000000000	24.1096000000000	35.2138000000000
10 C	35.6399000000000	25.6189000000000	36.5453000000000
11 C	36.8079000000000	25.5404000000000	37.2772000000000
12 C	35.2642000000000	27.7615000000000	37.5762000000000

1

1 P	33.5037000000000	20.9037000000000	33.6167000000000
2 O	34.4123000000000	22.0767000000000	33.4217000000000
3 C	32.7498000000000	20.3422000000000	32.0799000000000
4 N	33.6327000000000	19.7641000000000	31.2325000000000
5 C	33.1995000000000	19.4176000000000	30.0277000000000
6 H	33.8085000000000	19.0016000000000	29.4289000000000
7 C	31.8975000000000	19.6356000000000	29.6031000000000
8 H	31.6268000000000	19.3841000000000	28.7279000000000
9 C	31.0059000000000	20.2205000000000	30.4677000000000
10 H	30.1086000000000	20.3651000000000	30.1914000000000
11 C	31.4091000000000	20.6089000000000	31.7622000000000
12 C	32.0781000000000	21.2760000000000	34.6379000000000
13 C	32.3238000000000	21.5148000000000	35.9744000000000
14 H	33.1785000000000	21.3106000000000	36.3355000000000
15 C	31.3338000000000	22.0539000000000	36.8102000000000
16 H	31.5175000000000	22.2195000000000	37.7274000000000
17 C	30.1088000000000	22.3365000000000	36.2925000000000
18 H	29.4471000000000	22.7221000000000	36.8548000000000
19 C	29.7931000000000	22.0720000000000	34.9391000000000
20 C	28.5042000000000	22.3539000000000	34.4348000000000
21 H	27.8413000000000	22.7135000000000	35.0126000000000
22 C	28.2023000000000	22.1153000000000	33.1280000000000
23 H	27.3355000000000	22.3168000000000	32.7954000000000
24 C	29.1758000000000	21.5703000000000	32.2725000000000
25 H	28.9512000000000	21.4209000000000	31.3616000000000
26 C	30.4503000000000	21.2429000000000	32.7066000000000
27 C	30.7917000000000	21.5166000000000	34.0733000000000
28 C	34.3881000000000	19.5381000000000	34.3925000000000
29 C	33.8031000000000	18.2942000000000	34.5952000000000
30 H	32.9101000000000	18.1351000000000	34.3127000000000
31 C	34.5310000000000	17.2829000000000	35.2139000000000
32 H	34.1421000000000	16.4249000000000	35.3375000000000
33 C	35.8229000000000	17.5275000000000	35.6494000000000
34 H	36.3133000000000	16.8386000000000	36.0822000000000
35 C	36.3983000000000	18.7565000000000	35.4602000000000
36 H	37.2833000000000	18.9164000000000	35.7665000000000
37 C	35.6910000000000	19.7734000000000	34.8201000000000

38 H	36.095800000000	20.620800000000	34.676800000000
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2

1 P	5.387900000000	34.275600000000	48.245700000000
2 O	4.608100000000	35.351500000000	48.921200000000
3 C	4.479000000000	32.765500000000	47.957200000000
4 C	3.988800000000	32.123300000000	49.079900000000
5 H	4.205600000000	32.461400000000	49.940800000000
6 C	3.179500000000	30.984600000000	48.974300000000
7 H	2.844000000000	30.562500000000	49.756500000000
8 C	2.878300000000	30.489500000000	47.750300000000
9 H	2.333500000000	29.714100000000	47.684300000000
10 C	3.359700000000	31.104800000000	46.560300000000
11 C	3.037000000000	30.560900000000	45.297700000000
12 H	2.492600000000	29.784300000000	45.242100000000
13 C	3.500400000000	31.141700000000	44.166500000000
14 H	3.279300000000	30.771600000000	43.320000000000
15 C	4.307400000000	32.290300000000	44.238700000000
16 H	4.616700000000	32.682200000000	43.430400000000
17 C	4.668600000000	32.871600000000	45.438800000000
18 C	4.185900000000	32.270000000000	46.654500000000
19 C	5.937100000000	34.734200000000	46.603500000000
20 C	5.537600000000	34.068700000000	45.431100000000
21 C	6.030000000000	34.620100000000	44.229700000000
22 H	5.800400000000	34.219700000000	43.399300000000
23 C	6.841600000000	35.734900000000	44.249200000000
24 H	7.151100000000	36.074300000000	43.417700000000
25 N	7.220000000000	36.367600000000	45.362200000000
26 C	6.765400000000	35.857300000000	46.502900000000
27 H	7.022300000000	36.287500000000	47.309900000000
28 C	6.873100000000	33.863300000000	49.173400000000
29 C	7.454800000000	34.853800000000	49.964100000000
30 H	7.029600000000	35.699400000000	50.045700000000
31 C	8.640600000000	34.619900000000	50.629100000000
32 H	9.029600000000	35.301000000000	51.165000000000
33 C	9.258900000000	33.392000000000	50.512300000000
34 H	10.080500000000	33.231900000000	50.961600000000
35 C	8.687800000000	32.391400000000	49.743000000000
36 H	9.111700000000	31.543900000000	49.675600000000
37 C	7.501000000000	32.625600000000	49.073200000000
38 H	7.113100000000	31.939400000000	48.543000000000

1(PO)···A

1 P	33.503700000000	20.903700000000	33.616700000000
2 O	34.412300000000	22.076700000000	33.421700000000
3 C	32.749800000000	20.342200000000	32.079900000000
4 N	33.632700000000	19.764100000000	31.232500000000
5 C	33.199500000000	19.417600000000	30.027700000000
6 H	33.808500000000	19.001600000000	29.428900000000
7 C	31.897500000000	19.635600000000	29.603100000000
8 H	31.626800000000	19.384100000000	28.727900000000
9 C	31.005900000000	20.220500000000	30.467700000000

10	H	30.108600000000	20.365100000000	30.191400000000
11	C	31.409100000000	20.608900000000	31.762200000000
12	C	32.078100000000	21.276000000000	34.637900000000
13	C	32.323800000000	21.514800000000	35.974400000000
14	H	33.178500000000	21.310600000000	36.335500000000
15	C	31.333800000000	22.053900000000	36.810200000000
16	H	31.517500000000	22.219500000000	37.727400000000
17	C	30.108800000000	22.336500000000	36.292500000000
18	H	29.447100000000	22.722100000000	36.854800000000
19	C	29.793100000000	22.072000000000	34.939100000000
20	C	28.504200000000	22.353900000000	34.434800000000
21	H	27.841300000000	22.713500000000	35.012600000000
22	C	28.202300000000	22.115300000000	33.128000000000
23	H	27.335500000000	22.316800000000	32.795400000000
24	C	29.175800000000	21.570300000000	32.272500000000
25	H	28.951200000000	21.420900000000	31.361600000000
26	C	30.450300000000	21.242900000000	32.706600000000
27	C	30.791700000000	21.516600000000	34.073300000000
28	C	34.388100000000	19.538100000000	34.392500000000
29	C	33.803100000000	18.294200000000	34.595200000000
30	H	32.910100000000	18.135100000000	34.312700000000
31	C	34.531000000000	17.282900000000	35.213900000000
32	H	34.142100000000	16.424900000000	35.337500000000
33	C	35.822900000000	17.527500000000	35.649400000000
34	H	36.313300000000	16.838600000000	36.082200000000
35	C	36.398300000000	18.756500000000	35.460200000000
36	H	37.283300000000	18.916400000000	35.766500000000
37	C	35.691000000000	19.773400000000	34.820100000000
38	H	36.095800000000	20.620800000000	34.676800000000
39	F	37.617100000000	24.466600000000	37.147100000000
40	F	38.362200000000	26.408300000000	38.794600000000
41	I	37.015500000000	29.192300000000	39.639600000000
42	C	36.432300000000	27.683000000000	38.308100000000
43	F	34.455000000000	28.835300000000	37.706300000000
44	F	33.709900000000	26.893600000000	36.058600000000
45	I	35.056600000000	24.109600000000	35.213800000000
46	C	35.639900000000	25.618900000000	36.545300000000
47	C	36.807900000000	25.540400000000	37.277200000000
48	C	35.264200000000	27.761500000000	37.576200000000
49	C	37.198100000000	26.544200000000	38.134300000000
50	C	34.874000000000	26.757600000000	36.719100000000

1(N)···A

1	P	42.110100000000	29.787300000000	46.092200000000
2	O	43.018600000000	30.960300000000	45.897200000000
3	C	41.356100000000	29.225900000000	44.555500000000
4	N	42.239100000000	28.647700000000	43.708000000000
5	C	41.805800000000	28.301200000000	42.503300000000
6	H	42.414900000000	27.885200000000	41.904400000000
7	C	40.503800000000	28.519200000000	42.078700000000
8	H	40.233200000000	28.267700000000	41.203400000000
9	C	39.612200000000	29.104100000000	42.943300000000
10	H	38.714900000000	29.248700000000	42.666900000000
11	C	40.015500000000	29.492600000000	44.237700000000

12 C	40.6844000000000	30.1597000000000	47.1135000000000
13 C	40.9301000000000	30.3984000000000	48.4500000000000
14 H	41.7849000000000	30.1942000000000	48.8110000000000
15 C	39.9402000000000	30.9375000000000	49.2857000000000
16 H	40.1238000000000	31.1031000000000	50.2029000000000
17 C	38.7151000000000	31.2202000000000	48.7681000000000
18 H	38.0535000000000	31.6057000000000	49.3304000000000
19 C	38.3995000000000	30.9556000000000	47.4146000000000
20 C	37.1105000000000	31.2375000000000	46.9104000000000
21 H	36.4477000000000	31.5971000000000	47.4881000000000
22 C	36.8086000000000	30.9990000000000	45.6036000000000
23 H	35.9418000000000	31.2004000000000	45.2710000000000
24 C	37.7822000000000	30.4539000000000	44.7481000000000
25 H	37.5576000000000	30.3045000000000	43.8371000000000
26 C	39.0566000000000	30.1265000000000	45.1821000000000
27 C	39.3980000000000	30.4002000000000	46.5488000000000
28 C	42.9945000000000	28.4217000000000	46.8681000000000
29 C	42.4095000000000	27.1779000000000	47.0708000000000
30 H	41.5165000000000	27.0187000000000	46.7882000000000
31 C	43.1373000000000	26.1665000000000	47.6895000000000
32 H	42.7485000000000	25.3085000000000	47.8131000000000
33 C	44.4293000000000	26.4112000000000	48.1250000000000
34 H	44.9197000000000	25.7222000000000	48.5578000000000
35 C	45.0047000000000	27.6401000000000	47.9357000000000
36 H	45.8896000000000	27.8001000000000	48.2420000000000
37 C	44.2974000000000	28.6570000000000	47.2956000000000
38 H	44.7021000000000	29.5045000000000	47.1524000000000
39 I	45.0516000000000	27.7681000000000	43.6968000000000
40 C	47.4544000000000	26.2573000000000	42.5354000000000
41 C	48.6891000000000	25.6405000000000	42.5381000000000
42 F	46.7289000000000	26.1987000000000	41.4035000000000
43 F	49.1093000000000	25.0465000000000	41.4158000000000
44 I	51.3859000000000	24.7608000000000	43.6322000000000
45 C	49.4833000000000	25.6282000000000	43.6762000000000
46 C	48.9833000000000	26.2718000000000	44.7935000000000
47 C	47.7486000000000	26.8884000000000	44.7909000000000
48 F	49.7087000000000	26.3303000000000	45.9254000000000
49 F	47.3283000000000	27.4825000000000	45.9132000000000
50 C	46.9543000000000	26.9008000000000	43.6528000000000

2(PO)---A

1 P	5.3879000000000	34.2756000000000	48.2457000000000
2 O	4.6081000000000	35.3515000000000	48.9212000000000
3 C	4.4790000000000	32.7655000000000	47.9572000000000
4 C	3.9888000000000	32.1233000000000	49.0799000000000
5 H	4.2056000000000	32.4614000000000	49.9408000000000
6 C	3.1795000000000	30.9846000000000	48.9743000000000
7 H	2.8440000000000	30.5625000000000	49.7565000000000
8 C	2.8783000000000	30.4895000000000	47.7503000000000
9 H	2.3335000000000	29.7141000000000	47.6843000000000
10 C	3.3597000000000	31.1048000000000	46.5603000000000
11 C	3.0370000000000	30.5609000000000	45.2977000000000
12 H	2.4926000000000	29.7843000000000	45.2421000000000
13 C	3.5004000000000	31.1417000000000	44.1665000000000

14 H	3.2793000000000	30.7716000000000	43.3200000000000
15 C	4.3074000000000	32.2903000000000	44.2387000000000
16 H	4.6167000000000	32.6822000000000	43.4304000000000
17 C	4.6686000000000	32.8716000000000	45.4388000000000
18 C	4.1859000000000	32.2700000000000	46.6545000000000
19 C	5.9371000000000	34.7342000000000	46.6035000000000
20 C	5.5376000000000	34.0687000000000	45.4311000000000
21 C	6.0300000000000	34.6201000000000	44.2297000000000
22 H	5.8004000000000	34.2197000000000	43.3993000000000
23 C	6.8416000000000	35.7349000000000	44.2492000000000
24 H	7.1511000000000	36.0743000000000	43.4177000000000
25 N	7.2200000000000	36.3676000000000	45.3622000000000
26 C	6.7654000000000	35.8573000000000	46.5029000000000
27 H	7.0223000000000	36.2875000000000	47.3099000000000
28 C	6.8731000000000	33.8633000000000	49.1734000000000
29 C	7.4548000000000	34.8538000000000	49.9641000000000
30 H	7.0296000000000	35.6994000000000	50.0457000000000
31 C	8.6406000000000	34.6199000000000	50.6291000000000
32 H	9.0296000000000	35.3010000000000	51.1650000000000
33 C	9.2589000000000	33.3920000000000	50.5123000000000
34 H	10.0805000000000	33.2319000000000	50.9616000000000
35 C	8.6878000000000	32.3914000000000	49.7430000000000
36 H	9.1117000000000	31.5439000000000	49.6756000000000
37 C	7.5010000000000	32.6256000000000	49.0732000000000
38 H	7.1131000000000	31.9394000000000	48.5430000000000
39 C	1.2167000000000	38.6898000000000	52.2893000000000
40 F	0.9628000000000	37.4577000000000	52.7636000000000
41 I	3.1899000000000	37.2650000000000	50.4232000000000
42 C	2.1520000000000	38.8671000000000	51.2808000000000
43 C	2.3548000000000	40.1626000000000	50.8336000000000
44 C	1.6669000000000	41.2275000000000	51.3628000000000
45 F	-0.3682000000000	39.5187000000000	53.7939000000000
46 F	3.2518000000000	40.3986000000000	49.8583000000000
47 F	1.9209000000000	42.4596000000000	50.8886000000000
48 I	-0.3062000000000	42.6523000000000	53.2289000000000
49 C	0.7317000000000	41.0502000000000	52.3714000000000
50 C	0.5289000000000	39.7547000000000	52.8186000000000

2(N)···A

1 C	0.6310000000000	35.0738000000000	40.7315000000000
2 H	1.0561000000000	34.2282000000000	40.6499000000000
3 C	-0.5548000000000	35.3078000000000	40.0665000000000
4 H	-0.9438000000000	34.6266000000000	39.5306000000000
5 C	-1.1732000000000	36.5356000000000	40.1833000000000
6 H	-1.9947000000000	36.6957000000000	39.7340000000000
7 C	-0.6020000000000	37.5362000000000	40.9526000000000
8 H	-1.0259000000000	38.3837000000000	41.0200000000000
9 C	0.5848000000000	37.3020000000000	41.6224000000000
10 H	0.9727000000000	37.9882000000000	42.1526000000000
11 I	-0.8320000000000	31.2715000000000	45.3368000000000
12 C	-2.1953000000000	29.6693000000000	45.3386000000000
13 C	-2.6493000000000	29.1163000000000	46.5223000000000
14 C	-3.5491000000000	28.0707000000000	46.5227000000000
15 F	-2.2143000000000	29.5954000000000	47.6947000000000

16 F	-3.9409000000000	27.5694000000000	47.7033000000000
17 I	-5.4035000000000	25.9231000000000	45.3588000000000
18 C	-4.0403000000000	27.5253000000000	45.3571000000000
19 C	-3.5863000000000	28.0783000000000	44.1733000000000
20 C	-2.6865000000000	29.1239000000000	44.1729000000000
21 F	-4.0213000000000	27.5992000000000	43.0010000000000
22 F	-2.2946000000000	29.6252000000000	42.9923000000000
23 P	2.6979000000000	35.6520000000000	42.4499000000000
24 O	3.4776000000000	34.5761000000000	41.7744000000000
25 C	3.6068000000000	37.1622000000000	42.7384000000000
26 C	4.0970000000000	37.8044000000000	41.6157000000000
27 H	3.8802000000000	37.4662000000000	40.7548000000000
28 C	4.9063000000000	38.9430000000000	41.7213000000000
29 H	5.2418000000000	39.3651000000000	40.9391000000000
30 C	5.2075000000000	39.4381000000000	42.9453000000000
31 N	0.8658000000000	33.5600000000000	45.3334000000000
32 C	1.3204000000000	34.0704000000000	44.1928000000000
33 H	1.0635000000000	33.6401000000000	43.3857000000000
34 C	1.2127000000000	36.0643000000000	41.5222000000000
35 H	5.7523000000000	40.2135000000000	43.0113000000000
36 C	4.7261000000000	38.8228000000000	44.1353000000000
37 C	5.0488000000000	39.3668000000000	45.3979000000000
38 H	5.5932000000000	40.1433000000000	45.4536000000000
39 C	2.1487000000000	35.1934000000000	44.0921000000000
40 C	2.0558000000000	35.3075000000000	46.4659000000000
41 H	2.2854000000000	35.7079000000000	47.2963000000000
42 C	1.2442000000000	34.1927000000000	46.4464000000000
43 C	2.5482000000000	35.8590000000000	45.2646000000000
44 H	0.9347000000000	33.8533000000000	47.2779000000000
45 C	4.5854000000000	38.7859000000000	46.5291000000000
46 H	4.8065000000000	39.1561000000000	47.3756000000000
47 C	3.7783000000000	37.6374000000000	46.4569000000000
48 H	3.4691000000000	37.2454000000000	47.2652000000000
49 C	3.4172000000000	37.0560000000000	45.2568000000000
50 C	3.8998000000000	37.6576000000000	44.0411000000000

1(PO)-A...(OP)1

1 P	33.5037000000000	20.9037000000000	33.6167000000000
2 O	34.4123000000000	22.0767000000000	33.4217000000000
3 C	32.7498000000000	20.3422000000000	32.0799000000000
4 N	33.6327000000000	19.7641000000000	31.2325000000000
5 C	33.1995000000000	19.4176000000000	30.0277000000000
6 H	33.8085000000000	19.0016000000000	29.4289000000000
7 C	31.8975000000000	19.6356000000000	29.6031000000000
8 H	31.6268000000000	19.3841000000000	28.7279000000000
9 C	31.0059000000000	20.2205000000000	30.4677000000000
10 H	30.1086000000000	20.3651000000000	30.1914000000000
11 C	31.4091000000000	20.6089000000000	31.7622000000000
12 C	32.0781000000000	21.2760000000000	34.6379000000000
13 C	32.3238000000000	21.5148000000000	35.9744000000000
14 H	33.1785000000000	21.3106000000000	36.3355000000000
15 C	31.3338000000000	22.0539000000000	36.8102000000000
16 H	31.5175000000000	22.2195000000000	37.7274000000000
17 C	30.1088000000000	22.3365000000000	36.2925000000000

18 H	29.4471000000000	22.7221000000000	36.8548000000000
19 C	29.7931000000000	22.0720000000000	34.9391000000000
20 C	28.5042000000000	22.3539000000000	34.4348000000000
21 H	27.8413000000000	22.7135000000000	35.0126000000000
22 C	28.2023000000000	22.1153000000000	33.1280000000000
23 H	27.3355000000000	22.3168000000000	32.7954000000000
24 C	29.1758000000000	21.5703000000000	32.2725000000000
25 H	28.9512000000000	21.4209000000000	31.3616000000000
26 C	30.4503000000000	21.2429000000000	32.7066000000000
27 C	30.7917000000000	21.5166000000000	34.0733000000000
28 C	34.3881000000000	19.5381000000000	34.3925000000000
29 C	33.8031000000000	18.2942000000000	34.5952000000000
30 H	32.9101000000000	18.1351000000000	34.3127000000000
31 C	34.5310000000000	17.2829000000000	35.2139000000000
32 H	34.1421000000000	16.4249000000000	35.3375000000000
33 C	35.8229000000000	17.5275000000000	35.6494000000000
34 H	36.3133000000000	16.8386000000000	36.0822000000000
35 C	36.3983000000000	18.7565000000000	35.4602000000000
36 H	37.2833000000000	18.9164000000000	35.7665000000000
37 C	35.6910000000000	19.7734000000000	34.8201000000000
38 H	36.0958000000000	20.6208000000000	34.6768000000000
39 I	37.0155000000000	29.1923000000000	39.6396000000000
40 C	36.4323000000000	27.6830000000000	38.3081000000000
41 C	35.2642000000000	27.7615000000000	37.5762000000000
42 C	34.8740000000000	26.7576000000000	36.7191000000000
43 F	34.4550000000000	28.8353000000000	37.7063000000000
44 F	38.3622000000000	26.4083000000000	38.7946000000000
45 C	41.2804000000000	31.7853000000000	40.7801000000000
46 C	37.6840000000000	33.7638000000000	40.4609000000000
47 F	33.7099000000000	26.8936000000000	36.0586000000000
48 C	38.2690000000000	35.0076000000000	40.2582000000000
49 H	39.1620000000000	35.1667000000000	40.5407000000000
50 C	37.5412000000000	36.0190000000000	39.6395000000000
51 H	37.9300000000000	36.8770000000000	39.5159000000000
52 H	42.6250000000000	30.5798000000000	37.9986000000000
53 C	42.2790000000000	31.2299000000000	39.9143000000000
54 C	43.5679000000000	30.9479000000000	40.4186000000000
55 C	36.2492000000000	35.7743000000000	39.2040000000000
56 P	38.5684000000000	32.3982000000000	41.2367000000000
57 O	37.6599000000000	31.2252000000000	41.4317000000000
58 C	39.3223000000000	32.9596000000000	42.7735000000000
59 N	38.4394000000000	33.5378000000000	43.6209000000000
60 C	38.8726000000000	33.8843000000000	44.8257000000000
61 H	38.2636000000000	34.3002000000000	45.4245000000000
62 C	40.1746000000000	33.6663000000000	45.2503000000000
63 H	40.4453000000000	33.9178000000000	46.1255000000000
64 C	41.0663000000000	33.0813000000000	44.3857000000000
65 H	41.9636000000000	32.9368000000000	44.6620000000000
66 C	40.6630000000000	32.6929000000000	43.0912000000000
67 H	44.2308000000000	30.5884000000000	39.8408000000000
68 C	43.8698000000000	31.1865000000000	41.7254000000000
69 H	44.7366000000000	30.9850000000000	42.0580000000000
70 C	42.8963000000000	31.7315000000000	42.5809000000000
71 H	43.1209000000000	31.8810000000000	43.4918000000000
72 C	41.6218000000000	32.0589000000000	42.1468000000000
73 C	36.8079000000000	25.5404000000000	37.2772000000000
74 C	37.1981000000000	26.5442000000000	38.1343000000000

75 C	39.9941000000000	32.0258000000000	40.2155000000000
76 F	37.6171000000000	24.4666000000000	37.1471000000000
77 H	38.8936000000000	31.9913000000000	38.5179000000000
78 C	39.7483000000000	31.7871000000000	38.8790000000000
79 C	40.7383000000000	31.2480000000000	38.0432000000000
80 H	40.5546000000000	31.0824000000000	37.1260000000000
81 H	35.7588000000000	36.4633000000000	38.7712000000000
82 C	35.6738000000000	34.5454000000000	39.3932000000000
83 H	34.7888000000000	34.3854000000000	39.0869000000000
84 C	36.3811000000000	33.5285000000000	40.0333000000000
85 H	35.9763000000000	32.6810000000000	40.1766000000000
86 I	35.0566000000000	24.1096000000000	35.2138000000000
87 C	35.6399000000000	25.6189000000000	36.5453000000000
88 C	41.9633000000000	30.9653000000000	38.5609000000000

1(PO)-A...(N)1, 1(N)-A...(OP)1

1 C	37.645306940000	16.362587720000	31.758491980000
2 H	37.925732840000	15.524179330000	31.410639010000
3 P	36.665343850000	20.571659000000	33.194352130000
4 O	37.663349470000	21.481428210000	32.549564680000
5 C	34.973728020000	20.913951910000	32.677975400000
6 N	34.4985000000000	22.0892000000000	33.1521000000000
7 C	33.302680710000	22.486425240000	32.738096980000
8 H	32.955414600000	23.304819520000	33.072997600000
9 C	32.536877940000	21.760643260000	31.838207050000
10 H	31.689180780000	22.083280260000	31.555746610000
11 C	33.0231430000000	20.568356810000	31.362225640000
12 C	36.456878940000	16.950105970000	31.264758190000
13 C	35.683099350000	16.289170500000	30.285162110000
14 H	35.957809990000	15.438256910000	29.964263270000
15 C	34.546964690000	16.859906830000	29.796167800000
16 H	34.037960700000	16.412096310000	29.130598090000
17 C	34.129140800000	18.112827150000	30.278205710000
18 H	33.340512590000	18.500854680000	29.917868790000
19 C	34.823402750000	18.803446700000	31.258508610000
20 H	32.502591580000	20.057548370000	30.753518140000
21 C	34.288011640000	20.094554030000	31.768213100000
22 C	36.874378120000	18.852193670000	32.732104650000
23 C	38.003370010000	18.219216000000	33.210120930000
24 H	38.523722330000	18.639632330000	33.884864700000
25 C	38.397051580000	16.965619470000	32.717517460000
26 H	39.179996980000	16.542996500000	33.050548690000
27 C	36.038073920000	18.228121550000	31.761218150000
28 C	36.783081200000	20.671505680000	34.990222030000
29 C	35.901672030000	20.002260640000	35.830463010000
30 H	35.199576400000	19.476947890000	35.464833480000
31 C	36.052282960000	20.104919760000	37.209605910000
32 H	35.440654550000	19.664837840000	37.788524810000
33 C	37.094059710000	20.849082370000	37.738375000000
34 H	37.201366200000	20.907532150000	38.680446570000
35 C	37.970805540000	21.501174380000	36.911791890000
36 H	38.685049180000	22.005293610000	37.283464630000
37 C	37.819404220000	21.428375190000	35.527663000000
38 H	38.419319040000	21.892300770000	34.955572870000

39	P	38.5684000000000	32.3982000000000	41.2367000000000
40	O	37.6599000000000	31.2252000000000	41.4317000000000
41	C	39.3223000000000	32.9596000000000	42.7735000000000
42	N	38.4394000000000	33.5378000000000	43.6209000000000
43	C	38.8726000000000	33.8843000000000	44.8257000000000
44	H	38.2636000000000	34.3002000000000	45.4245000000000
45	C	40.1746000000000	33.6663000000000	45.2503000000000
46	H	40.4453000000000	33.9178000000000	46.1255000000000
47	C	41.0663000000000	33.0813000000000	44.3857000000000
48	H	41.9636000000000	32.9368000000000	44.6620000000000
49	C	40.6630000000000	32.6929000000000	43.0912000000000
50	C	39.9941000000000	32.0258000000000	40.2155000000000
51	C	39.7483000000000	31.7871000000000	38.8790000000000
52	H	38.8936000000000	31.9913000000000	38.5179000000000
53	C	40.7383000000000	31.2480000000000	38.0432000000000
54	H	40.5546000000000	31.0824000000000	37.1260000000000
55	C	41.9633000000000	30.9653000000000	38.5609000000000
56	H	42.6250000000000	30.5798000000000	37.9986000000000
57	C	42.2790000000000	31.2299000000000	39.9143000000000
58	C	43.5679000000000	30.9479000000000	40.4186000000000
59	H	44.2308000000000	30.5884000000000	39.8408000000000
60	C	43.8698000000000	31.1865000000000	41.7254000000000
61	H	44.7366000000000	30.9850000000000	42.0580000000000
62	C	42.8963000000000	31.7315000000000	42.5809000000000
63	H	43.1209000000000	31.8810000000000	43.4918000000000
64	C	41.6218000000000	32.0589000000000	42.1468000000000
65	C	41.2804000000000	31.7853000000000	40.7801000000000
66	C	37.6840000000000	33.7638000000000	40.4609000000000
67	C	38.2690000000000	35.0076000000000	40.2582000000000
68	H	39.1620000000000	35.1667000000000	40.5407000000000
69	C	37.5412000000000	36.0190000000000	39.6395000000000
70	H	37.9300000000000	36.8770000000000	39.5159000000000
71	C	36.2492000000000	35.7743000000000	39.2040000000000
72	H	35.7588000000000	36.4633000000000	38.7712000000000
73	C	35.6738000000000	34.5454000000000	39.3932000000000
74	H	34.7888000000000	34.3854000000000	39.0869000000000
75	C	36.3811000000000	33.5285000000000	40.0333000000000
76	H	35.9763000000000	32.6810000000000	40.1766000000000
77	I	35.0566000000000	24.1096000000000	35.2138000000000
78	C	35.6399000000000	25.6189000000000	36.5453000000000
79	C	36.8079000000000	25.5404000000000	37.2772000000000
80	C	37.1981000000000	26.5442000000000	38.1343000000000
81	F	37.6171000000000	24.4666000000000	37.1471000000000
82	F	38.3622000000000	26.4083000000000	38.7946000000000
83	I	37.0155000000000	29.1923000000000	39.6396000000000
84	C	36.4323000000000	27.6830000000000	38.3081000000000
85	C	35.2642000000000	27.7615000000000	37.5762000000000
86	C	34.8740000000000	26.7576000000000	36.7191000000000
87	F	34.4550000000000	28.8353000000000	37.7063000000000
88	F	33.7099000000000	26.8936000000000	36.0586000000000

1(N)-A...(N)1

1	P	42.1101000000000	29.7873000000000	46.0922000000000
2	O	43.0186000000000	30.9603000000000	45.8972000000000

3 C	41.356100000000	29.225900000000	44.555500000000
4 N	42.239100000000	28.647700000000	43.708000000000
5 C	41.805800000000	28.301200000000	42.503300000000
6 H	42.414900000000	27.885200000000	41.904400000000
7 C	40.503800000000	28.519200000000	42.078700000000
8 H	40.233200000000	28.267700000000	41.203400000000
9 C	39.612200000000	29.104100000000	42.943300000000
10 H	38.714900000000	29.248700000000	42.666900000000
11 C	40.015500000000	29.492600000000	44.237700000000
12 C	40.684400000000	30.159700000000	47.113500000000
13 C	40.930100000000	30.398400000000	48.450000000000
14 H	41.784900000000	30.194200000000	48.811000000000
15 C	39.940200000000	30.937500000000	49.285700000000
16 H	40.123800000000	31.103100000000	50.202900000000
17 C	38.715100000000	31.220200000000	48.768100000000
18 H	38.053500000000	31.605700000000	49.330400000000
19 C	38.399500000000	30.955600000000	47.414600000000
20 C	37.110500000000	31.237500000000	46.910400000000
21 H	36.447700000000	31.597100000000	47.488100000000
22 C	36.808600000000	30.999000000000	45.603600000000
23 H	35.941800000000	31.200400000000	45.271000000000
24 C	37.782200000000	30.453900000000	44.748100000000
25 H	37.557600000000	30.304500000000	43.837100000000
26 C	39.056600000000	30.126500000000	45.182100000000
27 C	39.398000000000	30.400200000000	46.548800000000
28 C	42.994500000000	28.421700000000	46.868100000000
29 C	42.409500000000	27.177900000000	47.070800000000
30 H	41.516500000000	27.018700000000	46.788200000000
31 C	43.137300000000	26.166500000000	47.689500000000
32 H	42.748500000000	25.308500000000	47.813100000000
33 C	44.429300000000	26.411200000000	48.125000000000
34 H	44.919700000000	25.722200000000	48.557800000000
35 C	45.004700000000	27.640100000000	47.935700000000
36 H	45.889600000000	27.800100000000	48.242000000000
37 C	44.297400000000	28.657000000000	47.295600000000
38 H	44.702100000000	29.504500000000	47.152400000000
39 C	52.008300000000	26.117800000000	39.204000000000
40 H	51.518000000000	26.806700000000	38.771200000000
41 C	48.689100000000	25.640500000000	42.538100000000
42 C	51.432900000000	24.888800000000	39.393200000000
43 H	50.548000000000	24.728900000000	39.086900000000
44 H	53.689200000000	27.220400000000	39.515900000000
45 C	55.507500000000	22.130500000000	38.879000000000
46 C	52.140200000000	23.871900000000	40.033300000000
47 H	54.652700000000	22.334700000000	38.517900000000
48 C	56.497500000000	21.591400000000	38.043200000000
49 F	46.728900000000	26.198700000000	41.403500000000
50 F	49.109300000000	25.046500000000	41.415800000000
51 I	51.385900000000	24.760800000000	43.632200000000
52 C	49.483300000000	25.628200000000	43.676200000000
53 C	48.983300000000	26.271800000000	44.793500000000
54 C	47.748600000000	26.888400000000	44.790900000000
55 F	49.708700000000	26.330300000000	45.925400000000
56 F	47.328300000000	27.482500000000	45.913200000000
57 P	54.327500000000	22.741600000000	41.236700000000
58 O	53.419000000000	21.568600000000	41.431700000000

59 C	55.0815000000000	23.3031000000000	42.7735000000000
60 H	56.3138000000000	21.4259000000000	37.1260000000000
61 C	57.7225000000000	21.3088000000000	38.5609000000000
62 H	58.3841000000000	20.9233000000000	37.9986000000000
63 C	58.0382000000000	21.5733000000000	39.9143000000000
64 H	51.7355000000000	23.0245000000000	40.1766000000000
65 N	54.1986000000000	23.8812000000000	43.6209000000000
66 C	54.6318000000000	24.2277000000000	44.8257000000000
67 H	54.0228000000000	24.6437000000000	45.4245000000000
68 C	55.9338000000000	24.0097000000000	45.2503000000000
69 H	56.2045000000000	24.2612000000000	46.1255000000000
70 C	46.9543000000000	26.9008000000000	43.6528000000000
71 C	56.8254000000000	23.4248000000000	44.3857000000000
72 C	47.4544000000000	26.2573000000000	42.5354000000000
73 H	57.7227000000000	23.2802000000000	44.6620000000000
74 C	56.4221000000000	23.0364000000000	43.0912000000000
75 C	55.7532000000000	22.3693000000000	40.2155000000000
76 I	45.0516000000000	27.7681000000000	43.6968000000000
77 C	59.3271000000000	21.2914000000000	40.4186000000000
78 H	59.9899000000000	20.9319000000000	39.8408000000000
79 C	59.6290000000000	21.5300000000000	41.7254000000000
80 H	60.4958000000000	21.3285000000000	42.0580000000000
81 C	58.6554000000000	22.0750000000000	42.5809000000000
82 H	58.8800000000000	22.2244000000000	43.4918000000000
83 C	57.3810000000000	22.4024000000000	42.1468000000000
84 C	57.0396000000000	22.1287000000000	40.7801000000000
85 C	53.4431000000000	24.1072000000000	40.4609000000000
86 C	54.0282000000000	25.3511000000000	40.2582000000000
87 H	54.9212000000000	25.5102000000000	40.5407000000000
88 C	53.3003000000000	26.3624000000000	39.6395000000000

2(PO)-A...(OP)2

1 P	5.3879000000000	34.2756000000000	48.2457000000000
2 O	4.6081000000000	35.3515000000000	48.9212000000000
3 C	4.4790000000000	32.7655000000000	47.9572000000000
4 C	3.9888000000000	32.1233000000000	49.0799000000000
5 H	4.2056000000000	32.4614000000000	49.9408000000000
6 C	3.1795000000000	30.9846000000000	48.9743000000000
7 H	2.8440000000000	30.5625000000000	49.7565000000000
8 C	2.8783000000000	30.4895000000000	47.7503000000000
9 H	2.3335000000000	29.7141000000000	47.6843000000000
10 C	3.3597000000000	31.1048000000000	46.5603000000000
11 C	3.0370000000000	30.5609000000000	45.2977000000000
12 H	2.4926000000000	29.7843000000000	45.2421000000000
13 C	3.5004000000000	31.1417000000000	44.1665000000000
14 H	3.2793000000000	30.7716000000000	43.3200000000000
15 C	4.3074000000000	32.2903000000000	44.2387000000000
16 H	4.6167000000000	32.6822000000000	43.4304000000000
17 C	4.6686000000000	32.8716000000000	45.4388000000000
18 C	4.1859000000000	32.2700000000000	46.6545000000000
19 C	5.9371000000000	34.7342000000000	46.6035000000000
20 C	5.5376000000000	34.0687000000000	45.4311000000000
21 C	6.0300000000000	34.6201000000000	44.2297000000000
22 H	5.8004000000000	34.2197000000000	43.3993000000000

23 C	6.841600000000	35.734900000000	44.249200000000
24 H	7.151100000000	36.074300000000	43.417700000000
25 N	7.220000000000	36.367600000000	45.362200000000
26 C	6.765400000000	35.857300000000	46.502900000000
27 H	7.022300000000	36.287500000000	47.309900000000
28 C	6.873100000000	33.863300000000	49.173400000000
29 C	7.454800000000	34.853800000000	49.964100000000
30 H	7.029600000000	35.699400000000	50.045700000000
31 C	8.640600000000	34.619900000000	50.629100000000
32 H	9.029600000000	35.301000000000	51.165000000000
33 C	9.258900000000	33.392000000000	50.512300000000
34 H	10.080500000000	33.231900000000	50.961600000000
35 C	8.687800000000	32.391400000000	49.743000000000
36 H	9.111700000000	31.543900000000	49.675600000000
37 C	7.501000000000	32.625600000000	49.073200000000
38 H	7.113100000000	31.939400000000	48.543000000000
39 C	-4.617300000000	47.291700000000	54.578900000000
40 H	-4.229400000000	47.977900000000	55.109100000000
41 I	3.189900000000	37.265000000000	50.423200000000
42 C	2.152000000000	38.867100000000	51.280800000000
43 C	2.354800000000	40.162600000000	50.833600000000
44 C	1.666900000000	41.227500000000	51.362800000000
45 F	3.251800000000	40.398600000000	49.858300000000
46 F	1.920900000000	42.459600000000	50.888600000000
47 C	-1.423800000000	47.627000000000	59.413400000000
48 H	-1.733000000000	47.235100000000	60.221700000000
49 C	-1.784900000000	47.045700000000	58.213400000000
50 C	-1.302300000000	47.647300000000	56.997600000000
51 C	-3.053400000000	45.183000000000	57.048600000000
52 C	-5.804100000000	47.525900000000	53.909100000000
53 H	-6.228000000000	48.373400000000	53.976500000000
54 C	-2.653900000000	45.848600000000	58.221100000000
55 C	-3.146300000000	45.297200000000	59.422400000000
56 I	-0.306200000000	42.652300000000	53.228900000000
57 C	0.731700000000	41.050200000000	52.371400000000
58 C	0.528900000000	39.754700000000	52.818600000000
59 H	-2.916700000000	45.697600000000	60.252800000000
60 C	-3.957900000000	44.182300000000	59.402900000000
61 C	1.216700000000	38.689800000000	52.289300000000
62 H	-4.267400000000	43.842900000000	60.234500000000
63 F	-0.368200000000	39.518700000000	53.793900000000
64 F	0.962800000000	37.457700000000	52.763600000000
65 P	-2.504200000000	45.641700000000	55.406400000000
66 O	-1.724500000000	44.565800000000	54.730900000000
67 C	-1.595300000000	47.151800000000	55.695000000000
68 C	-1.105100000000	47.794000000000	54.572200000000
69 H	-1.321900000000	47.455800000000	53.711300000000
70 C	-0.295800000000	48.932600000000	54.677800000000
71 H	0.039700000000	49.354800000000	53.895600000000
72 C	0.005400000000	49.427700000000	55.901800000000
73 H	0.550200000000	50.203200000000	55.967800000000
74 C	-0.476000000000	48.812400000000	57.091800000000
75 C	-0.153300000000	49.356400000000	58.354500000000
76 H	0.391100000000	50.133000000000	58.410100000000
77 N	-4.336300000000	43.549700000000	58.290000000000
78 C	-3.881700000000	44.060000000000	57.149300000000

79 H	-4.1386000000000	43.6298000000000	56.3422000000000
80 C	-3.9894000000000	46.0540000000000	54.4787000000000
81 C	-4.5711000000000	45.0635000000000	53.6881000000000
82 H	-4.1460000000000	44.2179000000000	53.6064000000000
83 C	-5.7569000000000	45.2974000000000	53.0230000000000
84 H	-6.1459000000000	44.6163000000000	52.4871000000000
85 C	-6.3753000000000	46.5253000000000	53.1399000000000
86 H	-7.1968000000000	46.6854000000000	52.6905000000000
87 C	-0.6167000000000	48.7756000000000	59.4856000000000
88 H	-0.3956000000000	49.1457000000000	60.3321000000000

2(PO)-A...(N)2, 2(N)-A...(OP)2

1 P	-8.9335000000000	21.5426000000000	48.2457000000000
2 O	-9.7132000000000	22.6185000000000	48.9212000000000
3 C	-9.8424000000000	20.0325000000000	47.9572000000000
4 C	-10.3325000000000	19.3902000000000	49.0799000000000
5 H	-10.1157000000000	19.7284000000000	49.9408000000000
6 C	-11.1418000000000	18.2516000000000	48.9743000000000
7 H	-11.4773000000000	17.8295000000000	49.7565000000000
8 C	-11.4430000000000	17.7565000000000	47.7503000000000
9 H	-11.9878000000000	16.9811000000000	47.6843000000000
10 C	-10.9616000000000	18.3718000000000	46.5603000000000
11 C	-11.2843000000000	17.8279000000000	45.2977000000000
12 H	-11.8287000000000	17.0513000000000	45.2421000000000
13 C	-10.8209000000000	18.4087000000000	44.1665000000000
14 H	-11.0420000000000	18.0385000000000	43.3200000000000
15 C	-10.0139000000000	19.5572000000000	44.2387000000000
16 H	-9.7046000000000	19.9492000000000	43.4304000000000
17 C	-9.6527000000000	20.1386000000000	45.4388000000000
18 C	-10.1354000000000	19.5370000000000	46.6545000000000
19 C	-8.3842000000000	22.0012000000000	46.6035000000000
20 C	-8.7837000000000	21.3357000000000	45.4311000000000
21 C	-8.2913000000000	21.8871000000000	44.2297000000000
22 H	-8.5209000000000	21.4867000000000	43.3993000000000
23 C	-7.4797000000000	23.0019000000000	44.2492000000000
24 H	-7.1702000000000	23.3413000000000	43.4177000000000
25 N	-7.1013000000000	23.6346000000000	45.3622000000000
26 C	-7.5559000000000	23.1243000000000	46.5029000000000
27 H	-7.2990000000000	23.5545000000000	47.3099000000000
28 C	-7.4482000000000	21.1303000000000	49.1734000000000
29 C	-6.8665000000000	22.1208000000000	49.9641000000000
30 H	-7.2917000000000	22.9664000000000	50.0457000000000
31 C	-5.6807000000000	21.8868000000000	50.6291000000000
32 H	-5.2917000000000	22.5680000000000	51.1650000000000
33 C	-5.0624000000000	20.6590000000000	50.5123000000000
34 H	-4.2408000000000	20.4989000000000	50.9616000000000
35 C	-5.6335000000000	19.6584000000000	49.7430000000000
36 H	-5.2096000000000	18.8109000000000	49.6756000000000
37 C	-6.8203000000000	19.8926000000000	49.0732000000000
38 H	-7.2082000000000	19.2064000000000	48.5430000000000
39 H	0.1516000000000	40.8294000000000	45.7531000000000
40 C	0.6675000000000	39.0356000000000	46.6039000000000
41 H	0.5877000000000	39.3423000000000	47.4995000000000
42 C	1.0406000000000	37.7240000000000	46.3823000000000

43 C	1.1500000000000	37.2725000000000	45.0195000000000
44 C	1.6891000000000	35.4951000000000	47.4053000000000
45 C	1.3228000000000	36.8460000000000	47.5389000000000
46 C	1.2456000000000	37.3193000000000	48.8656000000000
47 H	1.0046000000000	38.2235000000000	49.0294000000000
48 C	1.5169000000000	36.4817000000000	49.9271000000000
49 H	1.4529000000000	36.8405000000000	50.8043000000000
50 N	1.8635000000000	35.1987000000000	49.8004000000000
51 C	1.9428000000000	34.7393000000000	48.5550000000000
52 H	2.1903000000000	33.8298000000000	48.4372000000000
53 C	3.4855000000000	34.0754000000000	45.6743000000000
54 C	3.7896000000000	32.7728000000000	46.0682000000000
55 I	-0.8376000000000	31.2649000000000	45.3405000000000
56 C	-2.1938000000000	29.6711000000000	45.3342000000000
57 H	3.0927000000000	32.1938000000000	46.3540000000000
58 C	5.0908000000000	32.3151000000000	46.0478000000000
59 H	5.2884000000000	31.4262000000000	46.3185000000000
60 C	6.1040000000000	33.1544000000000	45.6322000000000
61 H	7.0020000000000	32.8444000000000	45.6265000000000
62 C	5.8185000000000	34.4468000000000	45.2234000000000
63 H	6.5185000000000	35.0166000000000	44.9269000000000
64 C	4.5151000000000	34.9080000000000	45.2465000000000
65 H	4.3220000000000	35.7959000000000	44.9695000000000
66 C	-2.6452000000000	29.1210000000000	46.5229000000000
67 C	-3.5548000000000	28.0917000000000	46.5453000000000
68 C	0.4012000000000	39.9342000000000	45.5563000000000
69 F	-2.1835000000000	29.5952000000000	47.6949000000000
70 F	-3.9420000000000	27.5985000000000	47.7345000000000
71 I	-5.4222000000000	25.9641000000000	45.3656000000000
72 C	-4.0659000000000	27.5578000000000	45.3718000000000
73 C	-3.6145000000000	28.1079000000000	44.1831000000000
74 C	-2.7050000000000	29.1373000000000	44.1608000000000
75 F	-4.0763000000000	27.6337000000000	43.0111000000000
76 F	-2.3177000000000	29.6304000000000	42.9715000000000
77 P	1.7848000000000	34.6396000000000	45.8344000000000
78 O	0.8249000000000	33.5040000000000	45.7297000000000
79 C	1.5224000000000	35.9489000000000	44.6484000000000
80 C	1.6192000000000	35.5940000000000	43.3150000000000
81 H	1.8814000000000	34.7099000000000	43.0870000000000
82 C	1.3389000000000	36.5110000000000	42.2936000000000
83 H	1.4014000000000	36.2463000000000	41.3833000000000
84 C	0.9782000000000	37.7769000000000	42.6119000000000
85 H	0.7943000000000	38.3963000000000	41.9155000000000
86 C	0.8683000000000	38.2004000000000	43.9665000000000
87 C	0.4989000000000	39.5295000000000	44.2685000000000
88 H	0.3184000000000	40.1420000000000	43.5650000000000

2(N)-A...(N)2

1 P	-8.9335000000000	21.5426000000000	48.2457000000000
2 O	-9.7132000000000	22.6185000000000	48.9212000000000
3 C	-9.8424000000000	20.0325000000000	47.9572000000000
4 C	-10.3325000000000	19.3902000000000	49.0799000000000
5 H	-10.1157000000000	19.7284000000000	49.9408000000000
6 C	-11.1418000000000	18.2516000000000	48.9743000000000

7 H	-11.4773000000000	17.8295000000000	49.7565000000000
8 C	-11.4430000000000	17.7565000000000	47.7503000000000
9 H	-11.9878000000000	16.9811000000000	47.6843000000000
10 C	-10.9616000000000	18.3718000000000	46.5603000000000
11 C	-11.2843000000000	17.8279000000000	45.2977000000000
12 H	-11.8287000000000	17.0513000000000	45.2421000000000
13 C	-10.8209000000000	18.4087000000000	44.1665000000000
14 H	-11.0420000000000	18.0385000000000	43.3200000000000
15 C	-10.0139000000000	19.5572000000000	44.2387000000000
16 H	-9.7046000000000	19.9492000000000	43.4304000000000
17 C	-9.6527000000000	20.1386000000000	45.4388000000000
18 C	-10.1354000000000	19.5370000000000	46.6545000000000
19 C	-8.3842000000000	22.0012000000000	46.6035000000000
20 C	-8.7837000000000	21.3357000000000	45.4311000000000
21 C	-8.2913000000000	21.8871000000000	44.2297000000000
22 H	-8.5209000000000	21.4867000000000	43.3993000000000
23 C	-7.4797000000000	23.0019000000000	44.2492000000000
24 H	-7.1702000000000	23.3413000000000	43.4177000000000
25 N	-7.1013000000000	23.6346000000000	45.3622000000000
26 C	-7.5559000000000	23.1243000000000	46.5029000000000
27 H	-7.2990000000000	23.5545000000000	47.3099000000000
28 C	-7.4482000000000	21.1303000000000	49.1734000000000
29 C	-6.8665000000000	22.1208000000000	49.9641000000000
30 H	-7.2917000000000	22.9664000000000	50.0457000000000
31 C	-5.6807000000000	21.8868000000000	50.6291000000000
32 H	-5.2917000000000	22.5680000000000	51.1650000000000
33 C	-5.0624000000000	20.6590000000000	50.5123000000000
34 H	-4.2408000000000	20.4989000000000	50.9616000000000
35 C	-5.6335000000000	19.6584000000000	49.7430000000000
36 H	-5.2096000000000	18.8109000000000	49.6756000000000
37 C	-6.8203000000000	19.8926000000000	49.0732000000000
38 H	-7.2082000000000	19.2064000000000	48.5430000000000
39 C	3.4172000000000	37.0560000000000	45.2568000000000
40 C	4.5854000000000	38.7859000000000	46.5291000000000
41 C	3.8998000000000	37.6576000000000	44.0411000000000
42 C	2.1487000000000	35.1934000000000	44.0921000000000
43 C	2.5482000000000	35.8590000000000	45.2646000000000
44 C	2.0558000000000	35.3075000000000	46.4659000000000
45 H	2.2854000000000	35.7079000000000	47.2963000000000
46 C	1.2442000000000	34.1927000000000	46.4464000000000
47 H	0.9347000000000	33.8533000000000	47.2779000000000
48 N	0.8658000000000	33.5600000000000	45.3334000000000
49 C	1.3204000000000	34.0704000000000	44.1928000000000
50 H	1.0635000000000	33.6401000000000	43.3857000000000
51 C	1.2127000000000	36.0643000000000	41.5222000000000
52 C	0.6310000000000	35.0738000000000	40.7315000000000
53 H	1.0561000000000	34.2282000000000	40.6499000000000
54 C	-0.5548000000000	35.3078000000000	40.0665000000000
55 H	-0.9438000000000	34.6266000000000	39.5306000000000
56 C	-1.1732000000000	36.5356000000000	40.1833000000000
57 H	-1.9947000000000	36.6957000000000	39.7340000000000
58 C	-0.6020000000000	37.5362000000000	40.9526000000000
59 H	-1.0259000000000	38.3837000000000	41.0200000000000
60 C	0.5848000000000	37.3020000000000	41.6224000000000
61 H	4.8065000000000	39.1561000000000	47.3756000000000
62 C	3.7783000000000	37.6374000000000	46.4569000000000
63 H	3.4691000000000	37.2454000000000	47.2652000000000

64 H	0.9727000000000	37.9882000000000	42.1526000000000
65 I	-0.8320000000000	31.2715000000000	45.3368000000000
66 C	-2.1953000000000	29.6693000000000	45.3386000000000
67 C	-2.6493000000000	29.1163000000000	46.5223000000000
68 C	-3.5491000000000	28.0707000000000	46.5227000000000
69 F	-2.2143000000000	29.5954000000000	47.6947000000000
70 F	-3.9409000000000	27.5694000000000	47.7033000000000
71 I	-5.4035000000000	25.9231000000000	45.3588000000000
72 C	-4.0403000000000	27.5253000000000	45.3571000000000
73 C	-3.5863000000000	28.0783000000000	44.1733000000000
74 C	-2.6865000000000	29.1239000000000	44.1729000000000
75 F	-4.0213000000000	27.5992000000000	43.0010000000000
76 F	-2.2946000000000	29.6252000000000	42.9923000000000
77 C	5.0488000000000	39.3668000000000	45.3979000000000
78 H	5.5932000000000	40.1433000000000	45.4536000000000
79 P	2.6979000000000	35.6520000000000	42.4499000000000
80 O	3.4776000000000	34.5761000000000	41.7744000000000
81 C	3.6068000000000	37.1622000000000	42.7384000000000
82 C	4.0970000000000	37.8044000000000	41.6157000000000
83 H	3.8802000000000	37.4662000000000	40.7548000000000
84 C	4.9063000000000	38.9430000000000	41.7213000000000
85 H	5.2418000000000	39.3651000000000	40.9391000000000
86 C	5.2075000000000	39.4381000000000	42.9453000000000
87 H	5.7523000000000	40.2135000000000	43.0113000000000
88 C	4.7261000000000	38.8228000000000	44.1353000000000

1...1

1 P	16.2910000000000	3.1364000000000	8.6655000000000
2 O	17.1996000000000	4.3094000000000	8.4705000000000
3 C	15.5371000000000	2.5750000000000	7.1288000000000
4 N	16.4200000000000	1.9968000000000	6.2813000000000
5 C	15.9868000000000	1.6503000000000	5.0766000000000
6 H	16.5958000000000	1.2343000000000	4.4777000000000
7 C	14.6848000000000	1.8683000000000	4.6520000000000
8 H	14.4141000000000	1.6168000000000	3.7767000000000
9 C	13.7932000000000	2.4532000000000	5.5166000000000
10 H	12.8959000000000	2.5978000000000	5.2402000000000
11 C	14.1964000000000	2.8417000000000	6.8110000000000
12 C	14.8653000000000	3.5087000000000	9.6868000000000
13 C	15.1111000000000	3.7475000000000	11.0233000000000
14 H	15.9658000000000	3.5433000000000	11.3843000000000
15 C	14.1211000000000	4.2866000000000	11.8590000000000
16 H	14.3048000000000	4.4522000000000	12.7762000000000
17 C	12.8961000000000	4.5693000000000	11.3414000000000
18 H	12.2344000000000	4.9548000000000	11.9037000000000
19 C	12.5804000000000	4.3047000000000	9.9879000000000
20 C	11.2915000000000	4.5866000000000	9.4837000000000
21 H	10.6286000000000	4.9462000000000	10.0614000000000
22 C	10.9896000000000	4.3481000000000	8.1769000000000
23 H	10.1228000000000	4.5495000000000	7.8443000000000
24 C	11.9631000000000	3.8030000000000	7.3214000000000
25 H	11.7385000000000	3.6536000000000	6.4104000000000
26 C	13.2376000000000	3.4756000000000	7.7554000000000
27 C	13.5790000000000	3.7493000000000	9.1221000000000

28 C	17.1754000000000	1.7708000000000	9.4414000000000
29 C	16.5904000000000	0.5269000000000	9.6441000000000
30 H	15.6974000000000	0.3678000000000	9.3615000000000
31 C	17.3183000000000	-0.4844000000000	10.2628000000000
32 H	16.9294000000000	-1.3424000000000	10.3864000000000
33 C	18.6102000000000	-0.2397000000000	10.6983000000000
34 H	19.1006000000000	-0.9287000000000	11.1311000000000
35 C	19.1856000000000	0.9892000000000	10.5090000000000
36 H	20.0706000000000	1.1492000000000	10.8153000000000
37 C	18.4783000000000	2.0061000000000	9.8689000000000
38 H	18.8831000000000	2.8535000000000	9.7257000000000
39 P	12.7493000000000	5.7472000000000	3.8100000000000
40 O	11.8408000000000	4.5743000000000	4.0050000000000
41 C	13.5033000000000	6.3087000000000	5.3468000000000
42 N	12.6203000000000	6.8868000000000	6.1942000000000
43 C	13.0536000000000	7.2333000000000	7.3990000000000
44 H	12.4445000000000	7.6493000000000	7.9978000000000
45 C	14.3556000000000	7.0153000000000	7.8236000000000
46 H	14.6263000000000	7.2668000000000	8.6988000000000
47 C	15.2472000000000	6.4304000000000	6.9590000000000
48 H	16.1445000000000	6.2858000000000	7.2353000000000
49 C	14.8439000000000	6.0420000000000	5.6645000000000
50 C	14.1750000000000	5.3749000000000	2.7888000000000
51 C	13.9293000000000	5.1361000000000	1.4523000000000
52 H	13.0745000000000	5.3403000000000	1.0912000000000
53 C	14.9193000000000	4.5970000000000	0.6165000000000
54 H	14.7356000000000	4.4315000000000	-0.3007000000000
55 C	16.1443000000000	4.3144000000000	1.1342000000000
56 H	16.8059000000000	3.9289000000000	0.5719000000000
57 C	16.4600000000000	4.5789000000000	2.4876000000000
58 C	17.7489000000000	4.2970000000000	2.9919000000000
59 H	18.4117000000000	3.9375000000000	2.4141000000000
60 C	18.0508000000000	4.5356000000000	4.2987000000000
61 H	18.9176000000000	4.3341000000000	4.6313000000000
62 C	17.0772000000000	5.0806000000000	5.1542000000000
63 H	17.3018000000000	5.2301000000000	6.0651000000000
64 C	15.8028000000000	5.4080000000000	4.7201000000000
65 C	15.4614000000000	5.1343000000000	3.3534000000000
66 C	11.8649000000000	7.1128000000000	3.0342000000000
67 C	12.4499000000000	8.3567000000000	2.8315000000000
68 H	13.3430000000000	8.5158000000000	3.1140000000000
69 C	11.7221000000000	9.3680000000000	2.2128000000000
70 H	12.1109000000000	10.2260000000000	2.0892000000000
71 C	10.4301000000000	9.1234000000000	1.7773000000000
72 H	9.9398000000000	9.8123000000000	1.3445000000000
73 C	9.8547000000000	7.8944000000000	1.9665000000000
74 H	8.9698000000000	7.7345000000000	1.6602000000000
75 C	10.5620000000000	6.8775000000000	2.6066000000000
76 H	10.1573000000000	6.0301000000000	2.7499000000000

2...2

1 P	3.1940000000000	4.3066000000000	9.3762000000000
2 O	2.4143000000000	5.3825000000000	10.0517000000000
3 C	2.2851000000000	2.7965000000000	9.0876000000000

4 C	1.794900000000	2.154300000000	10.210400000000
5 H	2.011700000000	2.492500000000	11.071300000000
6 C	0.985600000000	1.015700000000	10.104800000000
7 H	0.650100000000	0.593500000000	10.886900000000
8 C	0.684400000000	0.520500000000	8.880700000000
9 H	0.139600000000	-0.254900000000	8.814800000000
10 C	1.165800000000	1.135900000000	7.690800000000
11 C	0.843100000000	0.591900000000	6.428100000000
12 H	0.298700000000	-0.184700000000	6.372500000000
13 C	1.306500000000	1.172700000000	5.297000000000
14 H	1.085400000000	0.802600000000	4.450500000000
15 C	2.113600000000	2.321300000000	5.369100000000
16 H	2.422800000000	2.713200000000	4.560900000000
17 C	2.474700000000	2.902600000000	6.569200000000
18 C	1.992000000000	2.301000000000	7.785000000000
19 C	3.743200000000	4.765300000000	7.734000000000
20 C	3.343700000000	4.099700000000	6.561500000000
21 C	3.836100000000	4.651100000000	5.360100000000
22 H	3.606500000000	4.250700000000	4.529800000000
23 C	4.647700000000	5.766000000000	5.379700000000
24 H	4.957200000000	6.105400000000	4.548100000000
25 N	5.026100000000	6.398600000000	6.492600000000
26 C	4.571500000000	5.888300000000	7.633300000000
27 H	4.828400000000	6.318500000000	8.440400000000
28 C	4.679200000000	3.894300000000	10.303900000000
29 C	5.260900000000	4.884800000000	11.094500000000
30 H	4.835700000000	5.730400000000	11.176100000000
31 C	6.446700000000	4.650900000000	11.759600000000
32 H	6.835700000000	5.332000000000	12.295500000000
33 C	7.065100000000	3.423000000000	11.642700000000
34 H	7.886600000000	3.262900000000	12.092100000000
35 C	6.493900000000	2.422400000000	10.873500000000
36 H	6.917800000000	1.574900000000	10.806100000000
37 C	5.307100000000	2.656600000000	10.203700000000
38 H	4.919200000000	1.970400000000	9.673500000000
39 P	0.504000000000	5.683100000000	3.580400000000
40 O	1.283700000000	4.607100000000	2.904800000000
41 C	1.412900000000	7.193200000000	3.868900000000
42 C	1.903100000000	7.835400000000	2.746100000000
43 H	1.686300000000	7.497200000000	1.885200000000
44 C	2.712400000000	8.974000000000	2.851700000000
45 H	3.047900000000	9.396200000000	2.069600000000
46 C	3.013600000000	9.469100000000	4.075800000000
47 H	3.558400000000	10.244600000000	4.141800000000
48 C	2.532200000000	8.853800000000	5.265700000000
49 C	2.854900000000	9.397800000000	6.528400000000
50 H	3.399300000000	10.174300000000	6.584000000000
51 C	2.391500000000	8.816900000000	7.659600000000
52 H	2.612600000000	9.187100000000	8.506100000000
53 C	1.584400000000	7.668400000000	7.587400000000
54 H	1.275200000000	7.276400000000	8.395600000000
55 C	1.223300000000	7.087100000000	6.387300000000
56 C	1.705900000000	7.688600000000	5.171500000000
57 C	-0.045200000000	5.224400000000	5.222600000000
58 C	0.354300000000	5.890000000000	6.395000000000
59 C	-0.138100000000	5.338600000000	7.596400000000

60	H	0.091500000000	5.738900000000	8.426700000000
61	C	-0.949700000000	4.223700000000	7.576800000000
62	H	-1.259200000000	3.884300000000	8.408400000000
63	N	-1.328100000000	3.591100000000	6.463900000000
64	C	-0.873500000000	4.101400000000	5.323200000000
65	H	-1.130400000000	3.671100000000	4.516100000000
66	C	-0.981200000000	6.095400000000	2.652700000000
67	C	-1.562900000000	5.104900000000	1.862000000000
68	H	-1.137700000000	4.259300000000	1.780400000000
69	C	-2.748700000000	5.338800000000	1.196900000000
70	H	-3.137700000000	4.657600000000	0.661000000000
71	C	-3.367100000000	6.566700000000	1.313800000000
72	H	-4.188600000000	6.726700000000	0.864500000000
73	C	-2.795900000000	7.567300000000	2.083100000000
74	H	-3.219800000000	8.414800000000	2.150400000000
75	C	-1.609100000000	7.333000000000	2.752800000000
76	H	-1.221200000000	8.019200000000	3.283100000000

Dim¹(PO)···A

1	P	5.387900000000	34.275600000000	48.245700000000
2	O	4.608100000000	35.351500000000	48.921200000000
3	C	4.479000000000	32.765500000000	47.957200000000
4	C	3.988800000000	32.123300000000	49.079900000000
5	H	4.205600000000	32.461400000000	49.940800000000
6	C	3.179500000000	30.984600000000	48.974300000000
7	H	2.844000000000	30.562500000000	49.756500000000
8	C	2.878300000000	30.489500000000	47.750300000000
9	H	2.333500000000	29.714100000000	47.684300000000
10	C	3.359700000000	31.104800000000	46.560300000000
11	C	3.037000000000	30.560900000000	45.297700000000
12	H	2.492600000000	29.784300000000	45.242100000000
13	C	3.500400000000	31.141700000000	44.166500000000
14	H	3.279300000000	30.771600000000	43.320000000000
15	C	4.307400000000	32.290300000000	44.238700000000
16	H	4.616700000000	32.682200000000	43.430400000000
17	C	4.668600000000	32.871600000000	45.438800000000
18	C	4.185900000000	32.270000000000	46.654500000000
19	C	5.937100000000	34.734200000000	46.603500000000
20	C	5.537600000000	34.068700000000	45.431100000000
21	C	6.030000000000	34.620100000000	44.229700000000
22	H	5.800400000000	34.219700000000	43.399300000000
23	C	6.841600000000	35.734900000000	44.249200000000
24	H	7.151100000000	36.074300000000	43.417700000000
25	N	7.220000000000	36.367600000000	45.362200000000
26	C	6.765400000000	35.857300000000	46.502900000000
27	H	7.022300000000	36.287500000000	47.309900000000
28	C	6.873100000000	33.863300000000	49.173400000000
29	C	7.454800000000	34.853800000000	49.964100000000
30	H	7.029600000000	35.699400000000	50.045700000000
31	C	8.640600000000	34.619900000000	50.629100000000
32	H	9.029600000000	35.301000000000	51.165000000000
33	C	9.258900000000	33.392000000000	50.512300000000
34	H	10.080500000000	33.231900000000	50.961600000000
35	C	8.687800000000	32.391400000000	49.743000000000

36	H	9.1117000000000	31.5439000000000	49.6756000000000
37	C	7.5010000000000	32.6256000000000	49.0732000000000
38	H	7.1131000000000	31.9394000000000	48.5430000000000
39	C	4.5854000000000	38.7859000000000	46.5291000000000
40	H	4.8065000000000	39.1561000000000	47.3756000000000
41	C	3.7783000000000	37.6374000000000	46.4569000000000
42	H	3.4691000000000	37.2454000000000	47.2652000000000
43	C	3.4172000000000	37.0560000000000	45.2568000000000
44	C	3.8998000000000	37.6576000000000	44.0411000000000
45	C	2.1487000000000	35.1934000000000	44.0921000000000
46	C	2.5482000000000	35.8590000000000	45.2646000000000
47	C	2.0558000000000	35.3075000000000	46.4659000000000
48	H	2.2854000000000	35.7079000000000	47.2963000000000
49	C	1.2442000000000	34.1927000000000	46.4464000000000
50	H	0.9347000000000	33.8533000000000	47.2779000000000
51	N	0.8658000000000	33.5600000000000	45.3334000000000
52	C	1.3204000000000	34.0704000000000	44.1928000000000
53	H	1.0635000000000	33.6401000000000	43.3857000000000
54	C	1.2127000000000	36.0643000000000	41.5222000000000
55	C	0.6310000000000	35.0738000000000	40.7315000000000
56	H	1.0561000000000	34.2282000000000	40.6499000000000
57	C	-0.5548000000000	35.3078000000000	40.0665000000000
58	H	-0.9438000000000	34.6266000000000	39.5306000000000
59	C	-1.1732000000000	36.5356000000000	40.1833000000000
60	H	-1.9947000000000	36.6957000000000	39.7340000000000
61	C	-0.6020000000000	37.5362000000000	40.9526000000000
62	H	-1.0259000000000	38.3837000000000	41.0200000000000
63	C	0.5848000000000	37.3020000000000	41.6224000000000
64	H	0.9727000000000	37.9882000000000	42.1526000000000
65	F	-0.3682000000000	39.5187000000000	53.7939000000000
66	F	0.9628000000000	37.4577000000000	52.7636000000000
67	I	3.1899000000000	37.2650000000000	50.4232000000000
68	C	2.1520000000000	38.8671000000000	51.2808000000000
69	C	2.3548000000000	40.1626000000000	50.8336000000000
70	C	1.6669000000000	41.2275000000000	51.3628000000000
71	F	3.2518000000000	40.3986000000000	49.8583000000000
72	F	1.9209000000000	42.4596000000000	50.8886000000000
73	I	-0.3062000000000	42.6523000000000	53.2289000000000
74	C	0.7317000000000	41.0502000000000	52.3714000000000
75	C	0.5289000000000	39.7547000000000	52.8186000000000
76	C	1.2167000000000	38.6898000000000	52.2893000000000
77	P	2.6979000000000	35.6520000000000	42.4499000000000
78	O	3.4776000000000	34.5761000000000	41.7744000000000
79	C	3.6068000000000	37.1622000000000	42.7384000000000
80	C	4.0970000000000	37.8044000000000	41.6157000000000
81	H	3.8802000000000	37.4662000000000	40.7548000000000
82	C	4.9063000000000	38.9430000000000	41.7213000000000
83	H	5.2418000000000	39.3651000000000	40.9391000000000
84	C	5.2075000000000	39.4381000000000	42.9453000000000
85	H	5.7523000000000	40.2135000000000	43.0113000000000
86	C	4.7261000000000	38.8228000000000	44.1353000000000
87	C	5.0488000000000	39.3668000000000	45.3979000000000
88	H	5.5932000000000	40.1433000000000	45.4536000000000

1 P	42.110100000000	29.787300000000	46.092200000000
2 O	43.018600000000	30.960300000000	45.897200000000
3 C	41.356100000000	29.225900000000	44.555500000000
4 N	42.239100000000	28.647700000000	43.708000000000
5 C	41.805800000000	28.301200000000	42.503300000000
6 H	42.414900000000	27.885200000000	41.904400000000
7 C	40.503800000000	28.519200000000	42.078700000000
8 H	40.233200000000	28.267700000000	41.203400000000
9 C	39.612200000000	29.104100000000	42.943300000000
10 H	38.714900000000	29.248700000000	42.666900000000
11 C	40.015500000000	29.492600000000	44.237700000000
12 C	40.684400000000	30.159700000000	47.113500000000
13 C	40.930100000000	30.398400000000	48.450000000000
14 H	41.784900000000	30.194200000000	48.811000000000
15 C	39.940200000000	30.937500000000	49.285700000000
16 H	40.123800000000	31.103100000000	50.202900000000
17 C	38.715100000000	31.220200000000	48.768100000000
18 H	38.053500000000	31.605700000000	49.330400000000
19 C	38.399500000000	30.955600000000	47.414600000000
20 C	37.110500000000	31.237500000000	46.910400000000
21 H	36.447700000000	31.597100000000	47.488100000000
22 C	36.808600000000	30.999000000000	45.603600000000
23 H	35.941800000000	31.200400000000	45.271000000000
24 C	37.782200000000	30.453900000000	44.748100000000
25 H	37.557600000000	30.304500000000	43.837100000000
26 C	39.056600000000	30.126500000000	45.182100000000
27 C	39.398000000000	30.400200000000	46.548800000000
28 C	42.994500000000	28.421700000000	46.868100000000
29 C	42.409500000000	27.177900000000	47.070800000000
30 H	41.516500000000	27.018700000000	46.788200000000
31 C	43.137300000000	26.166500000000	47.689500000000
32 H	42.748500000000	25.308500000000	47.813100000000
33 C	44.429300000000	26.411200000000	48.125000000000
34 H	44.919700000000	25.722200000000	48.557800000000
35 C	45.004700000000	27.640100000000	47.935700000000
36 H	45.889600000000	27.800100000000	48.242000000000
37 C	44.297400000000	28.657000000000	47.295600000000
38 H	44.702100000000	29.504500000000	47.152400000000
39 C	39.748300000000	31.787100000000	38.879000000000
40 H	38.893600000000	31.991300000000	38.517900000000
41 C	40.738300000000	31.248000000000	38.043200000000
42 H	40.554600000000	31.082400000000	37.126000000000
43 C	41.963300000000	30.965300000000	38.560900000000
44 H	42.625000000000	30.579800000000	37.998600000000
45 C	42.279000000000	31.229900000000	39.914300000000
46 C	43.567900000000	30.947900000000	40.418600000000
47 H	44.230800000000	30.588400000000	39.840800000000
48 C	43.869800000000	31.186500000000	41.725400000000
49 H	44.736600000000	30.985000000000	42.058000000000
50 C	42.896300000000	31.731500000000	42.580900000000
51 H	43.120900000000	31.881000000000	43.491800000000
52 C	41.621800000000	32.058900000000	42.146800000000
53 C	41.280400000000	31.785300000000	40.780100000000
54 C	37.684000000000	33.763800000000	40.460900000000
55 C	38.269000000000	35.007600000000	40.258200000000
56 H	39.162000000000	35.166700000000	40.540700000000
57 C	37.541200000000	36.019000000000	39.639500000000

58 H	37.9300000000000	36.8770000000000	39.5159000000000
59 C	36.2492000000000	35.7743000000000	39.2040000000000
60 H	35.7588000000000	36.4633000000000	38.7712000000000
61 C	35.6738000000000	34.5454000000000	39.3932000000000
62 H	34.7888000000000	34.3854000000000	39.0869000000000
63 C	36.3811000000000	33.5285000000000	40.0333000000000
64 H	35.9763000000000	32.6810000000000	40.1766000000000
65 C	48.6891000000000	25.6405000000000	42.5381000000000
66 F	46.7289000000000	26.1987000000000	41.4035000000000
67 F	49.1093000000000	25.0465000000000	41.4158000000000
68 I	51.3859000000000	24.7608000000000	43.6322000000000
69 C	49.4833000000000	25.6282000000000	43.6762000000000
70 C	48.9833000000000	26.2718000000000	44.7935000000000
71 C	47.7486000000000	26.8884000000000	44.7909000000000
72 F	49.7087000000000	26.3303000000000	45.9254000000000
73 F	47.3283000000000	27.4825000000000	45.9132000000000
74 C	46.9543000000000	26.9008000000000	43.6528000000000
75 I	45.0516000000000	27.7681000000000	43.6968000000000
76 C	47.4544000000000	26.2573000000000	42.5354000000000
77 P	38.5684000000000	32.3982000000000	41.2367000000000
78 O	37.6599000000000	31.2252000000000	41.4317000000000
79 C	39.3223000000000	32.9596000000000	42.7735000000000
80 N	38.4394000000000	33.5378000000000	43.6209000000000
81 C	38.8726000000000	33.8843000000000	44.8257000000000
82 H	38.2636000000000	34.3002000000000	45.4245000000000
83 C	40.1746000000000	33.6663000000000	45.2503000000000
84 H	40.4453000000000	33.9178000000000	46.1255000000000
85 C	41.0663000000000	33.0813000000000	44.3857000000000
86 H	41.9636000000000	32.9368000000000	44.6620000000000
87 C	40.6630000000000	32.6929000000000	43.0912000000000
88 C	39.9941000000000	32.0258000000000	40.2155000000000

Dim²(N)···A

1 C	0.6310000000000	35.0738000000000	40.7315000000000
2 H	1.0561000000000	34.2282000000000	40.6499000000000
3 C	-0.5548000000000	35.3078000000000	40.0665000000000
4 H	-0.9438000000000	34.6266000000000	39.5306000000000
5 C	-1.1732000000000	36.5356000000000	40.1833000000000
6 H	-1.9947000000000	36.6957000000000	39.7340000000000
7 C	-0.6020000000000	37.5362000000000	40.9526000000000
8 H	-1.0259000000000	38.3837000000000	41.0200000000000
9 C	0.5848000000000	37.3020000000000	41.6224000000000
10 H	0.9727000000000	37.9882000000000	42.1526000000000
11 I	-0.8320000000000	31.2715000000000	45.3368000000000
12 C	-2.1953000000000	29.6693000000000	45.3386000000000
13 C	-2.6493000000000	29.1163000000000	46.5223000000000
14 C	-3.5491000000000	28.0707000000000	46.5227000000000
15 F	-2.2143000000000	29.5954000000000	47.6947000000000
16 F	-3.9409000000000	27.5694000000000	47.7033000000000
17 I	-5.4035000000000	25.9231000000000	45.3588000000000
18 C	-4.0403000000000	27.5253000000000	45.3571000000000
19 C	-3.5863000000000	28.0783000000000	44.1733000000000
20 C	-2.6865000000000	29.1239000000000	44.1729000000000
21 F	-4.0213000000000	27.5992000000000	43.0010000000000

22	F	-2.2946000000000	29.6252000000000	42.9923000000000
23	P	2.6979000000000	35.6520000000000	42.4499000000000
24	O	3.4776000000000	34.5761000000000	41.7744000000000
25	C	3.6068000000000	37.1622000000000	42.7384000000000
26	C	4.0970000000000	37.8044000000000	41.6157000000000
27	H	3.8802000000000	37.4662000000000	40.7548000000000
28	C	4.9063000000000	38.9430000000000	41.7213000000000
29	H	5.2418000000000	39.3651000000000	40.9391000000000
30	C	5.2075000000000	39.4381000000000	42.9453000000000
31	N	0.8658000000000	33.5600000000000	45.3334000000000
32	C	1.3204000000000	34.0704000000000	44.1928000000000
33	H	1.0635000000000	33.6401000000000	43.3857000000000
34	C	1.2127000000000	36.0643000000000	41.5222000000000
35	H	5.7523000000000	40.2135000000000	43.0113000000000
36	C	4.7261000000000	38.8228000000000	44.1353000000000
37	C	5.0488000000000	39.3668000000000	45.3979000000000
38	H	5.5932000000000	40.1433000000000	45.4536000000000
39	P	5.3879000000000	34.2756000000000	48.2457000000000
40	O	4.6081000000000	35.3515000000000	48.9212000000000
41	C	4.4790000000000	32.7655000000000	47.9572000000000
42	C	3.9888000000000	32.1233000000000	49.0799000000000
43	H	4.2056000000000	32.4614000000000	49.9408000000000
44	C	3.1795000000000	30.9846000000000	48.9743000000000
45	H	2.8440000000000	30.5625000000000	49.7565000000000
46	C	2.8783000000000	30.4895000000000	47.7503000000000
47	H	2.3335000000000	29.7141000000000	47.6843000000000
48	C	3.3597000000000	31.1048000000000	46.5603000000000
49	C	3.0370000000000	30.5609000000000	45.2977000000000
50	H	2.4926000000000	29.7843000000000	45.2421000000000
51	C	3.5004000000000	31.1417000000000	44.1665000000000
52	H	3.2793000000000	30.7716000000000	43.3200000000000
53	C	4.3074000000000	32.2903000000000	44.2387000000000
54	H	4.6167000000000	32.6822000000000	43.4304000000000
55	C	4.6686000000000	32.8716000000000	45.4388000000000
56	C	4.1859000000000	32.2700000000000	46.6545000000000
57	C	5.9371000000000	34.7342000000000	46.6035000000000
58	C	5.5376000000000	34.0687000000000	45.4311000000000
59	C	6.0300000000000	34.6201000000000	44.2297000000000
60	H	5.8004000000000	34.2197000000000	43.3993000000000
61	C	6.8416000000000	35.7349000000000	44.2492000000000
62	H	7.1511000000000	36.0743000000000	43.4177000000000
63	N	7.2200000000000	36.3676000000000	45.3622000000000
64	C	6.7654000000000	35.8573000000000	46.5029000000000
65	H	7.0223000000000	36.2875000000000	47.3099000000000
66	C	6.8731000000000	33.8633000000000	49.1734000000000
67	C	7.4548000000000	34.8538000000000	49.9641000000000
68	H	7.0296000000000	35.6994000000000	50.0457000000000
69	C	8.6406000000000	34.6199000000000	50.6291000000000
70	H	9.0296000000000	35.3010000000000	51.1650000000000
71	C	9.2589000000000	33.3920000000000	50.5123000000000
72	H	10.0805000000000	33.2319000000000	50.9616000000000
73	C	8.6878000000000	32.3914000000000	49.7430000000000
74	H	9.1117000000000	31.5439000000000	49.6756000000000
75	C	7.5010000000000	32.6256000000000	49.0732000000000
76	H	7.1131000000000	31.9394000000000	48.5430000000000
77	C	4.5854000000000	38.7859000000000	46.5291000000000
78	H	4.8065000000000	39.1561000000000	47.3756000000000

79 C	3.7783000000000	37.6374000000000	46.4569000000000
80 H	3.4691000000000	37.2454000000000	47.2652000000000
81 C	3.4172000000000	37.0560000000000	45.2568000000000
82 C	3.8998000000000	37.6576000000000	44.0411000000000
83 C	2.1487000000000	35.1934000000000	44.0921000000000
84 C	2.5482000000000	35.8590000000000	45.2646000000000
85 C	2.0558000000000	35.3075000000000	46.4659000000000
86 H	2.2854000000000	35.7079000000000	47.2963000000000
87 C	1.2442000000000	34.1927000000000	46.4464000000000
88 H	0.9347000000000	33.8533000000000	47.2779000000000

Dim¹(PO)-A...(OP)Dim¹

1 P	33.5037000000000	20.9037000000000	33.6167000000000
2 O	34.4123000000000	22.0767000000000	33.4217000000000
3 C	32.7498000000000	20.3422000000000	32.0799000000000
4 N	33.6327000000000	19.7641000000000	31.2325000000000
5 C	33.1995000000000	19.4176000000000	30.0277000000000
6 H	33.8085000000000	19.0016000000000	29.4289000000000
7 C	31.8975000000000	19.6356000000000	29.6031000000000
8 H	31.6268000000000	19.3841000000000	28.7279000000000
9 C	31.0059000000000	20.2205000000000	30.4677000000000
10 H	30.1086000000000	20.3651000000000	30.1914000000000
11 C	31.4091000000000	20.6089000000000	31.7622000000000
12 C	32.0781000000000	21.2760000000000	34.6379000000000
13 C	32.3238000000000	21.5148000000000	35.9744000000000
14 H	33.1785000000000	21.3106000000000	36.3355000000000
15 C	31.3338000000000	22.0539000000000	36.8102000000000
16 H	31.5175000000000	22.2195000000000	37.7274000000000
17 C	30.1088000000000	22.3365000000000	36.2925000000000
18 H	29.4471000000000	22.7221000000000	36.8548000000000
19 C	29.7931000000000	22.0720000000000	34.9391000000000
20 C	28.5042000000000	22.3539000000000	34.4348000000000
21 H	27.8413000000000	22.7135000000000	35.0126000000000
22 C	28.2023000000000	22.1153000000000	33.1280000000000
23 H	27.3355000000000	22.3168000000000	32.7954000000000
24 C	29.1758000000000	21.5703000000000	32.2725000000000
25 H	28.9512000000000	21.4209000000000	31.3616000000000
26 C	30.4503000000000	21.2429000000000	32.7066000000000
27 C	30.7917000000000	21.5166000000000	34.0733000000000
28 C	34.3881000000000	19.5381000000000	34.3925000000000
29 C	33.8031000000000	18.2942000000000	34.5952000000000
30 H	32.9101000000000	18.1351000000000	34.3127000000000
31 C	34.5310000000000	17.2829000000000	35.2139000000000
32 H	34.1421000000000	16.4249000000000	35.3375000000000
33 C	35.8229000000000	17.5275000000000	35.6494000000000
34 H	36.3133000000000	16.8386000000000	36.0822000000000
35 C	36.3983000000000	18.7565000000000	35.4602000000000
36 H	37.2833000000000	18.9164000000000	35.7665000000000
37 C	35.6910000000000	19.7734000000000	34.8201000000000
38 H	36.0958000000000	20.6208000000000	34.6768000000000
39 P	42.1101000000000	29.7873000000000	46.0922000000000
40 O	43.0186000000000	30.9603000000000	45.8972000000000
41 C	41.3561000000000	29.2259000000000	44.5555000000000
42 N	42.2391000000000	28.6477000000000	43.7080000000000

43 C	41.8058000000000	28.3012000000000	42.5033000000000
44 H	42.4149000000000	27.8852000000000	41.9044000000000
45 C	40.5038000000000	28.5192000000000	42.0787000000000
46 H	40.2332000000000	28.2677000000000	41.2034000000000
47 C	39.6122000000000	29.1041000000000	42.9433000000000
48 H	38.7149000000000	29.2487000000000	42.6669000000000
49 C	40.0155000000000	29.4926000000000	44.2377000000000
50 C	40.6844000000000	30.1597000000000	47.1135000000000
51 C	40.9301000000000	30.3984000000000	48.4500000000000
52 H	41.7849000000000	30.1942000000000	48.8110000000000
53 C	39.9402000000000	30.9375000000000	49.2857000000000
54 H	40.1238000000000	31.1031000000000	50.2029000000000
55 C	38.7151000000000	31.2202000000000	48.7681000000000
56 H	38.0535000000000	31.6057000000000	49.3304000000000
57 C	38.3995000000000	30.9556000000000	47.4146000000000
58 C	37.1105000000000	31.2375000000000	46.9104000000000
59 H	36.4477000000000	31.5971000000000	47.4881000000000
60 C	36.8086000000000	30.9990000000000	45.6036000000000
61 H	35.9418000000000	31.2004000000000	45.2710000000000
62 C	37.7822000000000	30.4539000000000	44.7481000000000
63 H	37.5576000000000	30.3045000000000	43.8371000000000
64 C	39.0566000000000	30.1265000000000	45.1821000000000
65 C	39.3980000000000	30.4002000000000	46.5488000000000
66 C	42.9945000000000	28.4217000000000	46.8681000000000
67 C	42.4095000000000	27.1779000000000	47.0708000000000
68 H	41.5165000000000	27.0187000000000	46.7882000000000
69 C	43.1373000000000	26.1665000000000	47.6895000000000
70 H	42.7485000000000	25.3085000000000	47.8131000000000
71 C	44.4293000000000	26.4112000000000	48.1250000000000
72 H	44.9197000000000	25.7222000000000	48.5578000000000
73 C	45.0047000000000	27.6401000000000	47.9357000000000
74 H	45.8896000000000	27.8001000000000	48.2420000000000
75 C	44.2974000000000	28.6570000000000	47.2956000000000
76 H	44.7021000000000	29.5045000000000	47.1524000000000
77 P	29.9620000000000	23.5145000000000	28.7612000000000
78 O	29.0535000000000	22.3415000000000	28.9562000000000
79 C	30.7160000000000	24.0760000000000	30.2979000000000
80 N	29.8331000000000	24.6541000000000	31.1454000000000
81 C	30.2663000000000	25.0060000000000	32.3501000000000
82 H	29.6572000000000	25.4166000000000	32.9490000000000
83 C	31.5683000000000	24.7826000000000	32.7747000000000
84 H	31.8390000000000	25.0341000000000	33.6500000000000
85 C	32.4599000000000	24.1977000000000	31.9101000000000
86 H	33.3572000000000	24.0531000000000	32.1865000000000
87 C	32.0566000000000	23.8093000000000	30.6157000000000
88 C	31.3877000000000	23.1422000000000	27.7399000000000
89 C	31.1420000000000	22.9034000000000	26.4034000000000
90 H	30.2872000000000	23.1076000000000	26.0424000000000
91 C	32.1320000000000	22.3643000000000	25.5677000000000
92 H	31.9483000000000	22.1988000000000	24.6505000000000
93 C	33.3570000000000	22.0817000000000	26.0853000000000
94 H	34.0186000000000	21.6961000000000	25.5230000000000
95 C	33.6727000000000	22.3462000000000	27.4388000000000
96 C	34.9616000000000	22.0643000000000	27.9430000000000
97 H	35.6244000000000	21.7048000000000	27.3653000000000
98 C	35.2635000000000	22.3029000000000	29.2498000000000
99 H	36.1303000000000	22.1014000000000	29.5824000000000

100 C	34.2899000000000	22.8479000000000	30.1053000000000
101 H	34.5145000000000	22.9973000000000	31.0163000000000
102 C	33.0155000000000	23.1753000000000	29.6713000000000
103 C	32.6741000000000	22.9016000000000	28.3046000000000
104 C	29.0776000000000	24.8801000000000	27.9853000000000
105 C	29.6627000000000	26.1240000000000	27.7826000000000
106 H	30.5557000000000	26.2831000000000	28.0652000000000
107 C	28.9348000000000	27.1353000000000	27.1639000000000
108 H	29.3237000000000	27.9933000000000	27.0403000000000
109 C	27.6428000000000	26.8907000000000	26.7284000000000
110 H	27.1525000000000	27.5796000000000	26.2956000000000
111 C	27.0674000000000	25.6617000000000	26.9177000000000
112 H	26.1825000000000	25.5018000000000	26.6114000000000
113 C	27.7747000000000	24.6448000000000	27.5578000000000
114 H	27.3700000000000	23.7974000000000	27.7010000000000
115 P	38.5684000000000	32.3982000000000	41.2367000000000
116 O	37.6599000000000	31.2252000000000	41.4317000000000
117 C	39.3223000000000	32.9596000000000	42.7735000000000
118 N	38.4394000000000	33.5378000000000	43.6209000000000
119 C	38.8726000000000	33.8843000000000	44.8257000000000
120 H	38.2636000000000	34.3002000000000	45.4245000000000
121 C	40.1746000000000	33.6663000000000	45.2503000000000
122 H	40.4453000000000	33.9178000000000	46.1255000000000
123 C	41.0663000000000	33.0813000000000	44.3857000000000
124 H	41.9636000000000	32.9368000000000	44.6620000000000
125 C	40.6630000000000	32.6929000000000	43.0912000000000
126 C	39.9941000000000	32.0258000000000	40.2155000000000
127 C	39.7483000000000	31.7871000000000	38.8790000000000
128 H	38.8936000000000	31.9913000000000	38.5179000000000
129 C	40.7383000000000	31.2480000000000	38.0432000000000
130 H	40.5546000000000	31.0824000000000	37.1260000000000
131 C	41.9633000000000	30.9653000000000	38.5609000000000
132 H	42.6250000000000	30.5798000000000	37.9986000000000
133 C	42.2790000000000	31.2299000000000	39.9143000000000
134 C	43.5679000000000	30.9479000000000	40.4186000000000
135 H	44.2308000000000	30.5884000000000	39.8408000000000
136 C	43.8698000000000	31.1865000000000	41.7254000000000
137 H	44.7366000000000	30.9850000000000	42.0580000000000
138 C	42.8963000000000	31.7315000000000	42.5809000000000
139 H	43.1209000000000	31.8810000000000	43.4918000000000
140 C	41.6218000000000	32.0589000000000	42.1468000000000
141 C	41.2804000000000	31.7853000000000	40.7801000000000
142 C	37.6840000000000	33.7638000000000	40.4609000000000
143 C	38.2690000000000	35.0076000000000	40.2582000000000
144 H	39.1620000000000	35.1667000000000	40.5407000000000
145 C	37.5412000000000	36.0190000000000	39.6395000000000
146 H	37.9300000000000	36.8770000000000	39.5159000000000
147 C	36.2492000000000	35.7743000000000	39.2040000000000
148 H	35.7588000000000	36.4633000000000	38.7712000000000
149 C	35.6738000000000	34.5454000000000	39.3932000000000
150 H	34.7888000000000	34.3854000000000	39.0869000000000
151 C	36.3811000000000	33.5285000000000	40.0333000000000
152 H	35.9763000000000	32.6810000000000	40.1766000000000
153 I	35.0566000000000	24.1096000000000	35.2138000000000
154 C	35.6399000000000	25.6189000000000	36.5453000000000
155 C	36.8079000000000	25.5404000000000	37.2772000000000

156 C	37.198100000000	26.544200000000	38.134300000000
157 F	37.617100000000	24.466600000000	37.147100000000
158 F	38.362200000000	26.408300000000	38.794600000000
159 I	37.015500000000	29.192300000000	39.639600000000
160 C	36.432300000000	27.683000000000	38.308100000000
161 C	35.264200000000	27.761500000000	37.576200000000
162 C	34.874000000000	26.757600000000	36.719100000000
163 F	34.455000000000	28.835300000000	37.706300000000
164 F	33.709900000000	26.893600000000	36.058600000000

Dim¹(PO)-A...(N)Dim¹, Dim¹(N)-A...(OP)Dim¹

1 P	42.110100000000	29.787300000000	46.092200000000
2 O	43.018600000000	30.960300000000	45.897200000000
3 C	41.356100000000	29.225900000000	44.555500000000
4 N	42.239100000000	28.647700000000	43.708000000000
5 C	41.805800000000	28.301200000000	42.503300000000
6 H	42.414900000000	27.885200000000	41.904400000000
7 C	40.503800000000	28.519200000000	42.078700000000
8 H	40.233200000000	28.267700000000	41.203400000000
9 C	39.612200000000	29.104100000000	42.943300000000
10 H	38.714900000000	29.248700000000	42.666900000000
11 C	40.015500000000	29.492600000000	44.237700000000
12 C	40.684400000000	30.159700000000	47.113500000000
13 C	40.930100000000	30.398400000000	48.450000000000
14 H	41.784900000000	30.194200000000	48.811000000000
15 C	39.940200000000	30.937500000000	49.285700000000
16 H	40.123800000000	31.103100000000	50.202900000000
17 C	38.715100000000	31.220200000000	48.768100000000
18 H	38.053500000000	31.605700000000	49.330400000000
19 C	38.399500000000	30.955600000000	47.414600000000
20 C	37.110500000000	31.237500000000	46.910400000000
21 H	36.447700000000	31.597100000000	47.488100000000
22 C	36.808600000000	30.999000000000	45.603600000000
23 H	35.941800000000	31.200400000000	45.271000000000
24 C	37.782200000000	30.453900000000	44.748100000000
25 H	37.557600000000	30.304500000000	43.837100000000
26 C	39.056600000000	30.126500000000	45.182100000000
27 C	39.398000000000	30.400200000000	46.548800000000
28 C	42.994500000000	28.421700000000	46.868100000000
29 C	42.409500000000	27.177900000000	47.070800000000
30 H	41.516500000000	27.018700000000	46.788200000000
31 C	43.137300000000	26.166500000000	47.689500000000
32 H	42.748500000000	25.308500000000	47.813100000000
33 C	44.429300000000	26.411200000000	48.125000000000
34 H	44.919700000000	25.722200000000	48.557800000000
35 C	45.004700000000	27.640100000000	47.935700000000
36 H	45.889600000000	27.800100000000	48.242000000000
37 C	44.297400000000	28.657000000000	47.295600000000
38 H	44.702100000000	29.504500000000	47.152400000000
39 P	38.568400000000	32.398200000000	41.236700000000
40 O	37.659900000000	31.225200000000	41.431700000000
41 C	39.322300000000	32.959600000000	42.773500000000
42 N	38.439400000000	33.537800000000	43.620900000000
43 C	38.872600000000	33.884300000000	44.825700000000

44 H	38.2636000000000	34.3002000000000	45.4245000000000
45 C	40.1746000000000	33.6663000000000	45.2503000000000
46 H	40.4453000000000	33.9178000000000	46.1255000000000
47 C	41.0663000000000	33.0813000000000	44.3857000000000
48 H	41.9636000000000	32.9368000000000	44.6620000000000
49 C	40.6630000000000	32.6929000000000	43.0912000000000
50 C	39.9941000000000	32.0258000000000	40.2155000000000
51 C	39.7483000000000	31.7871000000000	38.8790000000000
52 H	38.8936000000000	31.9913000000000	38.5179000000000
53 C	40.7383000000000	31.2480000000000	38.0432000000000
54 H	40.5546000000000	31.0824000000000	37.1260000000000
55 C	41.9633000000000	30.9653000000000	38.5609000000000
56 H	42.6250000000000	30.5798000000000	37.9986000000000
57 C	42.2790000000000	31.2299000000000	39.9143000000000
58 C	43.5679000000000	30.9479000000000	40.4186000000000
59 H	44.2308000000000	30.5884000000000	39.8408000000000
60 C	43.8698000000000	31.1865000000000	41.7254000000000
61 H	44.7366000000000	30.9850000000000	42.0580000000000
62 C	42.8963000000000	31.7315000000000	42.5809000000000
63 H	43.1209000000000	31.8810000000000	43.4918000000000
64 C	41.6218000000000	32.0589000000000	42.1468000000000
65 C	41.2804000000000	31.7853000000000	40.7801000000000
66 C	37.6840000000000	33.7638000000000	40.4609000000000
67 C	38.2690000000000	35.0076000000000	40.2582000000000
68 H	39.1620000000000	35.1667000000000	40.5407000000000
69 C	37.5412000000000	36.0190000000000	39.6395000000000
70 H	37.9300000000000	36.8770000000000	39.5159000000000
71 C	36.2492000000000	35.7743000000000	39.2040000000000
72 H	35.7588000000000	36.4633000000000	38.7712000000000
73 C	35.6738000000000	34.5454000000000	39.3932000000000
74 H	34.7888000000000	34.3854000000000	39.0869000000000
75 C	36.3811000000000	33.5285000000000	40.0333000000000
76 H	35.9763000000000	32.6810000000000	40.1766000000000
77 I	35.0566000000000	24.1096000000000	35.2138000000000
78 C	35.6399000000000	25.6189000000000	36.5453000000000
79 C	36.8079000000000	25.5404000000000	37.2772000000000
80 C	37.1981000000000	26.5442000000000	38.1343000000000
81 F	37.6171000000000	24.4666000000000	37.1471000000000
82 F	38.3622000000000	26.4083000000000	38.7946000000000
83 I	37.0155000000000	29.1923000000000	39.6396000000000
84 C	36.4323000000000	27.6830000000000	38.3081000000000
85 C	35.2642000000000	27.7615000000000	37.5762000000000
86 C	34.8740000000000	26.7576000000000	36.7191000000000
87 F	34.4550000000000	28.8353000000000	37.7063000000000
88 F	33.7099000000000	26.8936000000000	36.0586000000000
89 P	33.4756000000000	16.4385000000000	32.3339000000000
90 O	34.2783000000000	16.7442000000000	31.1085000000000
91 C	32.0076000000000	17.4719000000000	32.4821000000000
92 N	31.0614000000000	17.1907000000000	31.5560000000000
93 C	29.9891000000000	17.9699000000000	31.5092000000000
94 H	29.3140000000000	17.7749000000000	30.8698000000000
95 C	29.8094000000000	19.0566000000000	32.3517000000000
96 H	29.0327000000000	19.5992000000000	32.2805000000000
97 C	30.7715000000000	19.3358000000000	33.2903000000000
98 H	30.6540000000000	20.0714000000000	33.8798000000000
99 C	31.9325000000000	18.5412000000000	33.3879000000000

100 C	34.353000000000	16.785500000000	33.858300000000
101 C	35.420900000000	15.963600000000	34.154700000000
102 H	35.546700000000	15.164300000000	33.656900000000
103 C	36.324600000000	16.287300000000	35.178300000000
104 H	37.059500000000	15.716100000000	35.368400000000
105 C	36.136500000000	17.427200000000	35.894900000000
106 H	36.762000000000	17.655700000000	36.572600000000
107 C	35.034600000000	18.282400000000	35.658400000000
108 C	34.851600000000	19.447900000000	36.434900000000
109 H	35.467500000000	19.652600000000	37.128600000000
110 C	33.800400000000	20.281700000000	36.198600000000
111 H	33.690600000000	21.068400000000	36.719800000000
112 C	32.878500000000	19.975800000000	35.182200000000
113 H	32.157800000000	20.574300000000	35.024000000000
114 C	32.980500000000	18.835300000000	34.402000000000
115 C	34.099400000000	17.963400000000	34.619700000000
116 C	32.999100000000	14.700400000000	32.363000000000
117 C	32.164400000000	14.175500000000	33.342000000000
118 H	31.814100000000	14.738500000000	34.022400000000
119 C	31.844100000000	12.821900000000	33.321300000000
120 H	31.258500000000	12.462000000000	33.977200000000
121 C	32.379300000000	11.999300000000	32.343800000000
122 H	32.168200000000	11.073000000000	32.339200000000
123 C	33.211000000000	12.512400000000	31.383500000000
124 H	33.577000000000	11.939500000000	30.719900000000
125 C	33.522500000000	13.871400000000	31.375900000000
126 H	34.088100000000	14.228800000000	30.701400000000
127 P	32.084200000000	22.841500000000	32.374200000000
128 O	31.281500000000	22.535700000000	33.599600000000
129 C	33.552300000000	21.808000000000	32.226100000000
130 N	34.498500000000	22.089200000000	33.152100000000
131 C	35.570800000000	21.310000000000	33.198900000000
132 H	36.245800000000	21.505100000000	33.838300000000
133 C	35.750500000000	20.223300000000	32.356400000000
134 H	36.527100000000	19.680800000000	32.427500000000
135 C	34.788400000000	19.944100000000	31.417800000000
136 H	34.905900000000	19.208500000000	30.828300000000
137 C	33.627300000000	20.738800000000	31.320300000000
138 C	31.206900000000	22.494400000000	30.849800000000
139 C	30.139000000000	23.316300000000	30.553400000000
140 H	30.013100000000	24.115700000000	31.051300000000
141 C	29.235300000000	22.992700000000	29.529800000000
142 H	28.500400000000	23.563900000000	29.339600000000
143 C	29.423400000000	21.852700000000	28.813200000000
144 H	28.798000000000	21.624300000000	28.135500000000
145 C	30.525300000000	20.997600000000	29.049700000000
146 C	30.708400000000	19.831900000000	28.273300000000
147 H	30.092400000000	19.627400000000	27.579600000000
148 C	31.759500000000	18.998200000000	28.509500000000
149 H	31.869300000000	18.211500000000	27.988300000000
150 C	32.681400000000	19.304100000000	29.526000000000
151 H	33.402000000000	18.705700000000	29.684100000000
152 C	32.579300000000	20.444700000000	30.306100000000
153 C	31.460500000000	21.316500000000	30.088400000000
154 C	32.560800000000	24.579600000000	32.345200000000
155 C	33.395500000000	25.104400000000	31.366100000000
156 H	33.745700000000	24.541500000000	30.685600000000

157 C	33.715800000000	26.458000000000	31.386900000000
158 H	34.301500000000	26.817900000000	30.730900000000
159 C	33.180700000000	27.280700000000	32.364400000000
160 H	33.391800000000	28.206900000000	32.368900000000
161 C	32.348900000000	26.767600000000	33.324600000000
162 H	31.982900000000	27.340400000000	33.988200000000
163 C	32.037300000000	25.408600000000	33.332300000000
164 H	31.471800000000	25.051100000000	34.006700000000

Dim¹(N)-A...(N)Dim¹

1 P	42.110100000000	29.787300000000	46.092200000000
2 O	43.018600000000	30.960300000000	45.897200000000
3 C	41.356100000000	29.225900000000	44.555500000000
4 N	42.239100000000	28.647700000000	43.708000000000
5 C	41.805800000000	28.301200000000	42.503300000000
6 H	42.414900000000	27.885200000000	41.904400000000
7 C	40.503800000000	28.519200000000	42.078700000000
8 H	40.233200000000	28.267700000000	41.203400000000
9 C	39.612200000000	29.104100000000	42.943300000000
10 H	38.714900000000	29.248700000000	42.666900000000
11 C	40.015500000000	29.492600000000	44.237700000000
12 C	40.684400000000	30.159700000000	47.113500000000
13 C	40.930100000000	30.398400000000	48.450000000000
14 H	41.784900000000	30.194200000000	48.811000000000
15 C	39.940200000000	30.937500000000	49.285700000000
16 H	40.123800000000	31.103100000000	50.202900000000
17 C	38.715100000000	31.220200000000	48.768100000000
18 H	38.053500000000	31.605700000000	49.330400000000
19 C	38.399500000000	30.955600000000	47.414600000000
20 C	37.110500000000	31.237500000000	46.910400000000
21 H	36.447700000000	31.597100000000	47.488100000000
22 C	36.808600000000	30.999000000000	45.603600000000
23 H	35.941800000000	31.200400000000	45.271000000000
24 C	37.782200000000	30.453900000000	44.748100000000
25 H	37.557600000000	30.304500000000	43.837100000000
26 C	39.056600000000	30.126500000000	45.182100000000
27 C	39.398000000000	30.400200000000	46.548800000000
28 C	42.994500000000	28.421700000000	46.868100000000
29 C	42.409500000000	27.177900000000	47.070800000000
30 H	41.516500000000	27.018700000000	46.788200000000
31 C	43.137300000000	26.166500000000	47.689500000000
32 H	42.748500000000	25.308500000000	47.813100000000
33 C	44.429300000000	26.411200000000	48.125000000000
34 H	44.919700000000	25.722200000000	48.557800000000
35 C	45.004700000000	27.640100000000	47.935700000000
36 H	45.889600000000	27.800100000000	48.242000000000
37 C	44.297400000000	28.657000000000	47.295600000000
38 H	44.702100000000	29.504500000000	47.152400000000
39 P	57.869200000000	20.130800000000	46.092200000000
40 O	58.777800000000	21.303800000000	45.897200000000
41 C	57.115300000000	19.569300000000	44.555500000000
42 N	57.998200000000	18.991200000000	43.708000000000
43 C	57.565000000000	18.644700000000	42.503300000000
44 H	58.174000000000	18.228700000000	41.904400000000

45 C	56.263000000000	18.862700000000	42.078700000000
46 H	55.992300000000	18.611200000000	41.203400000000
47 C	55.371400000000	19.447600000000	42.943300000000
48 H	54.474100000000	19.592200000000	42.666900000000
49 C	55.774600000000	19.836000000000	44.237700000000
50 C	56.443600000000	20.503100000000	47.113500000000
51 C	56.689300000000	20.741900000000	48.450000000000
52 H	57.544000000000	20.537700000000	48.811000000000
53 C	55.699300000000	21.281000000000	49.285700000000
54 H	55.883000000000	21.446600000000	50.202900000000
55 C	54.474300000000	21.563600000000	48.768100000000
56 H	53.812600000000	21.949200000000	49.330400000000
57 C	54.158600000000	21.299100000000	47.414600000000
58 C	52.869700000000	21.581000000000	46.910400000000
59 H	52.206800000000	21.940600000000	47.488100000000
60 C	52.567800000000	21.342400000000	45.603600000000
61 H	51.701000000000	21.543900000000	45.271000000000
62 C	53.541300000000	20.797400000000	44.748100000000
63 H	53.316700000000	20.648000000000	43.837100000000
64 C	54.815800000000	20.470000000000	45.182100000000
65 C	55.157200000000	20.743700000000	46.548800000000
66 C	58.753600000000	18.765200000000	46.868100000000
67 C	58.168600000000	17.521300000000	47.070800000000
68 H	57.275600000000	17.362200000000	46.788200000000
69 C	58.896500000000	16.510000000000	47.689500000000
70 H	58.507600000000	15.652000000000	47.813100000000
71 C	60.188400000000	16.754700000000	48.125000000000
72 H	60.678800000000	16.065700000000	48.557800000000
73 C	60.763800000000	17.983600000000	47.935700000000
74 H	61.648800000000	18.143500000000	48.242000000000
75 C	60.056500000000	19.000500000000	47.295600000000
76 H	60.461300000000	19.847900000000	47.152400000000
77 P	38.568400000000	32.398200000000	41.236700000000
78 O	37.659900000000	31.225200000000	41.431700000000
79 C	39.322300000000	32.959600000000	42.773500000000
80 N	38.439400000000	33.537800000000	43.620900000000
81 C	38.872600000000	33.884300000000	44.825700000000
82 H	38.263600000000	34.300200000000	45.424500000000
83 C	40.174600000000	33.666300000000	45.250300000000
84 H	40.445300000000	33.917800000000	46.125500000000
85 C	41.066300000000	33.081300000000	44.385700000000
86 H	41.963600000000	32.936800000000	44.662000000000
87 C	40.663000000000	32.692900000000	43.091200000000
88 C	39.994100000000	32.025800000000	40.215500000000
89 C	39.748300000000	31.787100000000	38.879000000000
90 H	38.893600000000	31.991300000000	38.517900000000
91 C	40.738300000000	31.248000000000	38.043200000000
92 H	40.554600000000	31.082400000000	37.126000000000
93 C	41.963300000000	30.965300000000	38.560900000000
94 H	42.625000000000	30.579800000000	37.998600000000
95 C	42.279000000000	31.229900000000	39.914300000000
96 C	43.567900000000	30.947900000000	40.418600000000
97 H	44.230800000000	30.588400000000	39.840800000000
98 C	43.869800000000	31.186500000000	41.725400000000
99 H	44.736600000000	30.985000000000	42.058000000000
100 C	42.896300000000	31.731500000000	42.580900000000
101 H	43.120900000000	31.881000000000	43.491800000000

102 C	41.6218000000000	32.0589000000000	42.1468000000000
103 C	41.2804000000000	31.7853000000000	40.7801000000000
104 C	37.6840000000000	33.7638000000000	40.4609000000000
105 C	38.2690000000000	35.0076000000000	40.2582000000000
106 H	39.1620000000000	35.1667000000000	40.5407000000000
107 C	37.5412000000000	36.0190000000000	39.6395000000000
108 H	37.9300000000000	36.8770000000000	39.5159000000000
109 C	36.2492000000000	35.7743000000000	39.2040000000000
110 H	35.7588000000000	36.4633000000000	38.7712000000000
111 C	35.6738000000000	34.5454000000000	39.3932000000000
112 H	34.7888000000000	34.3854000000000	39.0869000000000
113 C	36.3811000000000	33.5285000000000	40.0333000000000
114 H	35.9763000000000	32.6810000000000	40.1766000000000
115 P	54.3275000000000	22.7416000000000	41.2367000000000
116 O	53.4190000000000	21.5686000000000	41.4317000000000
117 C	55.0815000000000	23.3031000000000	42.7735000000000
118 N	54.1986000000000	23.8812000000000	43.6209000000000
119 C	54.6318000000000	24.2277000000000	44.8257000000000
120 H	54.0228000000000	24.6437000000000	45.4245000000000
121 C	55.9338000000000	24.0097000000000	45.2503000000000
122 H	56.2045000000000	24.2612000000000	46.1255000000000
123 C	56.8254000000000	23.4248000000000	44.3857000000000
124 H	57.7227000000000	23.2802000000000	44.6620000000000
125 C	56.4221000000000	23.0364000000000	43.0912000000000
126 C	55.7532000000000	22.3693000000000	40.2155000000000
127 C	55.5075000000000	22.1305000000000	38.8790000000000
128 H	54.6527000000000	22.3347000000000	38.5179000000000
129 C	56.4975000000000	21.5914000000000	38.0432000000000
130 H	56.3138000000000	21.4259000000000	37.1260000000000
131 C	57.7225000000000	21.3088000000000	38.5609000000000
132 H	58.3841000000000	20.9233000000000	37.9986000000000
133 C	58.0382000000000	21.5733000000000	39.9143000000000
134 C	59.3271000000000	21.2914000000000	40.4186000000000
135 H	59.9899000000000	20.9319000000000	39.8408000000000
136 C	59.6290000000000	21.5300000000000	41.7254000000000
137 H	60.4958000000000	21.3285000000000	42.0580000000000
138 C	58.6554000000000	22.0750000000000	42.5809000000000
139 H	58.8800000000000	22.2244000000000	43.4918000000000
140 C	57.3810000000000	22.4024000000000	42.1468000000000
141 C	57.0396000000000	22.1287000000000	40.7801000000000
142 C	53.4431000000000	24.1072000000000	40.4609000000000
143 C	54.0282000000000	25.3511000000000	40.2582000000000
144 H	54.9212000000000	25.5102000000000	40.5407000000000
145 C	53.3003000000000	26.3624000000000	39.6395000000000
146 H	53.6892000000000	27.2204000000000	39.5159000000000
147 C	52.0083000000000	26.1178000000000	39.2040000000000
148 H	51.5180000000000	26.8067000000000	38.7712000000000
149 C	51.4329000000000	24.8888000000000	39.3932000000000
150 H	50.5480000000000	24.7289000000000	39.0869000000000
151 C	52.1402000000000	23.8719000000000	40.0333000000000
152 H	51.7355000000000	23.0245000000000	40.1766000000000
153 I	45.0516000000000	27.7681000000000	43.6968000000000
154 C	46.9543000000000	26.9008000000000	43.6528000000000
155 C	47.4544000000000	26.2573000000000	42.5354000000000
156 C	48.6891000000000	25.6405000000000	42.5381000000000
157 F	46.7289000000000	26.1987000000000	41.4035000000000

158 F	49.1093000000000	25.0465000000000	41.4158000000000
159 I	51.3859000000000	24.7608000000000	43.6322000000000
160 C	49.4833000000000	25.6282000000000	43.6762000000000
161 C	48.9833000000000	26.2718000000000	44.7935000000000
162 C	47.7486000000000	26.8884000000000	44.7909000000000
163 F	49.7087000000000	26.3303000000000	45.9254000000000
164 F	47.3283000000000	27.4825000000000	45.9132000000000

Dim²(PO)-A...(OP)Dim²

1 P	5.3879000000000	34.2756000000000	48.2457000000000
2 O	4.6081000000000	35.3515000000000	48.9212000000000
3 C	4.4790000000000	32.7655000000000	47.9572000000000
4 C	3.9888000000000	32.1233000000000	49.0799000000000
5 H	4.2056000000000	32.4614000000000	49.9408000000000
6 C	3.1795000000000	30.9846000000000	48.9743000000000
7 H	2.8440000000000	30.5625000000000	49.7565000000000
8 C	2.8783000000000	30.4895000000000	47.7503000000000
9 H	2.3335000000000	29.7141000000000	47.6843000000000
10 C	3.3597000000000	31.1048000000000	46.5603000000000
11 C	3.0370000000000	30.5609000000000	45.2977000000000
12 H	2.4926000000000	29.7843000000000	45.2421000000000
13 C	3.5004000000000	31.1417000000000	44.1665000000000
14 H	3.2793000000000	30.7716000000000	43.3200000000000
15 C	4.3074000000000	32.2903000000000	44.2387000000000
16 H	4.6167000000000	32.6822000000000	43.4304000000000
17 C	4.6686000000000	32.8716000000000	45.4388000000000
18 C	4.1859000000000	32.2700000000000	46.6545000000000
19 C	5.9371000000000	34.7342000000000	46.6035000000000
20 C	5.5376000000000	34.0687000000000	45.4311000000000
21 C	6.0300000000000	34.6201000000000	44.2297000000000
22 H	5.8004000000000	34.2197000000000	43.3993000000000
23 C	6.8416000000000	35.7349000000000	44.2492000000000
24 H	7.1511000000000	36.0743000000000	43.4177000000000
25 N	7.2200000000000	36.3676000000000	45.3622000000000
26 C	6.7654000000000	35.8573000000000	46.5029000000000
27 H	7.0223000000000	36.2875000000000	47.3099000000000
28 C	6.8731000000000	33.8633000000000	49.1734000000000
29 C	7.4548000000000	34.8538000000000	49.9641000000000
30 H	7.0296000000000	35.6994000000000	50.0457000000000
31 C	8.6406000000000	34.6199000000000	50.6291000000000
32 H	9.0296000000000	35.3010000000000	51.1650000000000
33 C	9.2589000000000	33.3920000000000	50.5123000000000
34 H	10.0805000000000	33.2319000000000	50.9616000000000
35 C	8.6878000000000	32.3914000000000	49.7430000000000
36 H	9.1117000000000	31.5439000000000	49.6756000000000
37 C	7.5010000000000	32.6256000000000	49.0732000000000
38 H	7.1131000000000	31.9394000000000	48.5430000000000
39 P	0.1858000000000	44.2652000000000	61.2022000000000
40 O	-0.5940000000000	45.3411000000000	61.8778000000000
41 C	-0.7232000000000	42.7551000000000	60.9137000000000
42 C	-1.2133000000000	42.1129000000000	62.0364000000000
43 H	-0.9965000000000	42.4511000000000	62.8973000000000
44 C	-2.0226000000000	40.9743000000000	61.9309000000000
45 H	-2.3581000000000	40.5521000000000	62.7130000000000

46 C	-2.3238000000000	40.4792000000000	60.7068000000000
47 H	-2.8686000000000	39.7037000000000	60.6408000000000
48 C	-1.8424000000000	41.0945000000000	59.5168000000000
49 C	-2.1651000000000	40.5505000000000	58.2542000000000
50 H	-2.7095000000000	39.7740000000000	58.1986000000000
51 C	-1.7017000000000	41.1314000000000	57.1230000000000
52 H	-1.9228000000000	40.7612000000000	56.2765000000000
53 C	-0.8947000000000	42.2799000000000	57.1952000000000
54 H	-0.5854000000000	42.6719000000000	56.3870000000000
55 C	-0.5335000000000	42.8612000000000	58.3953000000000
56 C	-1.0162000000000	42.2597000000000	59.6110000000000
57 C	0.7350000000000	44.7239000000000	59.5600000000000
58 C	0.3355000000000	44.0583000000000	58.3876000000000
59 C	0.8279000000000	44.6097000000000	57.1862000000000
60 H	0.5983000000000	44.2094000000000	56.3559000000000
61 C	1.6395000000000	45.7246000000000	57.2058000000000
62 H	1.9490000000000	46.0640000000000	56.3742000000000
63 N	2.0179000000000	46.3572000000000	58.3187000000000
64 C	1.5633000000000	45.8469000000000	59.4594000000000
65 H	1.8202000000000	46.2772000000000	60.2665000000000
66 C	1.6710000000000	43.8529000000000	62.1299000000000
67 C	2.2527000000000	44.8434000000000	62.9206000000000
68 H	1.8275000000000	45.6890000000000	63.0022000000000
69 C	3.4385000000000	44.6095000000000	63.5856000000000
70 H	3.8275000000000	45.2907000000000	64.1216000000000
71 C	4.0568000000000	43.3816000000000	63.4688000000000
72 H	4.8784000000000	43.2216000000000	63.9181000000000
73 C	3.4857000000000	42.3810000000000	62.6995000000000
74 H	3.9096000000000	41.5335000000000	62.6321000000000
75 C	2.2989000000000	42.6153000000000	62.0297000000000
76 H	1.9110000000000	41.9291000000000	61.4995000000000
77 P	2.6979000000000	35.6520000000000	42.4499000000000
78 O	3.4776000000000	34.5761000000000	41.7744000000000
79 C	3.6068000000000	37.1622000000000	42.7384000000000
80 C	4.0970000000000	37.8044000000000	41.6157000000000
81 H	3.8802000000000	37.4662000000000	40.7548000000000
82 C	4.9063000000000	38.9430000000000	41.7213000000000
83 H	5.2418000000000	39.3651000000000	40.9391000000000
84 C	5.2075000000000	39.4381000000000	42.9453000000000
85 H	5.7523000000000	40.2135000000000	43.0113000000000
86 C	4.7261000000000	38.8228000000000	44.1353000000000
87 C	5.0488000000000	39.3668000000000	45.3979000000000
88 H	5.5932000000000	40.1433000000000	45.4536000000000
89 C	4.5854000000000	38.7859000000000	46.5291000000000
90 H	4.8065000000000	39.1561000000000	47.3756000000000
91 C	3.7783000000000	37.6374000000000	46.4569000000000
92 H	3.4691000000000	37.2454000000000	47.2652000000000
93 C	3.4172000000000	37.0560000000000	45.2568000000000
94 C	3.8998000000000	37.6576000000000	44.0411000000000
95 C	2.1487000000000	35.1934000000000	44.0921000000000
96 C	2.5482000000000	35.8590000000000	45.2646000000000
97 C	2.0558000000000	35.3075000000000	46.4659000000000
98 H	2.2854000000000	35.7079000000000	47.2963000000000
99 C	1.2442000000000	34.1927000000000	46.4464000000000
100 H	0.9347000000000	33.8533000000000	47.2779000000000
101 N	0.8658000000000	33.5600000000000	45.3334000000000

102	C	1.3204000000000	34.0704000000000	44.1928000000000
103	H	1.0635000000000	33.6401000000000	43.3857000000000
104	C	1.2127000000000	36.0643000000000	41.5222000000000
105	C	0.6310000000000	35.0738000000000	40.7315000000000
106	H	1.0561000000000	34.2282000000000	40.6499000000000
107	C	-0.5548000000000	35.3078000000000	40.0665000000000
108	H	-0.9438000000000	34.6266000000000	39.5306000000000
109	C	-1.1732000000000	36.5356000000000	40.1833000000000
110	H	-1.9947000000000	36.6957000000000	39.7340000000000
111	C	-0.6020000000000	37.5362000000000	40.9526000000000
112	H	-1.0259000000000	38.3837000000000	41.0200000000000
113	C	0.5848000000000	37.3020000000000	41.6224000000000
114	H	0.9727000000000	37.9882000000000	42.1526000000000
115	P	-2.5042000000000	45.6417000000000	55.4064000000000
116	O	-1.7245000000000	44.5658000000000	54.7309000000000
117	C	-1.5953000000000	47.1518000000000	55.6950000000000
118	C	-1.1051000000000	47.7940000000000	54.5722000000000
119	H	-1.3219000000000	47.4558000000000	53.7113000000000
120	C	-0.2958000000000	48.9326000000000	54.6778000000000
121	H	0.0397000000000	49.3548000000000	53.8956000000000
122	C	0.0054000000000	49.4277000000000	55.9018000000000
123	H	0.5502000000000	50.2032000000000	55.9678000000000
124	C	-0.4760000000000	48.8124000000000	57.0918000000000
125	C	-0.1533000000000	49.3564000000000	58.3545000000000
126	H	0.3911000000000	50.1330000000000	58.4101000000000
127	C	-0.6167000000000	48.7756000000000	59.4856000000000
128	H	-0.3956000000000	49.1457000000000	60.3321000000000
129	C	-1.4238000000000	47.6270000000000	59.4134000000000
130	H	-1.7330000000000	47.2351000000000	60.2217000000000
131	C	-1.7849000000000	47.0457000000000	58.2134000000000
132	C	-1.3023000000000	47.6473000000000	56.9976000000000
133	C	-3.0534000000000	45.1830000000000	57.0486000000000
134	C	-2.6539000000000	45.8486000000000	58.2211000000000
135	C	-3.1463000000000	45.2972000000000	59.4224000000000
136	H	-2.9167000000000	45.6976000000000	60.2528000000000
137	C	-3.9579000000000	44.1823000000000	59.4029000000000
138	H	-4.2674000000000	43.8429000000000	60.2345000000000
139	N	-4.3363000000000	43.5497000000000	58.2900000000000
140	C	-3.8817000000000	44.0600000000000	57.1493000000000
141	H	-4.1386000000000	43.6298000000000	56.3422000000000
142	C	-3.9894000000000	46.0540000000000	54.4787000000000
143	C	-4.5711000000000	45.0635000000000	53.6881000000000
144	H	-4.1460000000000	44.2179000000000	53.6064000000000
145	C	-5.7569000000000	45.2974000000000	53.0230000000000
146	H	-6.1459000000000	44.6163000000000	52.4871000000000
147	C	-6.3753000000000	46.5253000000000	53.1399000000000
148	H	-7.1968000000000	46.6854000000000	52.6905000000000
149	C	-5.8041000000000	47.5259000000000	53.9091000000000
150	H	-6.2280000000000	48.3734000000000	53.9765000000000
151	C	-4.6173000000000	47.2917000000000	54.5789000000000
152	H	-4.2294000000000	47.9779000000000	55.1091000000000
153	I	3.1899000000000	37.2650000000000	50.4232000000000
154	C	2.1520000000000	38.8671000000000	51.2808000000000
155	C	2.3548000000000	40.1626000000000	50.8336000000000
156	C	1.6669000000000	41.2275000000000	51.3628000000000
157	F	3.2518000000000	40.3986000000000	49.8583000000000
158	F	1.9209000000000	42.4596000000000	50.8886000000000

159 I	-0.306200000000	42.652300000000	53.228900000000
160 C	0.731700000000	41.050200000000	52.371400000000
161 C	0.528900000000	39.754700000000	52.818600000000
162 C	1.216700000000	38.689800000000	52.289300000000
163 F	-0.368200000000	39.518700000000	53.793900000000
164 F	0.962800000000	37.457700000000	52.763600000000

Dim²(PO)-A··(N)Dim², Dim²(N)-A··(OP)Dim²

1 P	-8.933500000000	21.542600000000	48.245700000000
2 O	-9.713200000000	22.618500000000	48.921200000000
3 C	-9.842400000000	20.032500000000	47.957200000000
4 C	-10.332500000000	19.390200000000	49.079900000000
5 H	-10.115700000000	19.728400000000	49.940800000000
6 C	-11.141800000000	18.251600000000	48.974300000000
7 H	-11.477300000000	17.829500000000	49.756500000000
8 C	-11.443000000000	17.756500000000	47.750300000000
9 H	-11.987800000000	16.981100000000	47.684300000000
10 C	-10.961600000000	18.371800000000	46.560300000000
11 C	-11.284300000000	17.827900000000	45.297700000000
12 H	-11.828700000000	17.051300000000	45.242100000000
13 C	-10.820900000000	18.408700000000	44.166500000000
14 H	-11.042000000000	18.038500000000	43.320000000000
15 C	-10.013900000000	19.557200000000	44.238700000000
16 H	-9.704600000000	19.949200000000	43.430400000000
17 C	-9.652700000000	20.138600000000	45.438800000000
18 C	-10.135400000000	19.537000000000	46.654500000000
19 C	-8.384200000000	22.001200000000	46.603500000000
20 C	-8.783700000000	21.335700000000	45.431100000000
21 C	-8.291300000000	21.887100000000	44.229700000000
22 H	-8.520900000000	21.486700000000	43.399300000000
23 C	-7.479700000000	23.001900000000	44.249200000000
24 H	-7.170200000000	23.341300000000	43.417700000000
25 N	-7.101300000000	23.634600000000	45.362200000000
26 C	-7.555900000000	23.124300000000	46.502900000000
27 H	-7.299000000000	23.554500000000	47.309900000000
28 C	-7.448200000000	21.130300000000	49.173400000000
29 C	-6.866500000000	22.120800000000	49.964100000000
30 H	-7.291700000000	22.966400000000	50.045700000000
31 C	-5.680700000000	21.886800000000	50.629100000000
32 H	-5.291700000000	22.568000000000	51.165000000000
33 C	-5.062400000000	20.659000000000	50.512300000000
34 H	-4.240800000000	20.498900000000	50.961600000000
35 C	-5.633500000000	19.658400000000	49.743000000000
36 H	-5.209600000000	18.810900000000	49.675600000000
37 C	-6.820300000000	19.892600000000	49.073200000000
38 H	-7.208200000000	19.206400000000	48.543000000000
39 P	-11.623400000000	22.919000000000	42.449900000000
40 O	-10.843700000000	21.843100000000	41.774400000000
41 C	-10.714500000000	24.429200000000	42.738400000000
42 C	-10.224300000000	25.071400000000	41.615700000000
43 H	-10.441100000000	24.733200000000	40.754800000000
44 C	-9.415000000000	26.210000000000	41.721300000000
45 H	-9.079600000000	26.632100000000	40.939100000000
46 C	-9.113800000000	26.705100000000	42.945300000000

47 H	-8.569000000000	27.480500000000	43.011300000000
48 C	-9.595200000000	26.089800000000	44.135300000000
49 C	-9.272500000000	26.633800000000	45.397900000000
50 H	-8.728100000000	27.410300000000	45.453600000000
51 C	-9.735900000000	26.052900000000	46.529100000000
52 H	-9.514800000000	26.423100000000	47.375600000000
53 C	-10.543000000000	24.904400000000	46.456900000000
54 H	-10.852200000000	24.512400000000	47.265200000000
55 C	-10.904200000000	24.323000000000	45.256800000000
56 C	-10.421500000000	24.924600000000	44.041100000000
57 C	-12.172600000000	22.460400000000	44.092100000000
58 C	-11.773200000000	23.125900000000	45.264600000000
59 C	-12.265500000000	22.574500000000	46.465900000000
60 H	-12.035900000000	22.974900000000	47.296300000000
61 C	-13.077100000000	21.459700000000	46.446400000000
62 H	-13.386600000000	21.120300000000	47.277900000000
63 N	-13.455500000000	20.827000000000	45.333400000000
64 C	-13.000900000000	21.337400000000	44.192800000000
65 H	-13.257900000000	20.907100000000	43.385700000000
66 C	-13.108600000000	23.331300000000	41.522200000000
67 C	-13.690300000000	22.340800000000	40.731500000000
68 H	-13.265200000000	21.495200000000	40.649900000000
69 C	-14.876100000000	22.574800000000	40.066500000000
70 H	-15.265100000000	21.893600000000	39.530600000000
71 C	-15.494500000000	23.802600000000	40.183300000000
72 H	-16.316100000000	23.962700000000	39.734000000000
73 C	-14.923300000000	24.803200000000	40.952600000000
74 H	-15.347300000000	25.650700000000	41.020000000000
75 C	-13.736500000000	24.569000000000	41.622400000000
76 H	-13.348600000000	25.255200000000	42.152600000000
77 P	1.784800000000	34.639600000000	45.834400000000
78 O	0.824900000000	33.504000000000	45.729700000000
79 C	1.522400000000	35.948900000000	44.648400000000
80 C	1.619200000000	35.594000000000	43.315000000000
81 H	1.881400000000	34.709900000000	43.087000000000
82 C	1.338900000000	36.511000000000	42.293600000000
83 H	1.401400000000	36.246300000000	41.383300000000
84 C	0.978200000000	37.776900000000	42.611900000000
85 H	0.794300000000	38.396300000000	41.915500000000
86 C	0.868300000000	38.200400000000	43.966500000000
87 C	0.498900000000	39.529500000000	44.268500000000
88 H	0.318400000000	40.142000000000	43.565000000000
89 C	0.401200000000	39.934200000000	45.556300000000
90 H	0.151600000000	40.829400000000	45.753100000000
91 C	0.667500000000	39.035600000000	46.603900000000
92 H	0.587700000000	39.342300000000	47.499500000000
93 C	1.040600000000	37.724000000000	46.382300000000
94 C	1.150000000000	37.272500000000	45.019500000000
95 C	1.689100000000	35.495100000000	47.405300000000
96 C	1.322800000000	36.846000000000	47.538900000000
97 C	1.245600000000	37.319300000000	48.865600000000
98 H	1.004600000000	38.223500000000	49.029400000000
99 C	1.516900000000	36.481700000000	49.927100000000
100 H	1.452900000000	36.840500000000	50.804300000000
101 N	1.863500000000	35.198700000000	49.800400000000
102 C	1.942800000000	34.739300000000	48.555000000000
103 H	2.190300000000	33.829800000000	48.437200000000

104 C	3.485500000000	34.075400000000	45.674300000000
105 C	3.789600000000	32.772800000000	46.068200000000
106 H	3.092700000000	32.193800000000	46.354000000000
107 C	5.090800000000	32.315100000000	46.047800000000
108 H	5.288400000000	31.426200000000	46.318500000000
109 C	6.104000000000	33.154400000000	45.632200000000
110 H	7.002000000000	32.844400000000	45.626500000000
111 C	5.818500000000	34.446800000000	45.223400000000
112 H	6.518500000000	35.016600000000	44.926900000000
113 C	4.515100000000	34.908000000000	45.246500000000
114 H	4.322000000000	35.795900000000	44.969500000000
115 P	-2.540600000000	38.290700000000	49.102900000000
116 O	-1.580800000000	39.426300000000	49.207500000000
117 C	-2.278300000000	36.981400000000	50.289000000000
118 C	-2.375000000000	37.336200000000	51.622300000000
119 H	-2.637200000000	38.220400000000	51.850300000000
120 C	-2.094700000000	36.419300000000	52.643700000000
121 H	-2.157200000000	36.684000000000	53.554000000000
122 C	-1.734000000000	35.153400000000	52.325400000000
123 H	-1.550100000000	34.534000000000	53.021800000000
124 C	-1.624100000000	34.729900000000	50.970800000000
125 C	-1.254800000000	33.400800000000	50.668800000000
126 H	-1.074200000000	32.788300000000	51.372200000000
127 C	-1.157100000000	32.996100000000	49.381000000000
128 H	-0.907500000000	32.100900000000	49.184200000000
129 C	-1.423400000000	33.894700000000	48.333400000000
130 H	-1.343500000000	33.588000000000	47.437800000000
131 C	-1.796400000000	35.206300000000	48.555000000000
132 C	-1.905900000000	35.657800000000	49.917700000000
133 C	-2.444900000000	37.435200000000	47.532000000000
134 C	-2.078600000000	36.084100000000	47.398300000000
135 C	-2.001400000000	35.611000000000	46.071700000000
136 H	-1.760400000000	34.706800000000	45.907900000000
137 C	-2.272700000000	36.448600000000	45.010200000000
138 H	-2.208700000000	36.089900000000	44.133000000000
139 N	-2.619300000000	37.731600000000	45.136900000000
140 C	-2.698600000000	38.190900000000	46.382300000000
141 H	-2.946100000000	39.100600000000	46.500100000000
142 C	-4.241300000000	38.854900000000	49.263000000000
143 C	-4.545400000000	40.157600000000	48.869100000000
144 H	-3.848600000000	40.736500000000	48.583300000000
145 C	-5.846700000000	40.615200000000	48.889500000000
146 H	-6.044200000000	41.504100000000	48.618700000000
147 C	-6.859900000000	39.776000000000	49.305000000000
148 H	-7.757900000000	40.085900000000	49.310800000000
149 C	-6.574300000000	38.483500000000	49.713900000000
150 H	-7.274300000000	37.913700000000	50.010300000000
151 C	-5.270900000000	38.022300000000	49.690700000000
152 H	-5.077800000000	37.134400000000	49.967800000000
153 I	-0.837600000000	31.264900000000	45.340500000000
154 C	-2.193800000000	29.671100000000	45.334200000000
155 C	-2.645200000000	29.121000000000	46.522900000000
156 C	-3.554800000000	28.091700000000	46.545300000000
157 F	-2.183500000000	29.595200000000	47.694900000000
158 F	-3.942000000000	27.598500000000	47.734500000000
159 I	-5.422200000000	25.964100000000	45.365600000000

160 C	-4.0659000000000	27.5578000000000	45.3718000000000
161 C	-3.6145000000000	28.1079000000000	44.1831000000000
162 C	-2.7050000000000	29.1373000000000	44.1608000000000
163 F	-4.0763000000000	27.6337000000000	43.0111000000000
164 F	-2.3177000000000	29.6304000000000	42.9715000000000

Dim²(N)-A...(N)Dim²

1 P	-8.9335000000000	21.5426000000000	48.2457000000000
2 O	-9.7132000000000	22.6185000000000	48.9212000000000
3 C	-9.8424000000000	20.0325000000000	47.9572000000000
4 C	-10.3325000000000	19.3902000000000	49.0799000000000
5 H	-10.1157000000000	19.7284000000000	49.9408000000000
6 C	-11.1418000000000	18.2516000000000	48.9743000000000
7 H	-11.4773000000000	17.8295000000000	49.7565000000000
8 C	-11.4430000000000	17.7565000000000	47.7503000000000
9 H	-11.9878000000000	16.9811000000000	47.6843000000000
10 C	-10.9616000000000	18.3718000000000	46.5603000000000
11 C	-11.2843000000000	17.8279000000000	45.2977000000000
12 H	-11.8287000000000	17.0513000000000	45.2421000000000
13 C	-10.8209000000000	18.4087000000000	44.1665000000000
14 H	-11.0420000000000	18.0385000000000	43.3200000000000
15 C	-10.0139000000000	19.5572000000000	44.2387000000000
16 H	-9.7046000000000	19.9492000000000	43.4304000000000
17 C	-9.6527000000000	20.1386000000000	45.4388000000000
18 C	-10.1354000000000	19.5370000000000	46.6545000000000
19 C	-8.3842000000000	22.0012000000000	46.6035000000000
20 C	-8.7837000000000	21.3357000000000	45.4311000000000
21 C	-8.2913000000000	21.8871000000000	44.2297000000000
22 H	-8.5209000000000	21.4867000000000	43.3993000000000
23 C	-7.4797000000000	23.0019000000000	44.2492000000000
24 H	-7.1702000000000	23.3413000000000	43.4177000000000
25 N	-7.1013000000000	23.6346000000000	45.3622000000000
26 C	-7.5559000000000	23.1243000000000	46.5029000000000
27 H	-7.2990000000000	23.5545000000000	47.3099000000000
28 C	-7.4482000000000	21.1303000000000	49.1734000000000
29 C	-6.8665000000000	22.1208000000000	49.9641000000000
30 H	-7.2917000000000	22.9664000000000	50.0457000000000
31 C	-5.6807000000000	21.8868000000000	50.6291000000000
32 H	-5.2917000000000	22.5680000000000	51.1650000000000
33 C	-5.0624000000000	20.6590000000000	50.5123000000000
34 H	-4.2408000000000	20.4989000000000	50.9616000000000
35 C	-5.6335000000000	19.6584000000000	49.7430000000000
36 H	-5.2096000000000	18.8109000000000	49.6756000000000
37 C	-6.8203000000000	19.8926000000000	49.0732000000000
38 H	-7.2082000000000	19.2064000000000	48.5430000000000
39 P	5.3879000000000	34.2756000000000	48.2457000000000
40 O	4.6081000000000	35.3515000000000	48.9212000000000
41 C	4.4790000000000	32.7655000000000	47.9572000000000
42 C	3.9888000000000	32.1233000000000	49.0799000000000
43 H	4.2056000000000	32.4614000000000	49.9408000000000
44 C	3.1795000000000	30.9846000000000	48.9743000000000
45 H	2.8440000000000	30.5625000000000	49.7565000000000
46 C	2.8783000000000	30.4895000000000	47.7503000000000
47 H	2.3335000000000	29.7141000000000	47.6843000000000

48 C	3.3597000000000	31.1048000000000	46.5603000000000
49 C	3.0370000000000	30.5609000000000	45.2977000000000
50 H	2.4926000000000	29.7843000000000	45.2421000000000
51 C	3.5004000000000	31.1417000000000	44.1665000000000
52 H	3.2793000000000	30.7716000000000	43.3200000000000
53 C	4.3074000000000	32.2903000000000	44.2387000000000
54 H	4.6167000000000	32.6822000000000	43.4304000000000
55 C	4.6686000000000	32.8716000000000	45.4388000000000
56 C	4.1859000000000	32.2700000000000	46.6545000000000
57 C	5.9371000000000	34.7342000000000	46.6035000000000
58 C	5.5376000000000	34.0687000000000	45.4311000000000
59 C	6.0300000000000	34.6201000000000	44.2297000000000
60 H	5.8004000000000	34.2197000000000	43.3993000000000
61 C	6.8416000000000	35.7349000000000	44.2492000000000
62 H	7.1511000000000	36.0743000000000	43.4177000000000
63 N	7.2200000000000	36.3676000000000	45.3622000000000
64 C	6.7654000000000	35.8573000000000	46.5029000000000
65 H	7.0223000000000	36.2875000000000	47.3099000000000
66 C	6.8731000000000	33.8633000000000	49.1734000000000
67 C	7.4548000000000	34.8538000000000	49.9641000000000
68 H	7.0296000000000	35.6994000000000	50.0457000000000
69 C	8.6406000000000	34.6199000000000	50.6291000000000
70 H	9.0296000000000	35.3010000000000	51.1650000000000
71 C	9.2589000000000	33.3920000000000	50.5123000000000
72 H	10.0805000000000	33.2319000000000	50.9616000000000
73 C	8.6878000000000	32.3914000000000	49.7430000000000
74 H	9.1117000000000	31.5439000000000	49.6756000000000
75 C	7.5010000000000	32.6256000000000	49.0732000000000
76 H	7.1131000000000	31.9394000000000	48.5430000000000
77 P	-11.6234000000000	22.9190000000000	42.4499000000000
78 O	-10.8437000000000	21.8431000000000	41.7744000000000
79 C	-10.7145000000000	24.4292000000000	42.7384000000000
80 C	-10.2243000000000	25.0714000000000	41.6157000000000
81 H	-10.4411000000000	24.7332000000000	40.7548000000000
82 C	-9.4150000000000	26.2100000000000	41.7213000000000
83 H	-9.0796000000000	26.6321000000000	40.9391000000000
84 C	-9.1138000000000	26.7051000000000	42.9453000000000
85 H	-8.5690000000000	27.4805000000000	43.0113000000000
86 C	-9.5952000000000	26.0898000000000	44.1353000000000
87 C	-9.2725000000000	26.6338000000000	45.3979000000000
88 H	-8.7281000000000	27.4103000000000	45.4536000000000
89 C	-9.7359000000000	26.0529000000000	46.5291000000000
90 H	-9.5148000000000	26.4231000000000	47.3756000000000
91 C	-10.5430000000000	24.9044000000000	46.4569000000000
92 H	-10.8522000000000	24.5124000000000	47.2652000000000
93 C	-10.9042000000000	24.3230000000000	45.2568000000000
94 C	-10.4215000000000	24.9246000000000	44.0411000000000
95 C	-12.1726000000000	22.4604000000000	44.0921000000000
96 C	-11.7732000000000	23.1259000000000	45.2646000000000
97 C	-12.2655000000000	22.5745000000000	46.4659000000000
98 H	-12.0359000000000	22.9749000000000	47.2963000000000
99 C	-13.0771000000000	21.4597000000000	46.4464000000000
100 H	-13.3866000000000	21.1203000000000	47.2779000000000
101 N	-13.4555000000000	20.8270000000000	45.3334000000000
102 C	-13.0009000000000	21.3374000000000	44.1928000000000
103 H	-13.2579000000000	20.9071000000000	43.3857000000000

104 C	-13.108600000000	23.331300000000	41.522200000000
105 C	-13.690300000000	22.340800000000	40.731500000000
106 H	-13.265200000000	21.495200000000	40.649900000000
107 C	-14.876100000000	22.574800000000	40.066500000000
108 H	-15.265100000000	21.893600000000	39.530600000000
109 C	-15.494500000000	23.802600000000	40.183300000000
110 H	-16.316100000000	23.962700000000	39.734000000000
111 C	-14.923300000000	24.803200000000	40.952600000000
112 H	-15.347300000000	25.650700000000	41.020000000000
113 C	-13.736500000000	24.569000000000	41.622400000000
114 H	-13.348600000000	25.255200000000	42.152600000000
115 P	2.697900000000	35.652000000000	42.449900000000
116 O	3.477600000000	34.576100000000	41.774400000000
117 C	3.606800000000	37.162200000000	42.738400000000
118 C	4.097000000000	37.804400000000	41.615700000000
119 H	3.880200000000	37.466200000000	40.754800000000
120 C	4.906300000000	38.943000000000	41.721300000000
121 H	5.241800000000	39.365100000000	40.939100000000
122 C	5.207500000000	39.438100000000	42.945300000000
123 H	5.752300000000	40.213500000000	43.011300000000
124 C	4.726100000000	38.822800000000	44.135300000000
125 C	5.048800000000	39.366800000000	45.397900000000
126 H	5.593200000000	40.143300000000	45.453600000000
127 C	4.585400000000	38.785900000000	46.529100000000
128 H	4.806500000000	39.156100000000	47.375600000000
129 C	3.778300000000	37.637400000000	46.456900000000
130 H	3.469100000000	37.245400000000	47.265200000000
131 C	3.417200000000	37.056000000000	45.256800000000
132 C	3.899800000000	37.657600000000	44.041100000000
133 C	2.148700000000	35.193400000000	44.092100000000
134 C	2.548200000000	35.859000000000	45.264600000000
135 C	2.055800000000	35.307500000000	46.465900000000
136 H	2.285400000000	35.707900000000	47.296300000000
137 C	1.244200000000	34.192700000000	46.446400000000
138 H	0.934700000000	33.853300000000	47.277900000000
139 N	0.865800000000	33.560000000000	45.333400000000
140 C	1.320400000000	34.070400000000	44.192800000000
141 H	1.063500000000	33.640100000000	43.385700000000
142 C	1.212700000000	36.064300000000	41.522200000000
143 C	0.631000000000	35.073800000000	40.731500000000
144 H	1.056100000000	34.228200000000	40.649900000000
145 C	-0.554800000000	35.307800000000	40.066500000000
146 H	-0.943800000000	34.626600000000	39.530600000000
147 C	-1.173200000000	36.535600000000	40.183300000000
148 H	-1.994700000000	36.695700000000	39.734000000000
149 C	-0.602000000000	37.536200000000	40.952600000000
150 H	-1.025900000000	38.383700000000	41.020000000000
151 C	0.584800000000	37.302000000000	41.622400000000
152 H	0.972700000000	37.988200000000	42.152600000000
153 I	-0.832000000000	31.271500000000	45.336800000000
154 C	-2.195300000000	29.669300000000	45.338600000000
155 C	-2.649300000000	29.116300000000	46.522300000000
156 C	-3.549100000000	28.070700000000	46.522700000000
157 F	-2.214300000000	29.595400000000	47.694700000000
158 F	-3.940900000000	27.569400000000	47.703300000000
159 I	-5.403500000000	25.923100000000	45.358800000000
160 C	-4.040300000000	27.525300000000	45.357100000000

161 C	-3.586300000000	28.078300000000	44.173300000000
162 C	-2.686500000000	29.123900000000	44.172900000000
163 F	-4.021300000000	27.599200000000	43.001000000000
164 F	-2.294600000000	29.625200000000	42.992300000000