

```
2 #p B3LYP/Def2TZVP opt=(CalcAll,MaxCycle=100,MaxStep=100,verytight)
3 Freq=Anharmonic pop=(full,NBO) IOp(6/7=3)
4
5 anti-3CP xyz coordinates:
6 0, 1
7 C -0.5596300000 1.4097770000 0.0000000000
8 C -0.8358610000 0.0473940000 0.0000000000
9 C 0.7692490000 1.8130050000 0.0000000000
10 H 1.0049340000 2.8695490000 0.0000000000
11 C 0.1716790000 -0.9036600000 0.0000000000
12 C 1.8008080000 0.8823570000 0.0000000000
13 H -0.0532390000 -1.9603600000 0.0000000000
14 H 2.8343700000 1.2095410000 0.0000000000
15 C 1.4979320000 -0.4774450000 0.0000000000
16 H -1.3645220000 2.1300770000 0.0000000000
17 O 2.4580200000 -1.4457570000 0.0000000000
18 Cl -2.4989730000 -0.4866160000 0.0000000000
19 H 3.3317880000 -1.0388510000 0.0000000000
20
21 syn 3CP xyz coordinates:
22 0, 1
23 C 0.5591320000 1.4150320000 0.0000000000
24 C 0.8320250000 0.0554040000 0.0000000000
25 C -0.7722350000 1.8211420000 0.0000000000
26 H -1.0029220000 2.8788380000 0.0000000000
27 C -0.1831760000 -0.8922000000 0.0000000000
28 C -1.8069110000 0.8984250000 0.0000000000
29 H 0.0590130000 -1.9476060000 0.0000000000
30 H -2.8423120000 1.2103770000 0.0000000000
31 C -1.5081950000 -0.4624750000 0.0000000000
32 H 1.3653670000 2.1338850000 0.0000000000
33 O -2.5542010000 -1.3370820000 0.0000000000
34 H -2.2262360000 -2.2434920000 -0.0000010000
35 Cl 2.4915790000 -0.4910190000 0.0000000000
36
37 anti-3FP xyz coordinates:
38 0, 1
39 C -1.2446410000 1.0700390000 0.0000000000
40 C -1.1883030000 -0.3140530000 0.0000000000
41 C -0.0412870000 1.7644220000 0.0000000000
42 H -0.0501530000 2.8467280000 0.0000000000
43 C -0.0014260000 -1.0204920000 0.0000000000
44 C 1.1751350000 1.0922320000 0.0000000000
45 H 0.0030620000 -2.1011360000 0.0000000000
46 H 2.1067860000 1.6462910000 0.0000000000
47 C 1.1917130000 -0.3018340000 0.0000000000
48 H -2.2003380000 1.5742280000 0.0000000000
49 O 2.3486510000 -1.0232180000 0.0000000000
50 F -2.3444800000 -1.0107730000 0.0000000000
51 H 3.1046090000 -0.4252870000 0.0000020000
52
53 syn-3FP xyz coordinates:
54 0, 1
55 C 1.2597650000 1.0567310000 0.0000000000
56 C 1.1806070000 -0.3228580000 0.0000000000
57 C 0.0647860000 1.7716450000 0.0000000000
58 H 0.0943760000 2.8536340000 0.0000000000
59 C -0.0229730000 -1.0069190000 0.0000000000
60 C -1.1625460000 1.1256820000 0.0000000000
61 H -0.0255190000 -2.0899380000 0.0000000000
62 H -2.0913650000 1.6791300000 0.0000000000
63 C -1.2039780000 -0.2676640000 0.0000000000
64 H 2.2235540000 1.5453220000 0.0000000000
65 O -2.4313510000 -0.8613170000 0.0000000000
66 H -2.3339130000 -1.8201650000 0.0000010000
67 F 2.3210790000 -1.0463510000 0.0000000000
68
69
```