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SUPPORTING INFORMATION

Title: A New N,P-Ligand with Achiral gem-Dimethyloxazoline for Palladium(II)-Catalyzed Cyclization of 1,6-Enynes: Transition State Probe for the *N*/*C trans* Mode in Mizoroki–Heck-Type C–C Bond Formation
Author(s): Manabu Hatano, Masahiro Yamanaka, Koichi Mikami*
Ref. No.: O03196

General:

^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra were measured on a Varian GEMINI 300 (300 MHz) and Varian GEMINI 400 (400 MHz) spectrometers. Chemical shift of ^{1}H NMR were expressed in parts per million downfield from tetramethylsilane as an internal standard (δ = 0) in $CDCl_3$, unless otherwise noted. Chemical shifts of ^{13}C NMR were expressed in parts per million downfield from $CDCl_3$ as an internal standard (δ = 77.1) in $CDCl_3$, unless otherwise noted. Chemical shifts of ^{31}P NMR were expressed in parts per million downfield from 85% H_3PO_4 as an internal standard (δ = 0) in $CDCl_3$, unless otherwise noted. IR spectra were measured on a JASCO FT/IR-5000 spectrometer. Optical rotations were measured on a JASCO DIP-370. Liquid chromatographic analyses (HPLC) were conducted on a JASCO PU-980, LG-980-02, DG-980-50, AS-950 and CO-966 instrument equipped with model UV-975 spectrometers as an ultra violet light. Peak area were calculated by JASCO-BORWIN (Windows NT) as an automatic integrator. Capillary gas chromatographic analyses (GC) were conducted on a Shimadzu GC-14B instrument equipped with FID detector by using N_2 (75 kPa) as a carrier gas; Peak area were calculated by a Shimadzu C-R6A as an automatic integrator; Chiral column were CP-Cyclodextrin-β-2,3,6-M-19 (i.d. 0.25 mm x 25 m; CHROMPACK; GL Sciences Inc.) and CP-Chirasil-Dex CB (i.d. 0.32 mm x 25 m; CHROMPACK; GL Sciences Inc.); Split ratio was 100:1. Analytical thin layer chromatography (TLC) were performed on a glass plates (Merck Kieselgal 60 F_{254}, layer thickness 0.25 and 0.2 mm). Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$ and phosphomolybdic acid. Column chromatography was performed on KANTO Silica Gel 60N (spherical, neutral). All experiments were carried out under argon atmosphere otherwise noted.

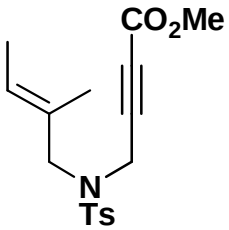
Materials:

$[(MeCN)_4Pd](BF_4)_2$ were purchased from Aldrich Chemical Co.

General procedure for Pd-catalyzed Ene-type cyclization of 1 under *"polar conditions"*.

Thoroughly degassed dimethylsulfoxide (DMSO) (2.0 mL) was injected under argon into a pyrex Schlenk tube containing $[(MeCN)_4Pd](BF_4)_2$ (4.4 mg, 0.010 mmol) and N,P-ligand **11** (10.7 mg, 0.020 mmol), and this suspension was stirred at room temperature for 5 min. Then **5** (67.4 mg, 0.200 mmol) and formic acid (7.5 μL, 0.20 mmol) were added, the tube was sealed with a screw cap. The mixture was stirred at 100 C for 3 h. The reaction mixture was washed with brine and ether-extracted organic layer was evaporated in vacuo and the residue was purified by short column chromatography (neutral-silica-gel, pentane/ether = 2/1) to afford 95% *ee* of (*S*)-(+)-**6** in quantitative yield.

4-[(2-Methyl-but-2-enyl)-(toluene-4-sulfonyl)-amino]-but-2-ynoic acid methyl ester (3).



^{1}H NMR (300 MHz, $CDCl_3$)

δ 1.58-1.66 (6H), 2.41 (s, 3H), 3.66 (s, 2H), 4.09 (s, 2H), 5.46 (m, 1H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 2H).

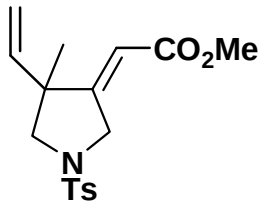
^{13}C NMR (75 MHz, $CDCl_3$)

δ 13.6, 13.6, 21.5, 35.1, 52.7, 54.9, 76.9, 80.8, 125.9, 127.7, 129.4, 129.7, 135.5, 143.8, 153.0.

IR (neat)

2958, 2922, 2866, 2244, 1717, 1601, 1437, 1450, 153, 1164 cm^{-1}.

[4-Methyl-1-(toluene-4-sulfonyl)-4-vinyl-pyrrolidin-3-ylidene]-acetic acid methyl ester (4).



^{1}H NMR (300 MHz, $CDCl_3$)
δ 1.27 (s, 3H), 2.43 (s, 3H), 3.09 (d, *J* = 9.6 Hz, 1H), 3.14 (d, *J* = 9.0 Hz, 1H), 3.68 (s, 3H), 4.19 (dd, *J* = 18.0, 2.7 Hz, 1H), 4.41 (dd, *J* = 18.3, 2.4 Hz, 1H), 5.15 (d, *J* = 11.1 Hz, 1H), 5.16 (d, *J* = 17.4 Hz, 1H), 5.60 (t, *J* = 2.7 Hz, 1H), 5.69 (dd, *J* = 17.4, 10.8 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H).

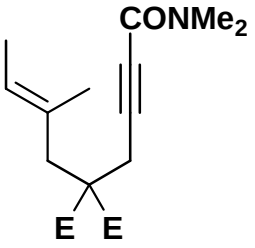
^{13}C NMR (75 MHz, $CDCl_3$)
δ 21.6, 23.1, 49.8, 51.5, 52.2, 58.3, 112.9, 115.4, 128.0, 129.8, 140.2, 143.9, 164.3, 166.3.

IR (neat)
2928, 2856, 1715 1667, 1601, 1437, 1340 cm^{-1}.

HPLC analysis (DAICEL CHIRALCEL OD-H, eluent, hexane/2-propanol = 95/5, flow rate 0.6 mL / min, 15 , detection 254 nm light)
t_R: 23.8 min ((*R*)-isomer) and 26.6 min ((*S*)-isomer).

$[\alpha]_D^{23}$ = + 15.47 (*c* = 0.865 in $CHCl_3$); 87%ee product (*S*).

2-(3-Dimethylcarbamoyl-prop-2-ynyl)-2-(2-methyl-but-2-enyl)-malonic acid diethyl ester (5).



E = CO_2Et

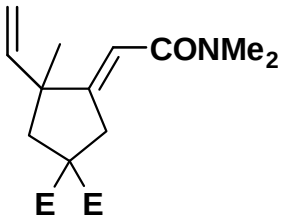
^{1}H NMR (300 MHz, $CDCl_3$)
δ 1.24 (t, *J* = 7.2 Hz, 6H), 1.51 (bs, 3H), 1.55 (d, *J* = 6.9 Hz, 3H), 2.76 (s, 2H), 2.93 (s, 3H), 2.95 (s, 2H), 3.15 (s, 3H), 3.18 (m, 4H), 5.38 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$)
δ 13.7, 14.0, 16.5, 23.2, 34.1, 38.2, 41.9, 56.4, 61.7, 65.9, 87.8, 125.5, 129.6, 154.2, 170.1.

IR (neat)
2984, 2256, 2222, 1734, 1634, 1446, 1396, 1288, 1187, 1100, 1062 cm^{-1}.

4-Dimethylcarbamoylmethylene-3-methyl-3-vinyl-cyclopentane-1,1-dicarboxylic acid

diethyl ester (6).



E = CO_2Et

^{1}H NMR (300 MHz, $CDCl_3$)
δ 1.19 (s, 3H), 1.22 (q, *J* = 3.9 Hz, 6H), 2.38 (d, *J* = 13.5 Hz, 1H), 2.54 (d, *J* = 13.5 Hz, 1H), 2.97 (s, 3H), 3.02 (s, 3H), 3.53 (2H), 4.15 (m, 4H), 4.98 (d, *J* = 9.9 Hz, 1H), 5.00 (d, *J* = 17.4 Hz, 1H), 5.78 (dd, *J* = 17.1, 10.5 Hz, 1H), 5.87 (t, *J* = 2.7 Hz, 1H).

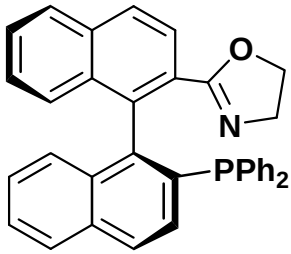
^{13}C NMR (75 MHz, $CDCl_3$)
δ 13.9, 25.8, 35.1, 37.5, 39.2, 45.9, 50.1, 58.3, 61.6, 61.7, 112.6, 113.7, 144.6, 162.2, 167.3, 171.5, 172.0.

IR (neat)
2980, 2934, 1734, 1661, 1628, 1398, 1259, 1185 cm^{-1}.

HPLC analysis (DAICEL CHIRALCEL OD-H, eluent, hexane/2-propanol = 95/5, flow rate 0.6 mL / min, 15 , detection 254 nm light)
t_R: 31.2 min ((*R*)-isomer) and 32.8 min ((*S*)-isomer).

$[\alpha]_D^{23}$ = + 5.02 (*c* = 1.835 in $CHCl_3$); 95%ee product (*S*).

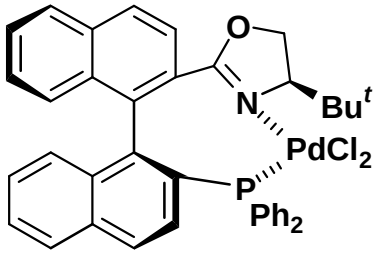
(*S*)-2-(2'-Diphenylphosphanyl-[1,1']binaphthalenyl-2-yl)-4,5-dihydro-oxazole (8).



^{1}H NMR (300 MHz, $CDCl_3$)
δ 3.38-3.66 (4H), 6.92-7.25 (3H), 7.25-7.34 (11H), 7.38-7.52 (3H), 7.80-7.94 (3H), 8.00 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$)
δ 54.5, 67.3, 126.0-129.0, 130.4, 133,2 (d, *J* = 19.4 Hz, 1H), 133.8 (d, *J* = 19.4 Hz, 1H).

Dichloro[(*R*,a*S*)-2-[4-(*tert*-butyl)oxazol-2-yl]-2'-diphenylphosphino-1,1'-binaphthyl]palladium (10a).



A mixture of $PdCl_2$(cod) (28.5 mg, 0.100 mmol) and N,P-ligand **7a** (58.1 mg, 0.103 mmol) in CH_2Cl_2 (4 mL) was stirred for 3 h at room temperature, then all the volatiles were removed under reduced pressure. To this residue pentane was added and remove the clear layer to remove COD released and then dry up under reduced pressure (73.9 mg, 72.7%). The yellow powder was dissolved in a minimum amount of AcOEt and recrystalized by slow diffusion of pentane into the concentrated AcOEt solution at room temperature to afforded orange prismatic crystals.

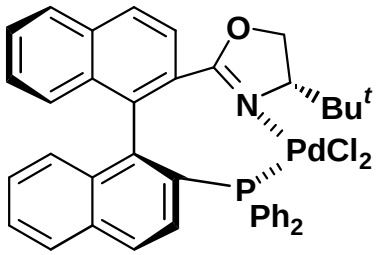
^{1}H NMR (300 MHz, $CDCl_3$)
δ 1.36 (s, 9H), 3.38 (dd, *J* = 10.5, 8.4 Hz, 1H), 3.48 (t, *J* = 10.5 Hz, 1H), 4.05 (dd, *J* = 10.2, 8.7 Hz, 1H), 6.18 (d, *J* = 8.1 Hz, 1H), 6.67 (m, 2H), 6.77 (m, 1H), 6.83 (m, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 7.21-7.37 (3H), 7.44-7.60 (6H), 7.80-8.00 (5H), 8.16 (d, *J* = 8.1 Hz, 1H), 8.22 (d, *J* = 8.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$, selected)
δ 26.8, 33.6, 71.3.

^{31}P NMR (109 MHz, $CDCl_3$)
δ 24.00 (s, 1P)

X-ray analysis: CCDC-179394

Dichloro[(*S*,a*S*)-2-[4-(*tert*-butyl)oxazol-2-yl]-2'-diphenylphosphino-1,1'-binaphthyl]palladium (10b).



A mixture of $PdCl_2$(cod) (14.8 mg, 0.052 mmol) and PN-ligand **7b** (30.6 mg, 0.054 mmol) in CH_2Cl_2 (2 mL) was stirred for 1 h at room temperature, then all the volatiles were removed under reduced pressure. To this residue pentane was added and remove the clear layer to remove COD released and then dry up under reduced pressure. Then the resultant residue was purified by neutral silicagel chromatography. The yellow residue was dissolved in a minimum amount of CH_2Cl_2 and recrystalized by slow diffusion of hexane into the concentrated CH_2Cl_2 solution at room temperature to afforded yellow prismatic crystals.

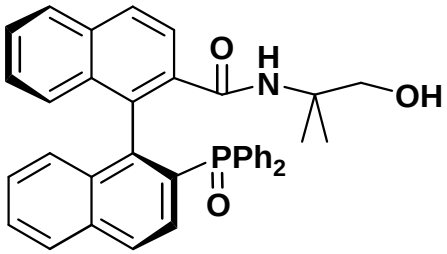
^{1}H NMR (300 MHz, $CDCl_3$)
δ 0.60 (s, 9H), 4.00 (dd, *J* = 9.3, 6.6 Hz, 1H), 4.52 (dd, *J* = 10.5, 9.0 Hz, 1H), 5.06 (dd, *J* = 10.5, 6.9

Hz, 1H), 6.37 (d, *J* = 8.4 Hz, 1H), 6.60-6.79 (m, 3H), 6.78 (d, *J* = 8.7 Hz, 1H), 6.93 (ddd, *J* = 8.7, 6.9, 1.2 Hz, 1H), 7.22 (t, 1H), 7.30 (t, *J* = 8.4 Hz, 1H), 7.35 (t, *J* = 9.0 Hz, 1H), 7.40-7.62 (m, 6H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 8.00 (br, 2H).

^{31}P NMR (109 MHz, $CDCl_3$)
δ 24.60 (s, 1P)

X-ray analysis: CCDC-179395

(*S*)-2'-(Diphenyl-phosphinoyl)-[1,1']binaphthalenyl-2-carboxylic acid (2-hydroxy-1,1-dimethyl-ethyl)-amide.

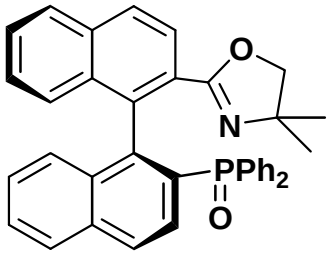


A mixture of (*S*)-2'-(diphenyl-phosphinoyl)-[1,1']binaphthalenyl-2-carboxylic acid methyl ester (4.23 g, 8.26 mmol), 2-amino-2-methyl-1-propanol (80 mL), and a small amount of sodium was heated at 100 for 2 h. The mixture was diluted with dichloromethane and neutralized wit acetic acid. The neutralized solution was washed with water and then brine and dried over $MgSO_4$. After the solvent was removed under reduced pressure, the residue was purified by neutral column chromatography with ethyl acetate/hexane (2/1 to AcOEt only) as an eluent to afford the titled compound. (2.97 g, 70.2%)

^{1}H NMR (300 MHz, $CDCl_3$)
δ 0.76 (s, 3H), 0.91 (s, 3H), 3.14 (m, 1H), 3.36 (m,1H), 5.09 (br, 1H), 6.52 (d, *J* = 8.7 Hz, 1H), 6.75-6.86 (3H), 6.97 (t, *J* = 7.5 Hz, 1H), 7.05-7.16 (3H), 7.18 (d, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 8.4 Hz, 1H), 7.44-7.64 (6H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.83-7.94 (3H), 7.97 (dd, *J* = 8.4, 2.4 Hz, 1H), 8.85 (bs, 1H)

^{13}C NMR (75 MHz, $CDCl_3$, selected)
δ 23.0, 23.8, 55.9, 70.4, 170.1.

(*S*)-2-[2'-(Diphenyl-phosphinoyl)-[1,1']binaphthalenyl-2-yl]-4,4-dimethyl-4,5-dihydro-oxazole.

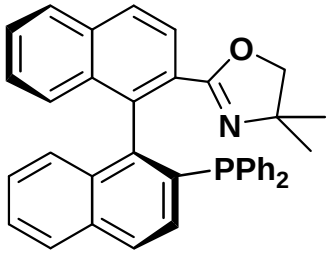


To a solution of (*S*)-2'-(diphenyl-phosphinoyl)-[1,1']binaphthalenyl-2-carboxylic acid (2-hydroxy-1,1-dimethyl-ethyl)-amide (2.97 g, 5.22 mmol), triethylamine (2.91 mL, 20.8 mmol), DMAP (31.8mg, 0.261 mmol)in CH_2Cl_2 (80 mL) was added methanesulfonyl chloride (0.484 mL, 6.26 mmol) at 0 . After stirring at room temperature for 8 h, the reaction solution was washed with water and brine, dried over $MgSO_4$, and concentrated under reduced pressure to provide a residue which was purified by column chromatography to afford the titled compound. (2.75 g, 86.8%)

^{1}H NMR (300 MHz, $CDCl_3$)
δ 0.87 (s, 3H), 1.00 (s, 3H), 3.41 (d, *J* = 8.1 Hz, 1H), 3.64 (d, *J* = 7.8 Hz, 1H), 6.98-7.60 (15H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.92 (dd, *J* = 8.4, 2.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$, selected)
δ 27.5, 27.8, 67.1, 78.7.

(*S*)-2-(2'-Diphenylphosphanyl-[1,1']binaphthalenyl-2-yl)-4,4-dimethyl-4,5-dihydro-oxazole (11).



To a mixture of (*S*)-2-[2'-(Diphenyl-phosphinoyl)-[1,1']binaphthalenyl-2-yl]-4,4 -dimethyl-4,5-dihydro-oxazole (1.146 g, 2.07 mmol) and triethylamine (8.6 mL, 62.1 mmol) in toluene (35 mL) was added trichlorosilane (2.09 ml, 20.7 mmol) at 0 , and the solution was stirred for 30 min at this temperature. It was then refluxed for 1.5 h under argen. After cooling to 0 , the reaction mixture was diluted with ether and quenched with a small amount of sat. $NaHCO_3$ solution. The resulting suspension was filtered through a pad of Celite and the filter cake was washed with ether, then the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography to afford the titled compound (600 mg, 54.0%).

^{1}H NMR (300 MHz, $CDCl_3$)
δ 0.89 (s, 3H), 0.92 (s, 3H), 3.31 (d, *J* = 7.8 Hz, 1H), 3.44 (d, *J* = 7.8 Hz, 1H), 6.92-6.95 (2H), 7.04-7.08 (2H), 7.08-7.26 (10H), 7.37 (m, 1H), 7.43 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.49 (dd, *J* = 6.3, 2.4 Hz, 1H), 7.84 (d, *J* = 6.6 Hz, 1H), 7.85 (d, *J* = 6.6 Hz, 1H), 7.88 (d, *J* = 6.0 Hz, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 8.11 (d, *J* = 8.7 Hz, 1H).

^{31}P NMR (109 MHz, $CDCl_3$)
δ -14.53 (s, 1P)

Computational details:

Computational method and chemical model

All calculations were performed with the GAUSSIAN 98 package.[1] Geometry optimization was performed by ONIOM (B3LYP:HF) method. The complexes, **CP1** and **CP2**, were divided into two layers as shown in Figure 1S. The small models (**CP1$_{model}$** and **CP2$_{model}$**) with H atoms and dienyl group instead of phenyl groups and biphenyl group, respectively, were treated at the higher-level method, B3LYP, with the basis set denoted as 631SDD consisting of Sttutgart's effective core potential[2] for Pd atoms and 6-31G(d) basis set[3] for the rest. The full real model (**CP1** and **CP2**) including phenyl and biphenyl groups was treated at the lower-level method, HF, with the basis set denoted as 321LAN consisting of LANL2DZ effective core potential[4] for Pd atoms and 3-21G basis set[3] for the rest. Cartesian coordinates and total energies are shown below.

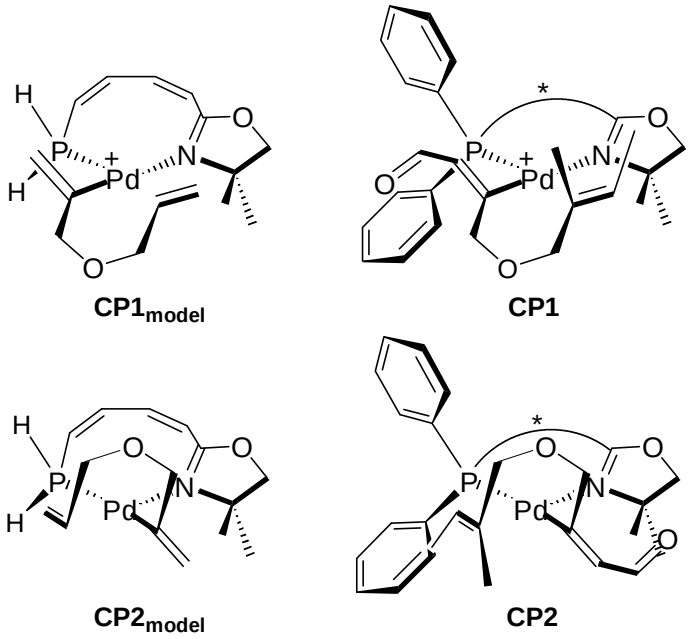


Figure 1S. Chemical models of Pd^{II} complex with (a*S*)-P,N-ligand **11**

Cartesian coordinates and total energies

CP1

```
E123= -1168.102622169198  -1180.954065831784  -2499.305486272116 a.u.
ONIOM: extrapolated energy =   -2512.156929934703 a.u.
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0        1.406770   -0.765813   -0.515989
    2         15             0        0.332299    0.461988    1.213321
    3          8             0       -2.040638   -3.123161   -1.492889
    4          7             0       -0.189865   -2.409438   -0.427283
    5          6             0       -2.321902    0.041611    0.244657
    6          6             0       -1.467943    0.074457    1.358612
    7          6             0       -2.003655   -0.164841    2.654880
```

8	1	0	-1.347493	-0.143354	3.497920
9	6	0	-3.321604	-0.418103	2.835746
10	1	0	-3.705153	-0.590120	3.822348
11	6	0	-5.591678	-0.742904	1.930569
12	1	0	-5.949435	-0.907209	2.927853
13	6	0	-6.437030	-0.797475	0.873141
14	1	0	-7.477487	-1.005351	1.020367
15	6	0	-5.948477	-0.580241	-0.435668
16	1	0	-6.626025	-0.628795	-1.263964
17	6	0	-4.636561	-0.312152	-0.649265
18	1	0	-4.279373	-0.149417	-1.642892
19	6	0	-3.721635	-0.243122	0.438616
20	6	0	-4.212761	-0.466515	1.741293
21	6	0	-1.864665	0.245045	-1.171590
22	6	0	-1.378612	-0.841274	-1.900084
23	6	0	-1.101566	-0.727785	-3.287759
24	1	0	-0.784223	-1.595183	-3.829242
25	6	0	-1.253736	0.462355	-3.916795
26	1	0	-1.042651	0.550520	-4.964330
27	6	0	-1.909132	2.839657	-3.883704
28	1	0	-1.647323	2.909818	-4.921062
29	6	0	-2.417092	3.909470	-3.224103
30	1	0	-2.556990	4.842113	-3.732037
31	6	0	-2.780833	3.797465	-1.862677
32	1	0	-3.196891	4.646020	-1.358717
33	6	0	-2.612711	2.627622	-1.197871
34	1	0	-2.903669	2.541581	-0.174360
35	6	0	-2.062018	1.493521	-1.850965
36	6	0	-1.725893	1.599481	-3.218892
37	6	0	0.351010	2.322869	1.484853
38	6	0	-0.817010	2.997583	1.805752
39	1	0	-1.743558	2.470496	1.867907
40	6	0	-0.792401	4.356600	2.072395
41	1	0	-1.702869	4.862367	2.324689
42	6	0	0.399178	5.053874	2.018482
43	1	0	0.417744	6.106160	2.218993
44	6	0	1.571435	4.384125	1.712559
45	1	0	2.503642	4.909423	1.666387
46	6	0	1.546999	3.026842	1.455779
47	1	0	2.465757	2.534124	1.238198
48	6	0	1.110830	-0.125276	2.816803
49	6	0	1.729172	-1.367651	2.866502
50	1	0	1.755755	-1.987724	1.993773
51	6	0	2.321880	-1.815261	4.033732
52	1	0	2.797616	-2.775337	4.057879
53	6	0	2.306397	-1.018952	5.164917
54	1	0	2.768762	-1.360662	6.068841
55	6	0	1.700605	0.224144	5.122117
56	1	0	1.693593	0.849224	5.992127
57	6	0	1.109668	0.671965	3.953658
58	1	0	0.658847	1.641906	3.929049
59	6	0	-1.164355	-2.145262	-1.232595
60	6	0	-0.485774	-3.758533	0.162524
61	6	0	-1.499639	-4.314320	-0.852935
62	1	0	-1.038651	-4.925566	-1.638354
63	1	0	-2.329453	-4.859029	-0.401175
64	6	0	-1.161495	-3.556444	1.544228
65	1	0	-2.068389	-2.976752	1.442188

66	1	0	-0.494974	-3.039073	2.218362
67	1	0	-1.406789	-4.523297	1.968338
68	6	0	0.756914	-4.661483	0.302448
69	1	0	1.220365	-4.848879	-0.656203
70	1	0	0.462218	-5.611166	0.732533
71	1	0	1.477633	-4.202960	0.966762
72	6	0	2.636710	0.830789	-0.700244
73	6	0	2.245210	1.825025	-1.515541
74	6	0	3.937089	0.796967	0.092758
75	1	0	1.316968	1.739816	-2.076149
76	6	0	2.937149	3.133179	-1.690643
77	8	0	4.948749	0.019335	-0.539269
78	1	0	3.751611	0.411531	1.106940
79	1	0	4.355473	1.800277	0.146762
80	6	0	4.590650	-1.325372	-0.771147
81	1	0	5.509785	-1.813868	-1.119964
82	6	0	3.551821	-1.468789	-1.863948
83	1	0	4.269387	-1.825417	0.156479
84	6	0	2.588703	-2.435779	-1.802245
85	1	0	2.605305	-3.093196	-0.936153
86	6	0	1.845901	-2.959847	-3.031055
87	6	0	3.883154	-0.700914	-3.143891
88	1	0	2.475758	-3.683413	-3.540486
89	1	0	1.613645	-2.170055	-3.730091
90	1	0	0.930077	-3.456900	-2.750665
91	1	0	2.996713	-0.390880	-3.676605
92	1	0	4.466292	-1.354206	-3.787300
93	1	0	4.473727	0.166584	-2.901221
94	8	0	3.818482	3.577233	-0.982181
95	1	0	2.553316	3.714131	-2.522772

CP2

E123= -1168.080198736206 -1180.940515814250 -2499.286641540400 a.u.
ONIOM: extrapolated energy = -2512.146958618444 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.810270	-0.090682	-0.193214
2	15	0	-0.038216	1.618335	0.225559
3	8	0	0.442066	-2.626627	-2.645794
4	7	0	-0.615760	-0.835446	-1.821296
5	6	0	2.201748	0.028570	-0.558110
6	6	0	1.578983	1.289091	-0.612494
7	6	0	2.210532	2.343565	-1.328480
8	1	0	1.749653	3.306641	-1.347407
9	6	0	3.379569	2.151768	-1.985669
10	1	0	3.837744	2.965374	-2.513249
11	6	0	5.226046	0.687363	-2.702685
12	1	0	5.651698	1.512683	-3.238729
13	6	0	5.830444	-0.524533	-2.702012
14	1	0	6.744794	-0.676163	-3.239066
15	6	0	5.254962	-1.600456	-1.987236
16	1	0	5.741036	-2.555061	-1.993790
17	6	0	4.100936	-1.434958	-1.295512

18	1	0	3.680795	-2.256405	-0.757795
19	6	0	3.435996	-0.175283	-1.276085
20	6	0	4.014044	0.892929	-1.992575
21	6	0	1.711501	-1.152716	0.238074
22	6	0	0.844255	-2.099446	-0.318431
23	6	0	0.579062	-3.335270	0.330387
24	1	0	-0.097460	-4.035628	-0.116290
25	6	0	1.146675	-3.598565	1.531862
26	1	0	0.941813	-4.525752	2.029413
27	6	0	2.629587	-2.962521	3.395929
28	1	0	2.394076	-3.891348	3.876802
29	6	0	3.497878	-2.089362	3.962150
30	1	0	3.958481	-2.317575	4.902125
31	6	0	3.810038	-0.873576	3.311289
32	1	0	4.501979	-0.195507	3.768150
33	6	0	3.244821	-0.564661	2.118523
34	1	0	3.483080	0.354503	1.628656
35	6	0	2.322501	-1.452203	1.502028
36	6	0	2.021545	-2.671652	2.147138
37	6	0	0.487458	1.804403	2.010370
38	6	0	1.496354	2.701669	2.347149
39	1	0	1.964066	3.294584	1.586889
40	6	0	1.899617	2.836316	3.660602
41	1	0	2.670606	3.536836	3.911669
42	6	0	1.312794	2.062696	4.650738
43	1	0	1.628005	2.166908	5.669353
44	6	0	0.330354	1.151005	4.319813
45	1	0	-0.112470	0.535842	5.077032
46	6	0	-0.078347	1.023384	3.001519
47	1	0	-0.822921	0.297602	2.753122
48	6	0	-0.505031	3.360846	-0.282638
49	6	0	-0.784720	3.611381	-1.622778
50	1	0	-0.657845	2.835952	-2.350392
51	6	0	-1.222304	4.854674	-2.031131
52	1	0	-1.423844	5.035912	-3.067939
53	6	0	-1.405869	5.865091	-1.099061
54	1	0	-1.749635	6.829791	-1.413230
55	6	0	-1.145266	5.620374	0.234424
56	1	0	-1.287209	6.394258	0.961700
57	6	0	-0.694486	4.373071	0.642772
58	1	0	-0.494075	4.203418	1.679066
59	6	0	0.194814	-1.821694	-1.608466
60	6	0	-0.822400	-0.761200	-3.302350
61	6	0	-0.474684	-2.200454	-3.703822
62	1	0	-1.330747	-2.883915	-3.688518
63	1	0	0.055496	-2.283454	-4.652904
64	6	0	0.234619	0.211918	-3.892344
65	1	0	1.236461	-0.121158	-3.656306
66	1	0	0.099231	1.200561	-3.483132
67	1	0	0.121833	0.259358	-4.969260
68	6	0	-2.238314	-0.300748	-3.697664
69	1	0	-2.998834	-0.944125	-3.284342
70	1	0	-2.333464	-0.295616	-4.776817
71	1	0	-2.402775	0.707614	-3.338120
72	6	0	-2.595834	-2.005386	-0.023315
73	6	0	-3.014953	-2.809258	-1.016019
74	6	0	-2.472402	-2.464994	1.426576
75	8	0	-3.634332	-2.083139	2.153815

76	6	0	-3.729454	-0.686386	2.342500
77	6	0	-3.872858	0.075918	1.042582
78	6	0	-3.248317	1.300236	0.869361
79	6	0	-3.774248	2.344187	-0.121547
80	1	0	-3.293390	-2.406491	-1.983114
81	6	0	-3.110141	-4.293161	-0.945250
82	1	0	-1.569836	-2.061834	1.907507
83	1	0	-2.430147	-3.550994	1.466989
84	1	0	-2.881307	-0.311500	2.932990
85	1	0	-4.642742	-0.527860	2.929129
86	6	0	-5.111124	-0.323637	0.231502
87	1	0	-2.664485	1.689123	1.702936
88	1	0	-3.080900	3.159689	-0.226971
89	1	0	-4.710566	2.740053	0.262379
90	1	0	-3.969044	1.922881	-1.098537
91	8	0	-2.495701	-5.005984	-0.173692
92	1	0	-3.756546	-4.728930	-1.700315
93	1	0	-5.005370	-0.115826	-0.822012
94	1	0	-5.951472	0.249517	0.614755
95	1	0	-5.312370	-1.373504	0.366796

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