Supplementary Materials

The C-3 Functionalization of 1*H*-Indazole through Suzuki-Miyaura Cross-Coupling Catalyzed by Ferrocene-Based Divalent Palladium Complex Immobilized over Ionic Liquid as well as Theoretical Insights into Reaction Mechanism

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S26. ESI-HRMS (TOF-SIMS) of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**) (Fig. S26)

S27. Optimized structures from calculations

S1. ^{1}H NMR spectrum of 3-iodo-1*H*-indazole (compound **2**)

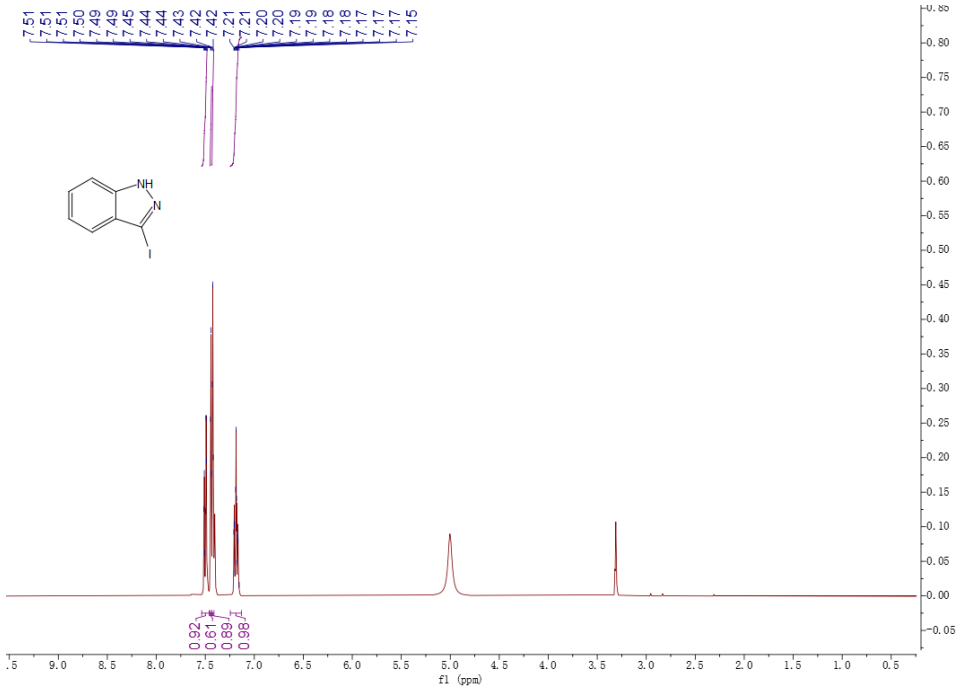


Fig. S1. ^{1}H NMR spectrum of 3-iodo-1*H*-indazole (compound **2**)

^{1}H NMR (400 MHz, Methanol-d_4) δ_H, ppm: 7.50 (1H, dt, J = 1.7, 7.4 Hz, Ar*H*), 7.44 (1H, d, J = 1.7 Hz, Ar*H*), 7.43 (1H, d, J = 1.7 Hz, Ar*H*), 7.19 (1H, m, Ar*H*). Herein, the peak appeared at δ_H = 3.31 ppm is the solvent peak of Methanol-d_4. The peak appeared at δ_H = 5.02 ppm means N*H* of compound **2** (not integrated due to influences of hydrogen bond as regular).

S2. ^{13}C NMR spectrum of 3-iodo-1*H*-indazole (compound **2**)

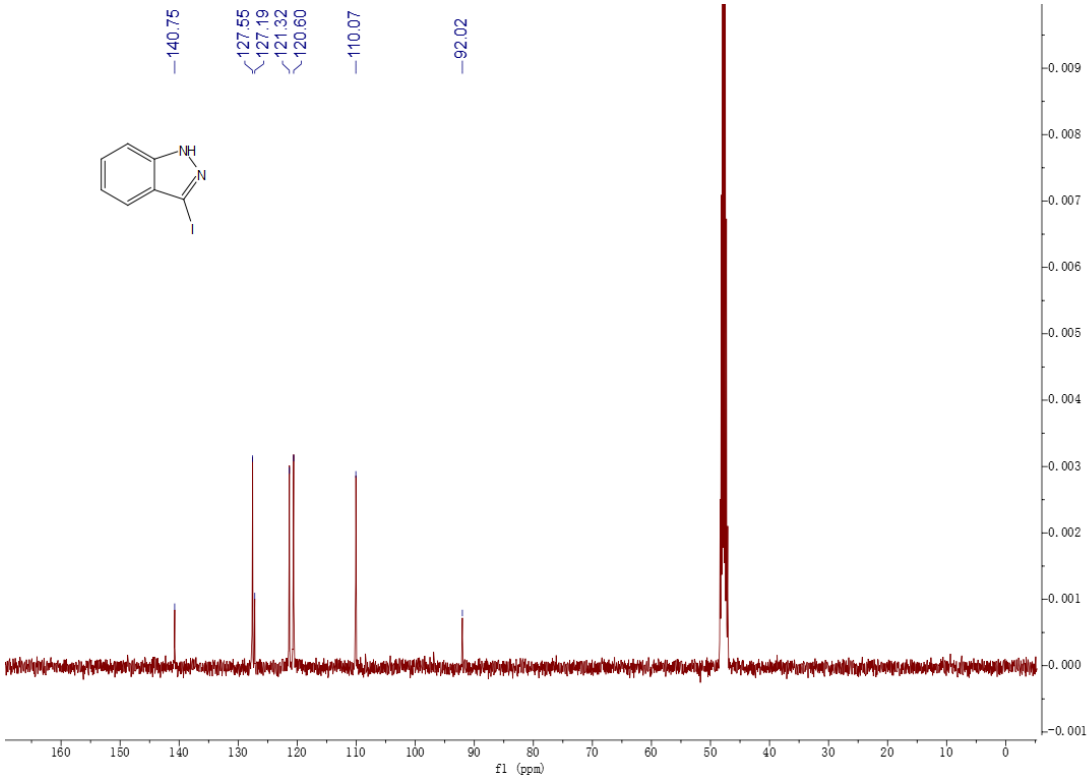


Fig. S2. ^{13}C NMR spectrum of 3-iodo-1*H*-indazole (compound **2**)

S3. ^{1}H NMR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

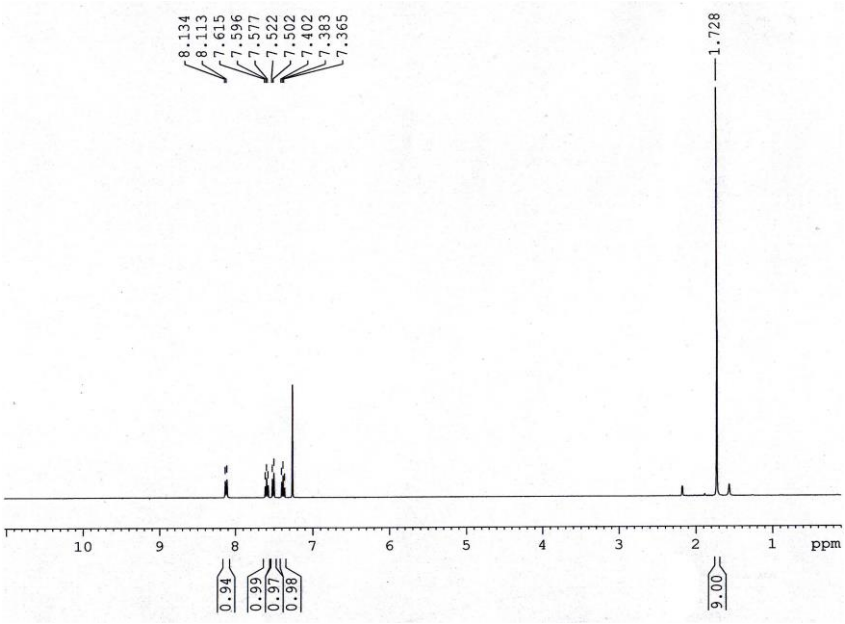


Fig. S3. ^{1}H NMR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate

(compound **3**)

S4. ^{13}C NMR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

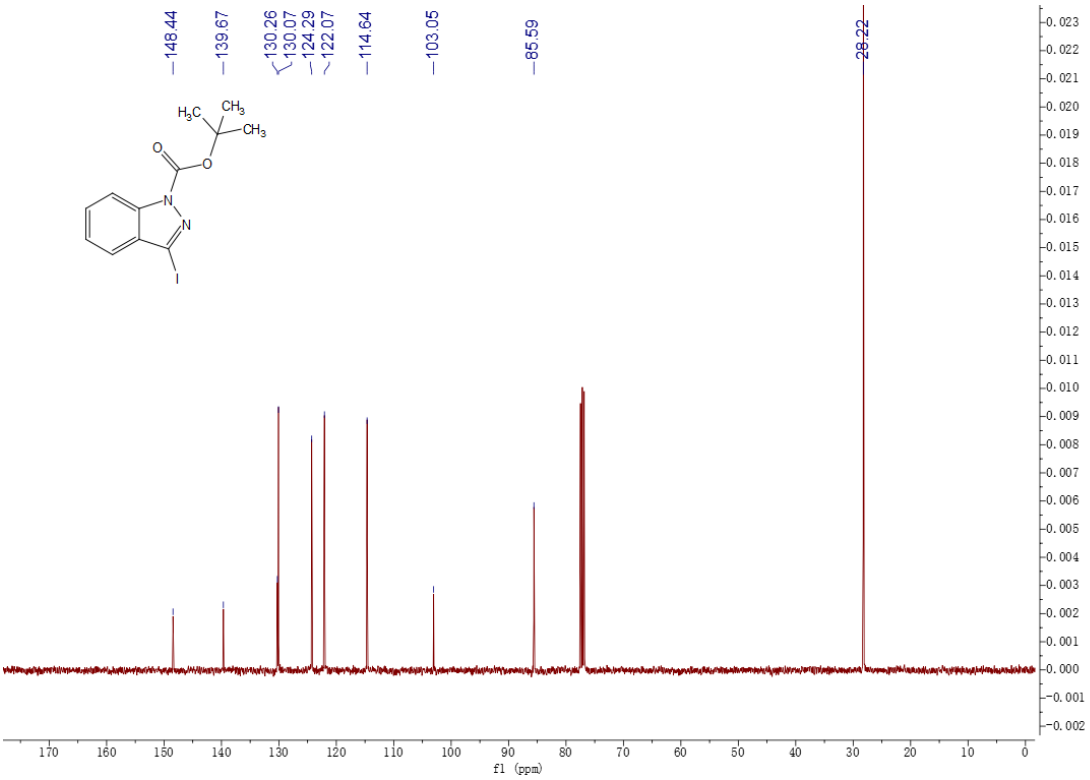


Fig. S4. ^{13}C NMR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

S5. ESI-HRMS of ^{13}C NMR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

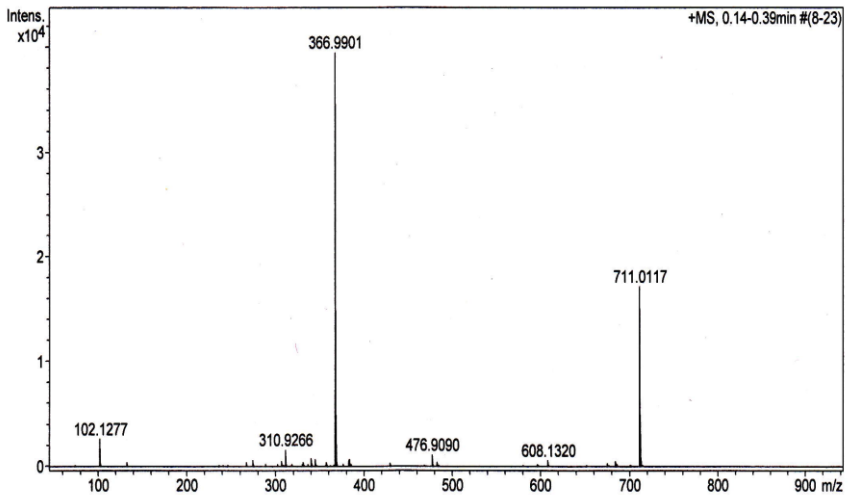


Fig. S5. ESI-HRMS of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

S6. FT-IR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

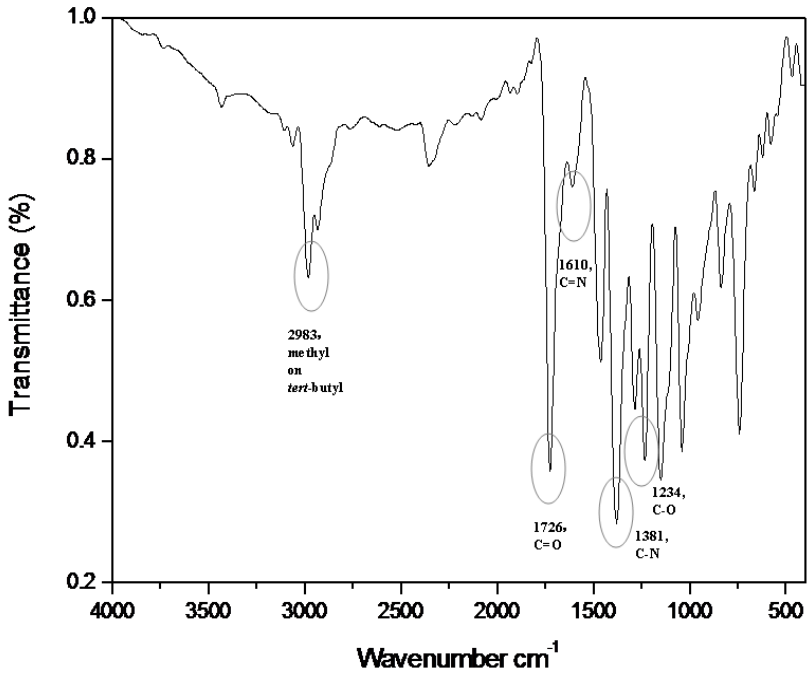


Fig. S6. FT-IR spectrum of *tert*-butyl-3-iodo-1*H*-indazole-1-carboxylate (compound **3**)

S7. ^{1}H NMR spectrum of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate

(compound **5**)

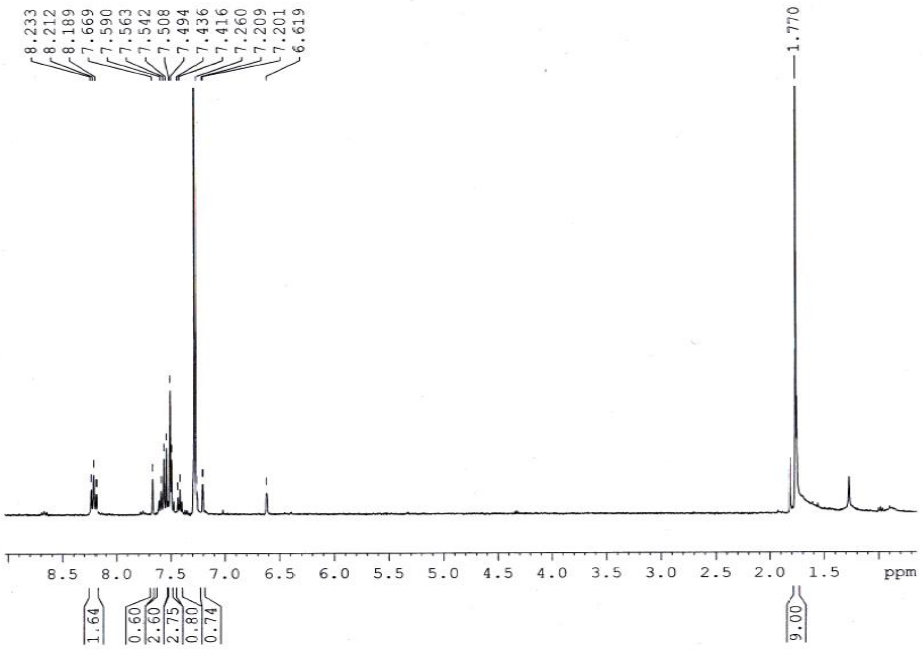


Fig. S7. ^{1}H NMR spectrum of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

S8. ^{13}C NMR spectrum of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

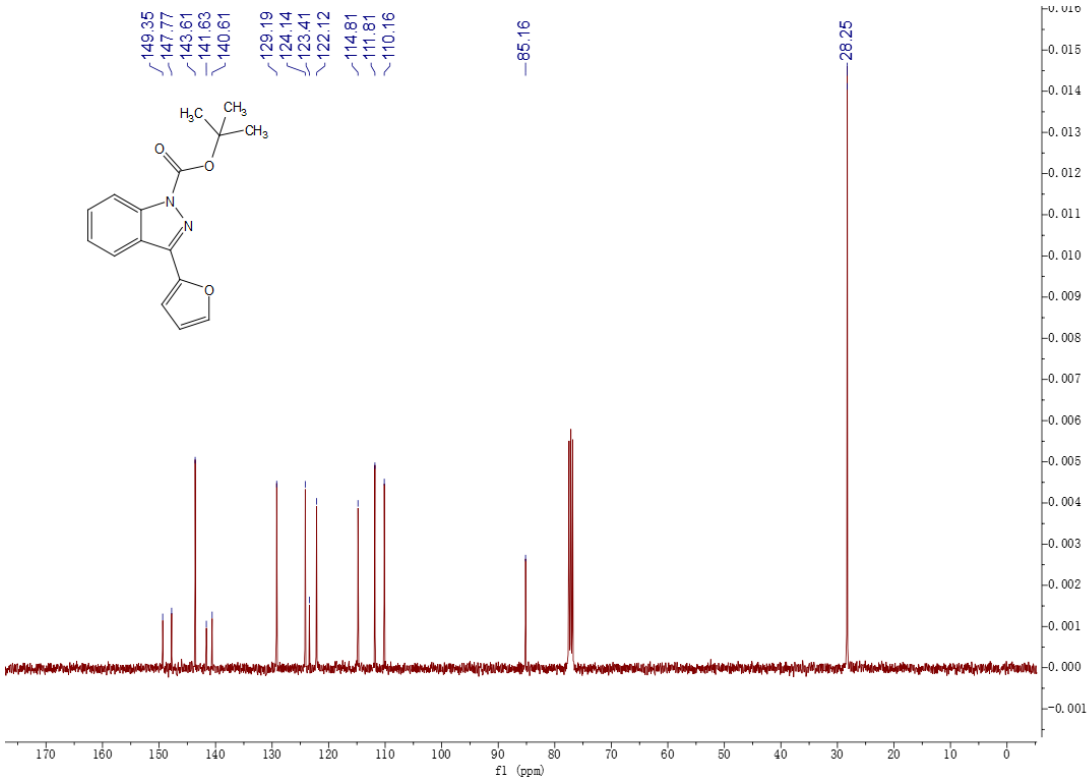


Fig. S8. ^{13}C NMR spectrum of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

S9. ESI-HRMS of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

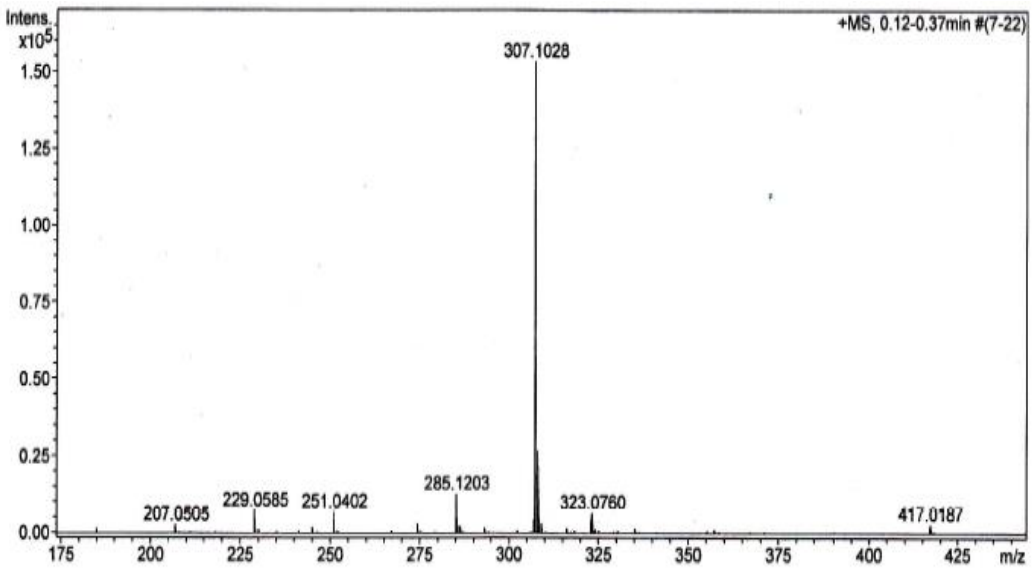


Fig. S9. ESI-HRMS of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound

5)

S10. FT-IR spectrum of ESI-HRMS of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

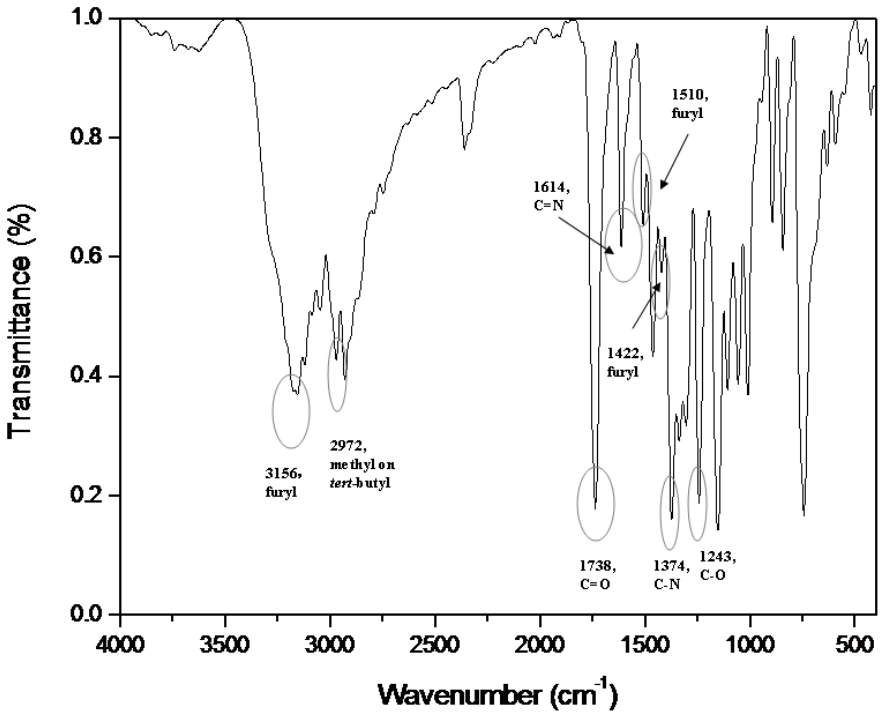


Fig. S10. FT-IR spectrum of ESI-HRMS of *tert*-butyl-3-(2-furyl)-1*H*-indazole-1-carboxylate (compound **5**)

S11. ^{1}H NMR spectrum of 3-(2-furyl)-1*H*-indazole (compound **6**)

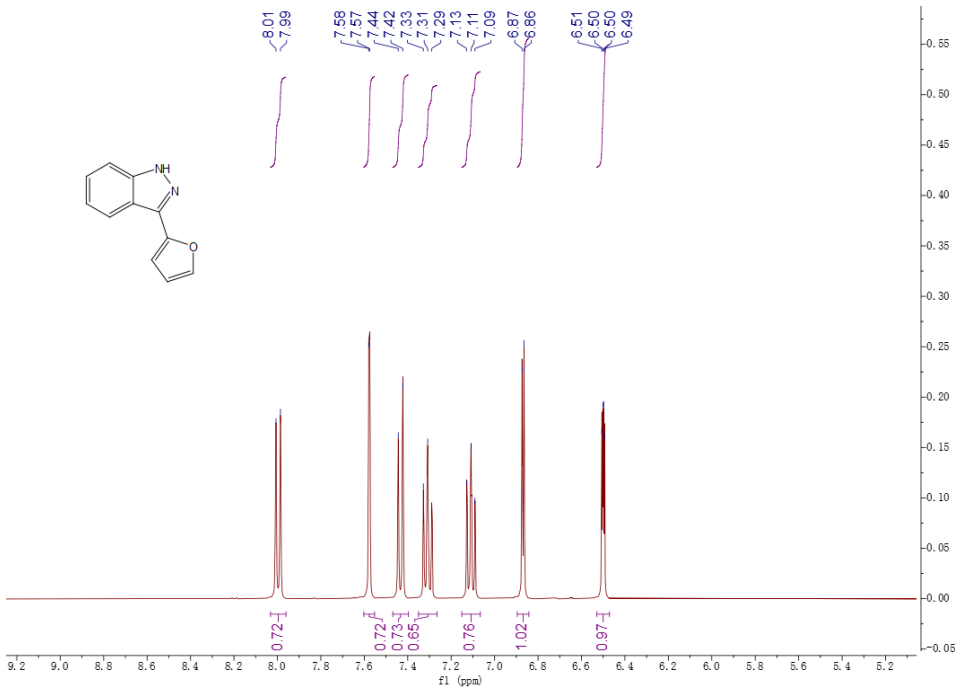


Fig. S11. ^{1}H NMR spectrum of 3-(2-furyl)-1*H*-indazole (compound **6**)

^{1}H NMR (400 MHz, $CDCl_3$) δ_H, ppm: 8.00 (1H, d, *J* = 8.2 Hz, Ar*H*), 7.58 (1H, d, *J* = 1.8 Hz, Ar*H*), 7.43 (1H, d, *J* = 8.4 Hz, *H* on furyl), 7.31 (1H, t, *J* = 7.6 Hz, Ar*H*), 7.11 (1H, t, *J* = 7.6 Hz, Ar*H*), 6.87 (1H, d, *J* = 3.4 Hz, *H* on furyl), 6.50 (1H, dd, *J* = 1.8, 3.4 Hz, *H* on furyl). Herein, the peak of N*H* of compound **6** was not found due to influences of hydrogen bond as regular.

S12. ^{13}C NMR spectrum of 3-(2-furyl)-1*H*-indazole (compound **6**)

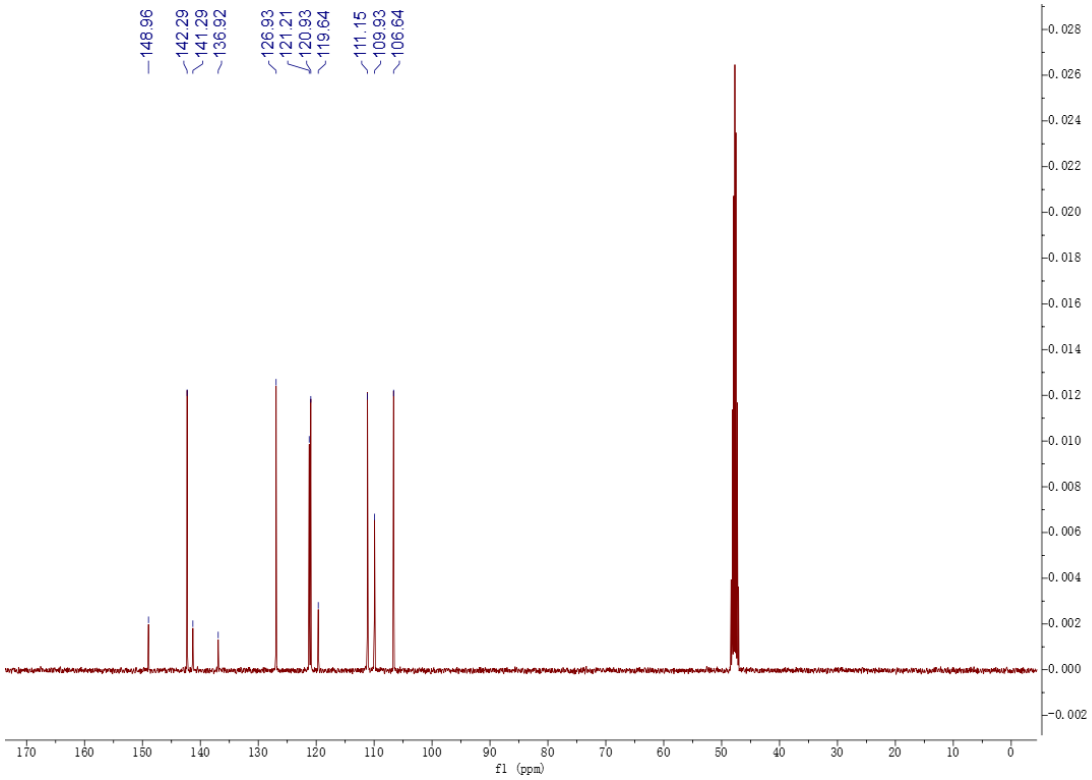


Fig. S12. ^{13}C NMR spectrum of 3-(2-furyl)-1*H*-indazole (compound **6**)

S13. ^{1}H NMR spectrum of *tert*-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **8**)

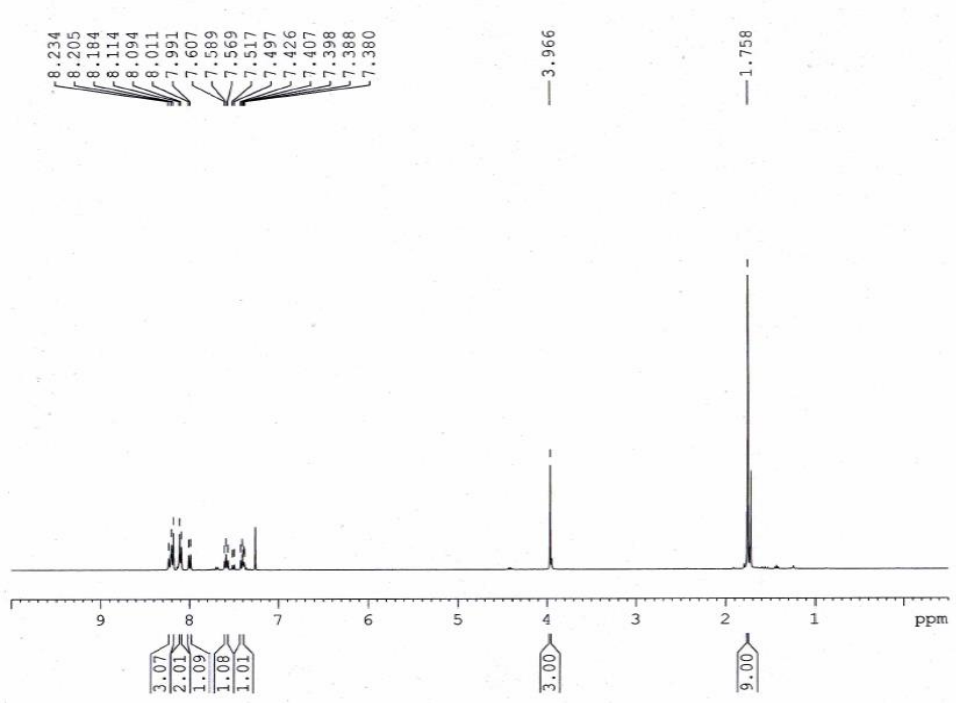


Fig. S13. ^{1}H NMR spectrum of

tert-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1- carboxylate (compound **8**)

S14. ^{13}C NMR spectrum of *tert*-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **8**)

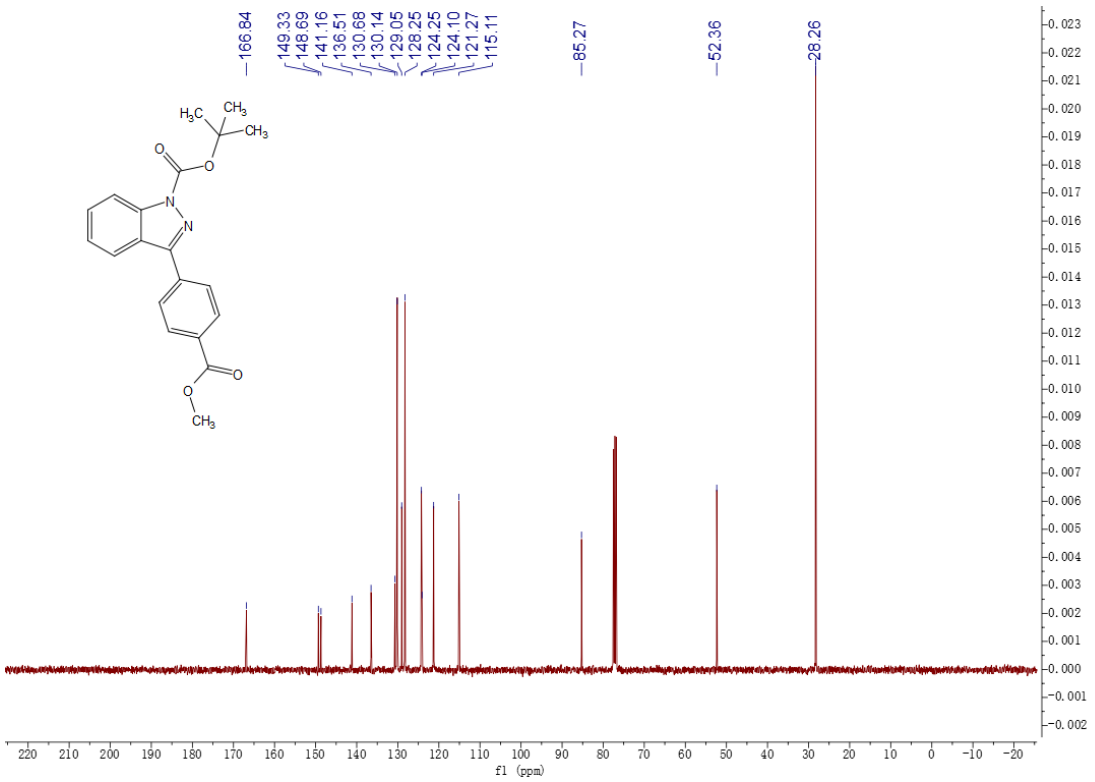


Fig. S14. ^{13}C NMR spectrum of

tert-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1- carboxylate (compound **8**)

S15. ESI-HRMS of *tert*-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **8**)

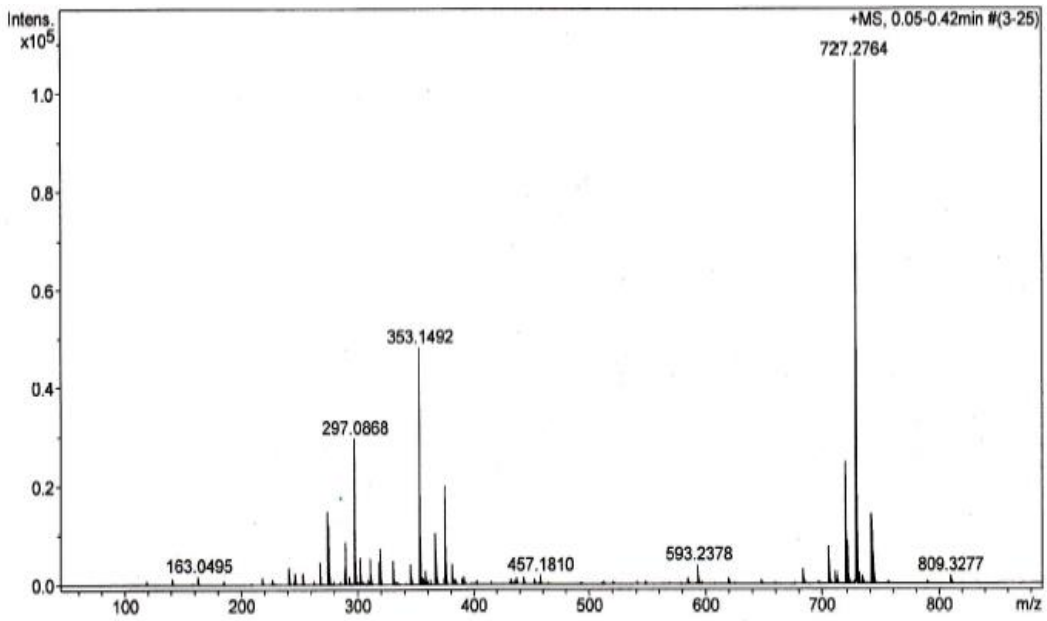


Fig. S15. ESI-HRMS of *tert*-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **8**)

S16. FT-IR spectrum of *tert*-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **8**)

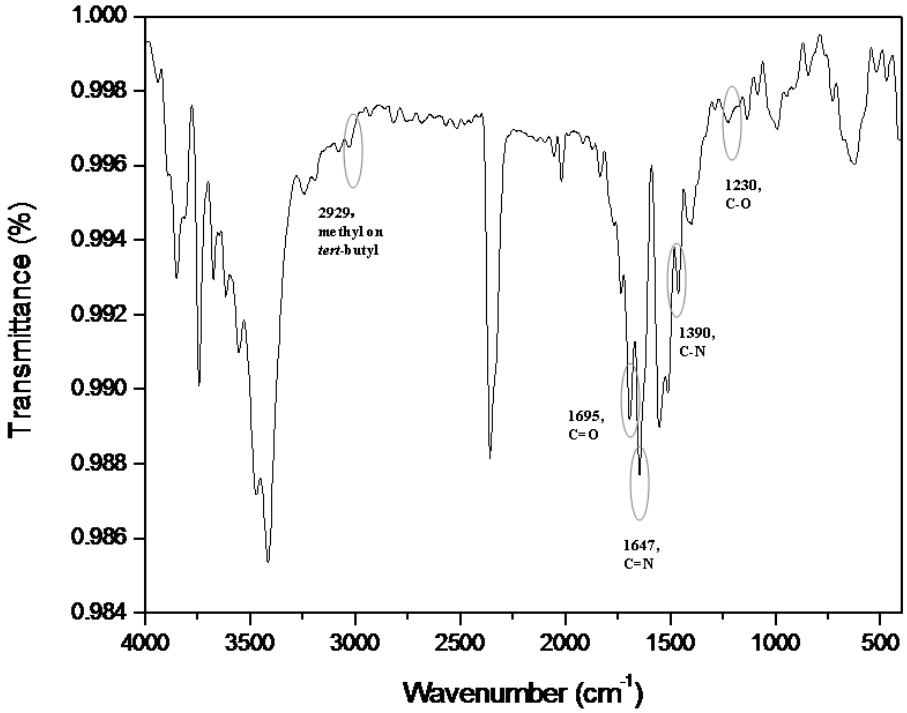


Fig. S16. FT-IR spectrum of

tert-butyl-3-(4-(methoxycarbonyl)phenyl)-1*H*-indazole-1- carboxylate (compound **8**)

S17. ^{1}H NMR spectrum of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

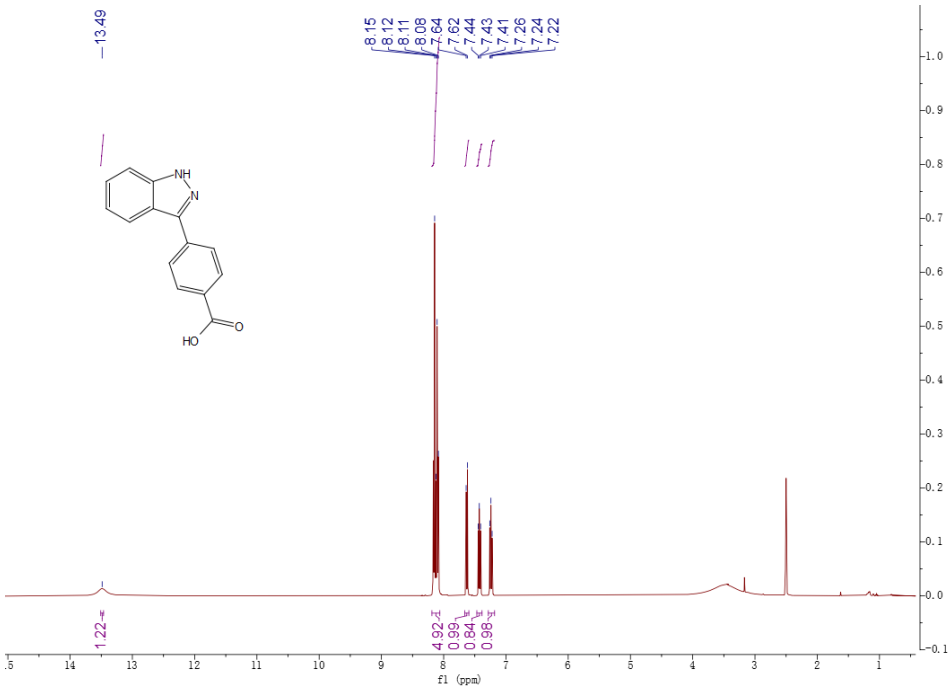


Fig. S17. ^{1}H NMR spectrum of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

^{1}H NMR (400 MHz, DMSO-d_6) δ_H, ppm: 13.49 (1H, s, COO*H*), 8.11 (5H, dd, *J* = 8.3, 16.0 Hz, Ar*H*), 7.63 (1H, d, *J* = 8.4 Hz, Ar*H*), 7.43 (1H, m, Ar*H*), 7.24 (1H, m, Ar*H*). Herein, the peak appeared at δ_H = 2.50 ppm means the solvent peak of DMSO-d_6. the peak of N*H* of compound **9** was not found due to influences of hydrogen bond as regular.

S18. ^{13}C NMR spectrum of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

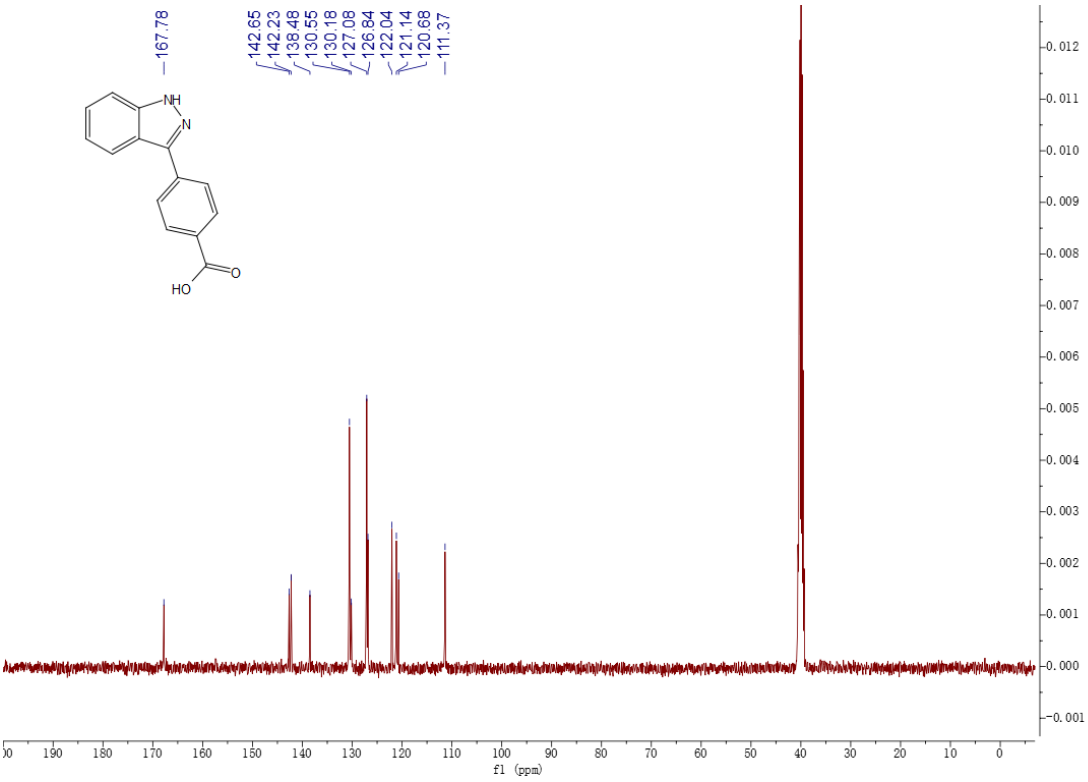


Fig. S18. ^{13}C NMR spectrum of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

S19. ESI-HRMS (TOF-SIMS) of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

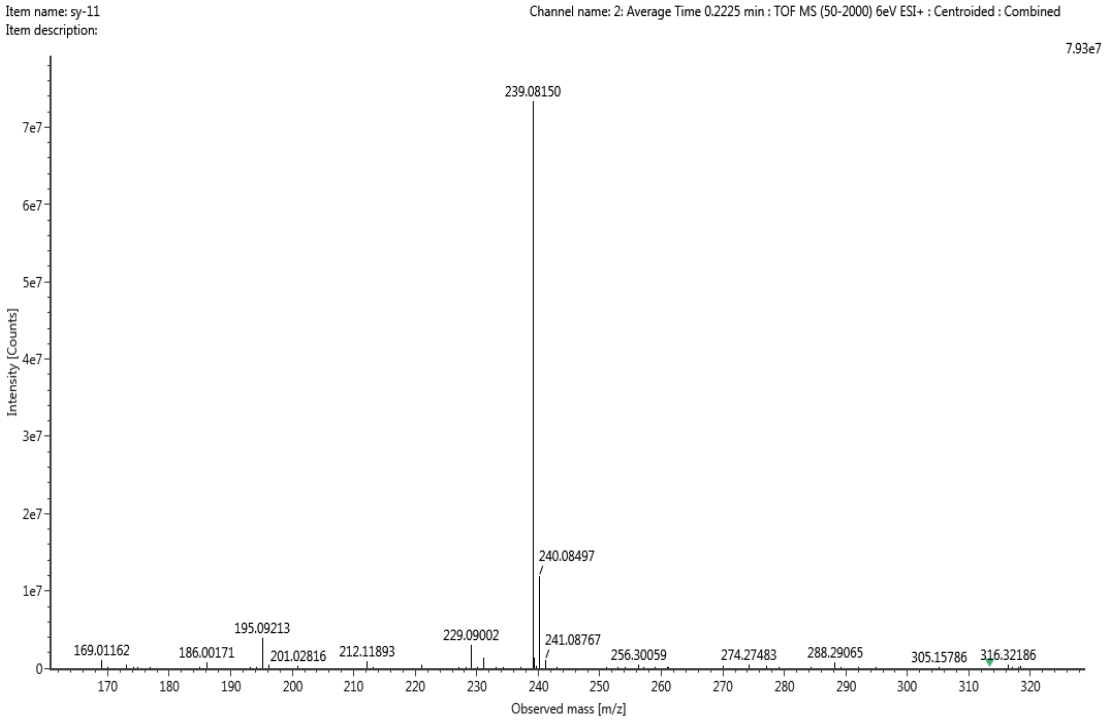


Fig. S19. ESI-HRMS (TOF-SIMS) of 4-(1*H*-indazole-3-yl)benzoic acid (compound **9**)

S20. ^{1}H NMR spectrum of *tert*-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

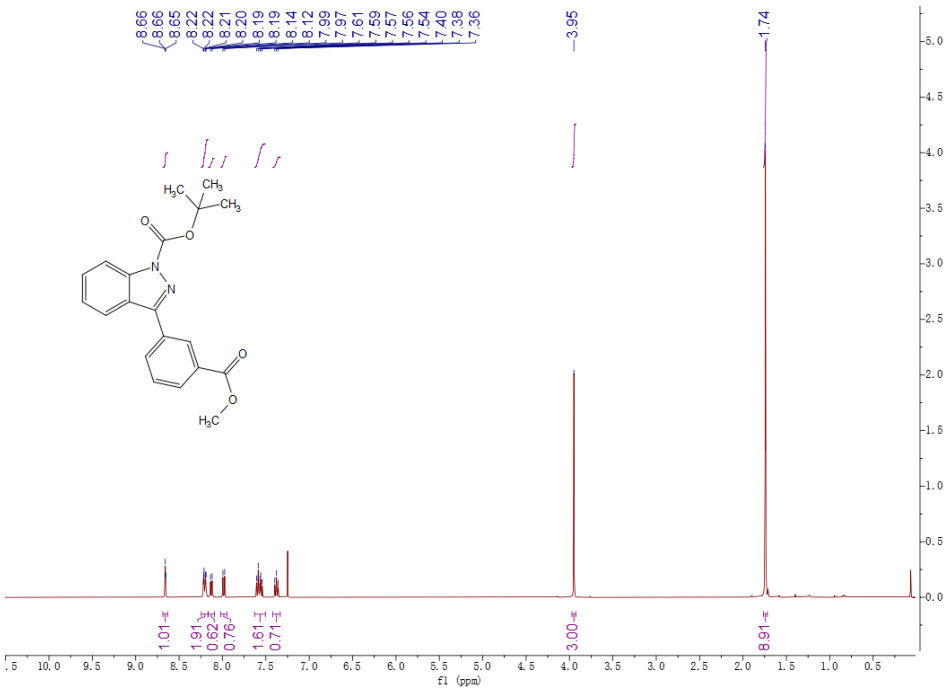


Fig. S20. ^{1}H NMR spectrum of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

S21. ^{13}C NMR spectrum of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

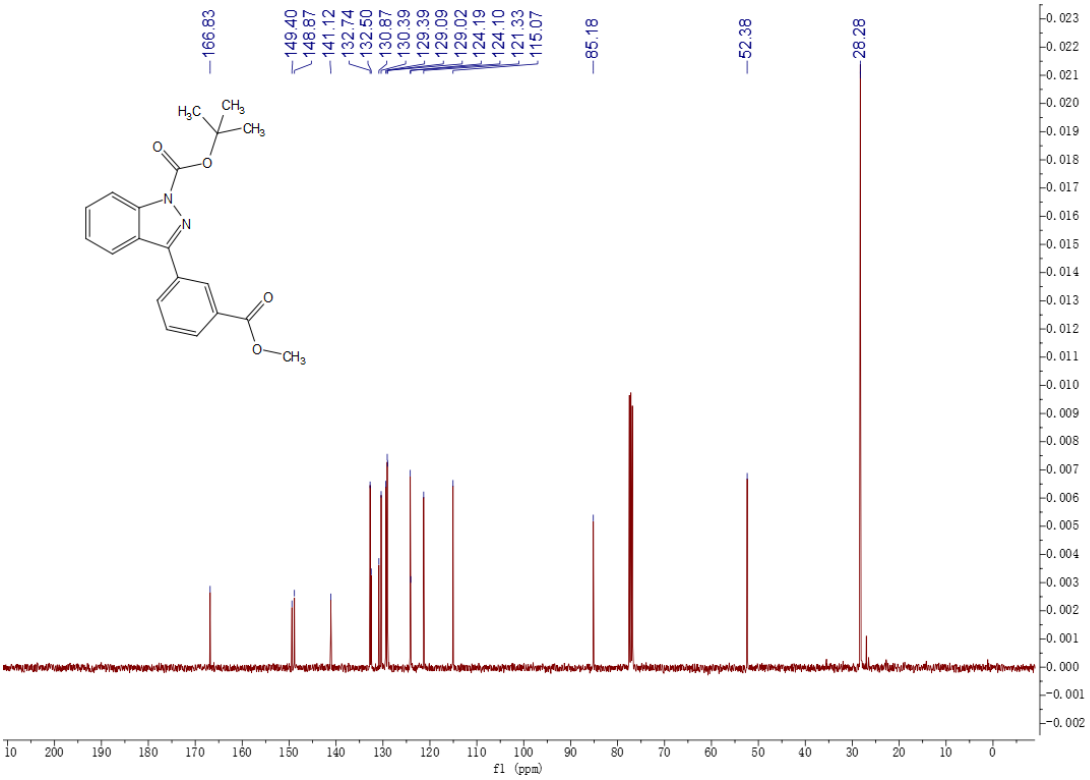


Fig. S21. ^{13}C NMR spectrum of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

S22. ESI-HRMS of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

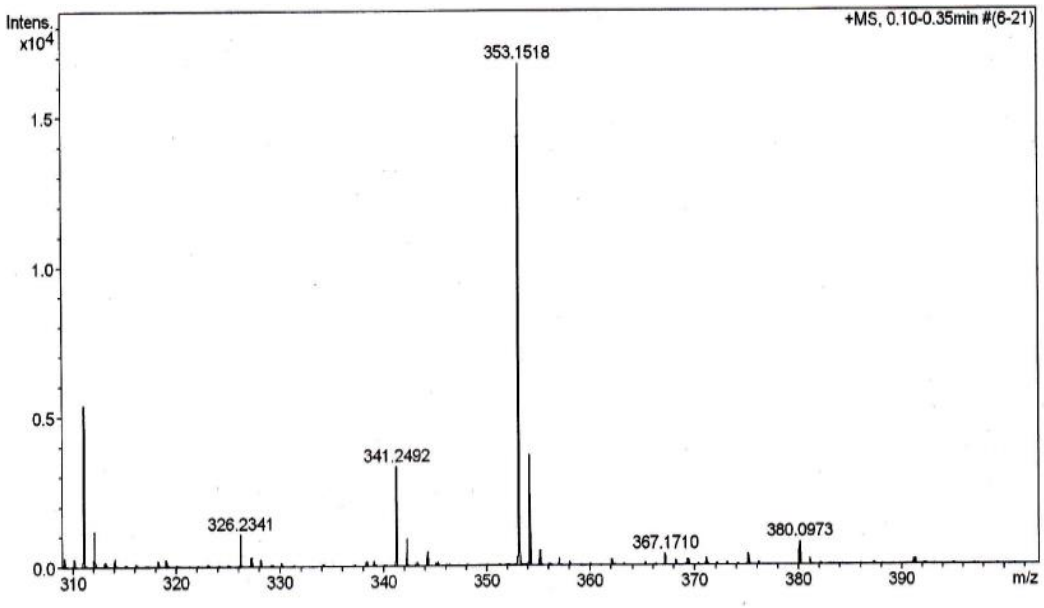


Fig. S22. ESI-HRMS of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

S23. FT-IR spectrum of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

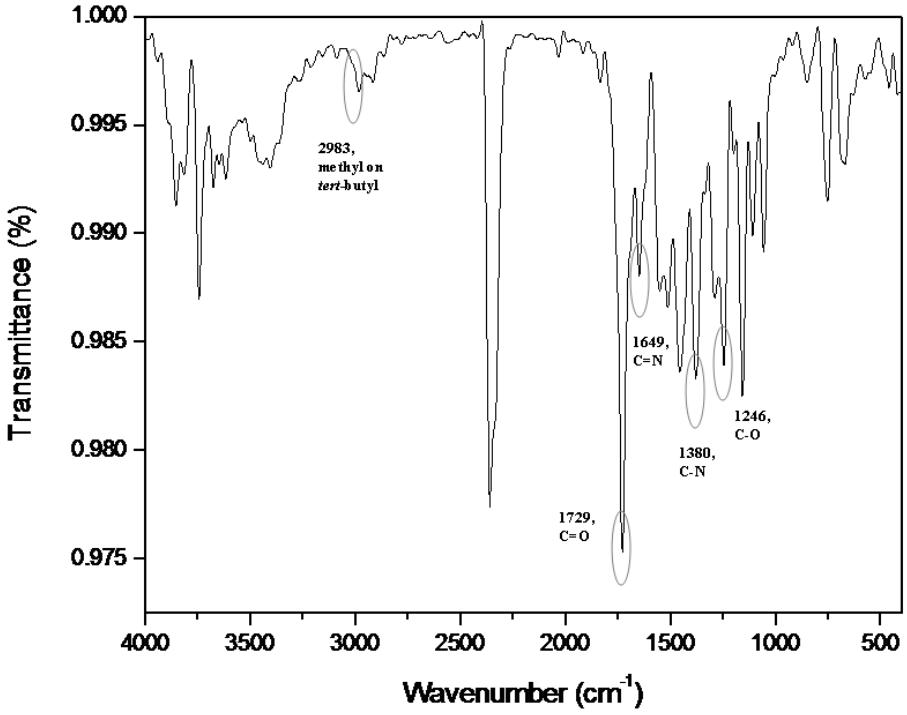


Fig. S23. FT-IR spectrum of

tert-butyl-3-(3-(methoxycarbonyl)phenyl)-1*H*-indazole-1-carboxylate (compound **11**)

S24. ^{1}H NMR spectrum of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

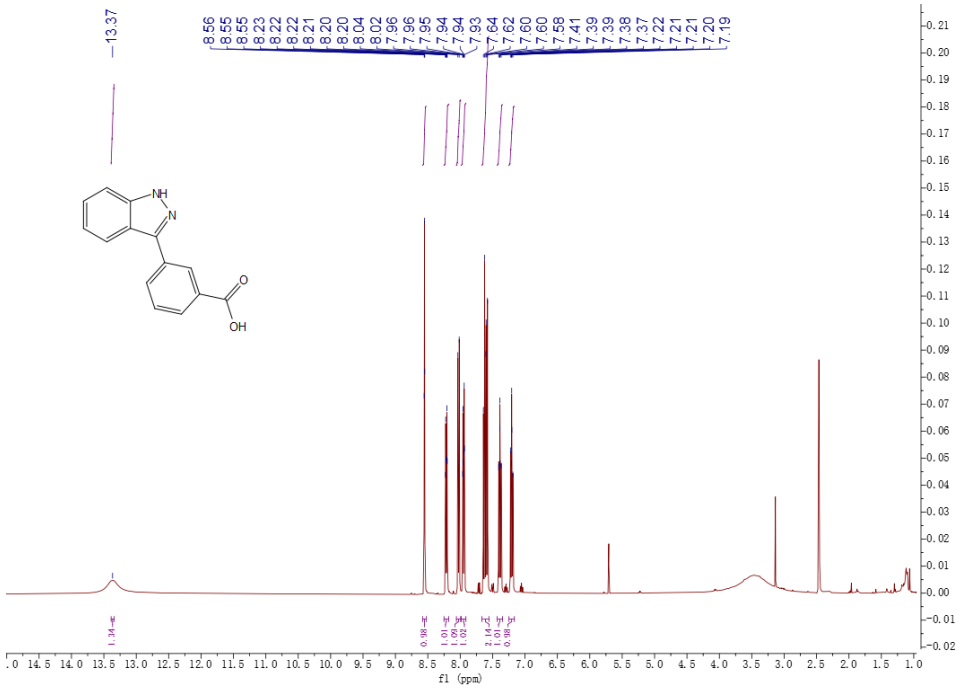


Fig. S24. ^{1}H NMR spectrum of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

S25. ^{13}C NMR spectrum of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

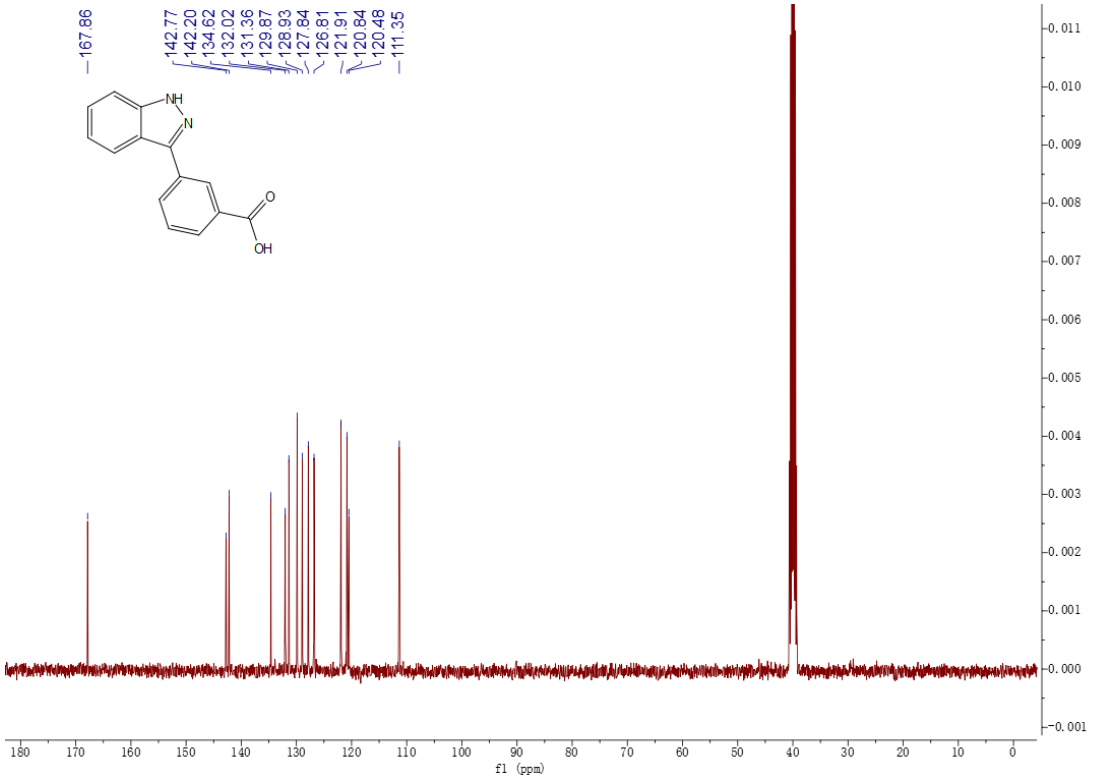


Fig. S25. ^{13}C NMR spectrum of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

S26. ESI-HRMS (TOF-SIMS) of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

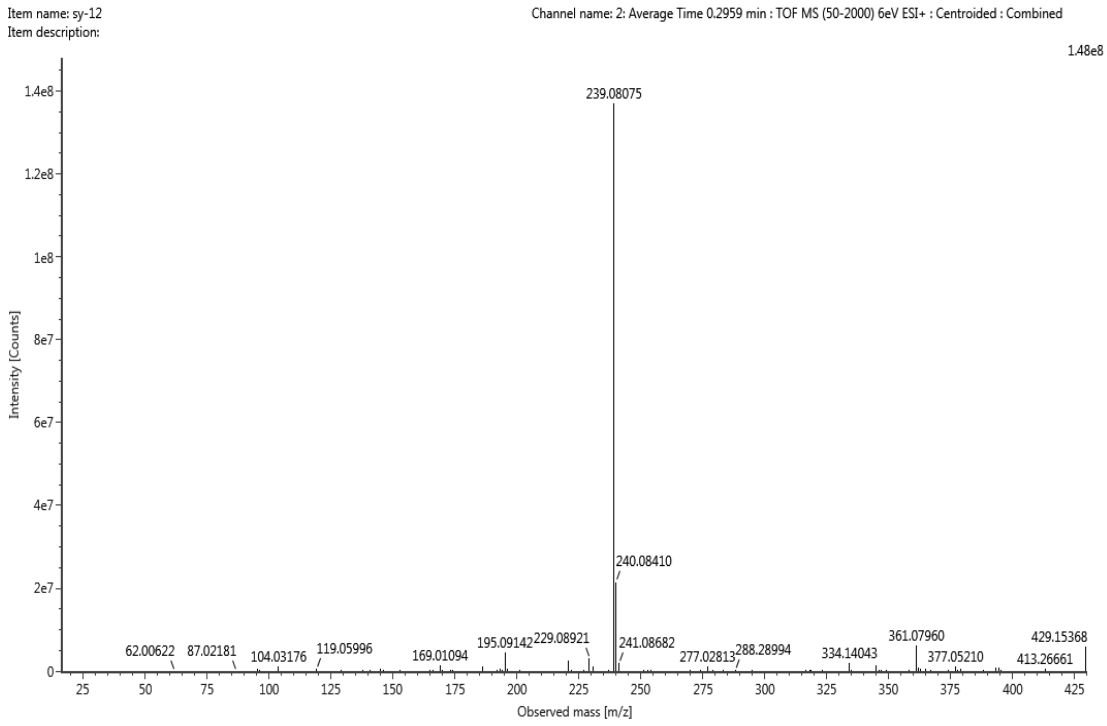


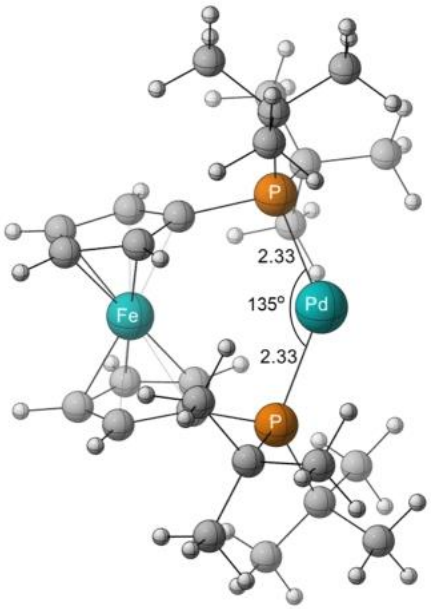
Fig. S26. ESI-HRMS (TOF-SIMS) of 3-(1*H*-indazole-3-yl)benzoic acid (compound **12**)

S27. Optimized structures from calculations

Optimized structures

(1) **L = dtbpf**

Precatalyst



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Zero-point correction= 0.640075 (Hartree/Particle)
Thermal correction to Energy= 0.676758
Thermal correction to Enthalpy= 0.677702
Thermal correction to Gibbs Free Energy= 0.577020
Sum of electronic and zero-point Energies= -3089.888203
Sum of electronic and thermal Energies= -3089.851521
Sum of electronic and thermal Enthalpies= -3089.850577
Sum of electronic and thermal Free Energies= -3089.951259

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C	1.03252600	2.92609400	1.66290700
C	1.61312400	3.45560400	0.47285300
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H	0.72128200	0.81651400	2.33016500
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H	1.68237600	4.50956100	0.20049100
H	2.55230300	2.46504500	-1.29065200
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H	-3.90898600	-2.69808900	1.61475600
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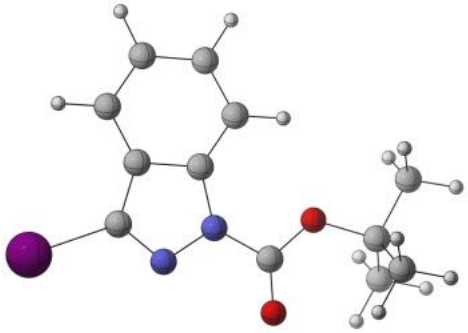
H	3.47388800	-2.19201300	-3.26192600
H	3.90814900	-2.69744100	-1.61516400
C	4.34068300	0.04025900	-1.88745900
H	4.29414700	1.08996400	-1.55430400
H	5.12899100	-0.46508500	-1.30644700
H	4.66953200	0.04258300	-2.94472600
C	3.49130600	-1.06412300	1.32967400
C	4.46305200	0.09537000	1.61562600
H	3.93232700	0.99786100	1.96163100
H	5.16616700	-0.20504200	2.41695900
H	5.06534400	0.37029900	0.73537900
C	4.28565700	-2.32672500	0.94572300
H	4.98626500	-2.15324700	0.11365600
H	4.88924000	-2.64850200	1.81556100
H	3.62154700	-3.16737300	0.67664600
C	2.71340400	-1.39394700	2.62223000
H	3.42851100	-1.71370500	3.40443100
H	2.16507100	-0.52539700	3.01860100
H	1.98910000	-2.21202700	2.46141000

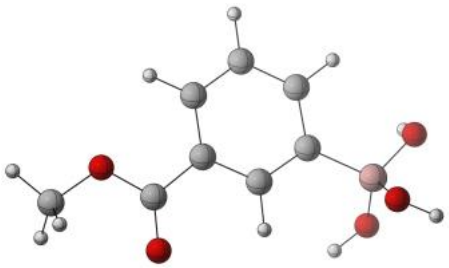
Substrate 3



E(RB3LYP) = -1022.30944128
Zero-point correction= 0.233336 (Hartree/Particle)
Thermal correction to Energy= 0.249463
Thermal correction to Enthalpy= 0.250407
Thermal correction to Gibbs Free Energy= 0.187522
Sum of electronic and zero-point Energies= -1022.076105
Sum of electronic and thermal Energies= -1022.059979
Sum of electronic and thermal Enthalpies= -1022.059034
Sum of electronic and thermal Free Energies= -1022.121919

C	0.34844600	1.10195600	0.00019600
C	-1.06543100	1.20090600	0.00016200
C	-1.70244200	2.45329100	0.00001900
C	-0.90491800	3.59151800	-0.00010100
C	0.50473700	3.48481500	-0.00000600
C	1.15494700	2.25282600	0.00016800
C	-1.50565700	-0.16893200	0.00014000
H	-2.79359000	2.52205700	-0.00000400
H	-1.36857500	4.58196300	-0.00026500
H	1.10725100	4.39812600	-0.00003500
H	2.24081300	2.18654600	0.00032600
N	-0.51293200	-1.01191700	0.00020800
N	0.63366100	-0.26672500	0.00034700
C	1.86794500	-0.96559400	0.00029700
O	2.86878300	-0.09757000	0.00039300
O	1.92532900	-2.16845200	0.00027700
C	4.29197200	-0.52223400	-0.00015000
C	5.04112900	0.81088200	-0.00025900
H	4.78789300	1.40238400	0.89619400
H	6.12894900	0.62815200	-0.00061100
H	4.78732900	1.40254800	-0.89644400
C	4.58732000	-1.31743300	1.27411200
H	4.04203600	-2.27314300	1.28913400
H	5.66893600	-1.53081500	1.32721900
H	4.30919500	-0.73203600	2.16783100
C	4.58650200	-1.31712300	-1.27478500
H	4.30772200	-0.73156700	-2.16819700
H	5.66810900	-1.53034900	-1.32864600
H	4.04134500	-2.27290700	-1.28965800
I	-3.49722100	-0.84153900	-0.00009100

Substrate 6



E(RB3LYP) = -711.551217003

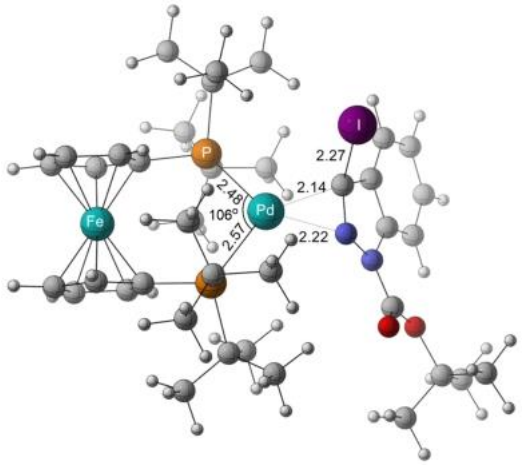
Zero-point correction= 0.178756 (Hartree/Particle)

Thermal correction to Energy= 0.193098

Thermal correction to Enthalpy= 0.194042
Thermal correction to Gibbs Free Energy= 0.137161
Sum of electronic and zero-point Energies= -711.372461
Sum of electronic and thermal Energies= -711.358119
Sum of electronic and thermal Enthalpies= -711.357175
Sum of electronic and thermal Free Energies= -711.414056

C	-1.12318100	0.28900300	0.00505700
C	0.11668600	-0.37608900	0.00990700
C	1.34747700	0.30625200	0.01662200
C	1.26972500	1.71248700	0.01525700
C	0.04801000	2.40197600	0.00801900
C	-1.15598500	1.69623400	0.00453800
H	0.09494400	-1.47176200	0.01175200
H	2.20797900	2.27887100	0.02182800
H	0.03399700	3.49777600	0.00813500
H	-2.11338700	2.22148500	0.00165700
C	-2.36796700	-0.52832200	-0.00108700
O	-3.48873800	0.22064500	0.00299200
O	-2.40297600	-1.74362400	-0.00958900
C	-4.73144900	-0.48019800	-0.00423900
H	-4.82220900	-1.12739800	0.88438000
H	-5.51535100	0.29082600	0.00691000
H	-4.82486500	-1.10377000	-0.90943400
B	2.80252200	-0.48624600	0.01957400
O	2.87566000	-1.23149800	1.28715400
H	3.74221000	-1.67222500	1.28077800
O	3.94538000	0.44478000	-0.04951000
H	4.02356700	0.73869000	-0.97008000
O	2.90325600	-1.37368800	-1.17112400
H	2.07996500	-1.88224300	-1.23763000

Int-1



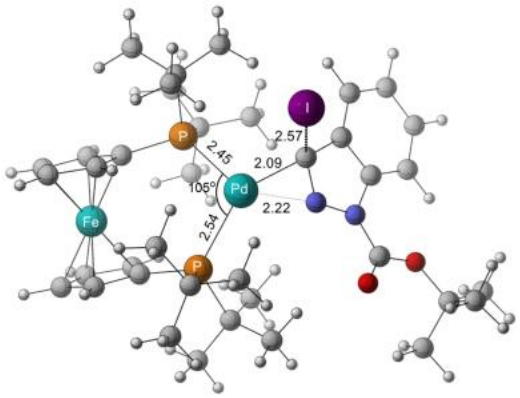
E(RB3LYP) = -4112.83489473
Zero-point correction= 0.874869 (Hartree/Particle)
Thermal correction to Energy= 0.929321
Thermal correction to Enthalpy= 0.930265
Thermal correction to Gibbs Free Energy= 0.788740
Sum of electronic and zero-point Energies= -4111.960025
Sum of electronic and thermal Energies= -4111.905574
Sum of electronic and thermal Enthalpies= -4111.904630
Sum of electronic and thermal Free Energies= -4112.046155

C	4.08613200	-0.53239800	0.65936400
C	5.43736700	-0.12944600	0.44760800
C	5.69220700	-0.18364100	-0.95429700
C	4.50308500	-0.63343500	-1.60336400
C	3.48454400	-0.86416900	-0.61010200
H	3.58661300	-0.56038200	1.62306400
H	6.13500500	0.19823300	1.21896700
H	6.62133000	0.09477300	-1.45306400
H	4.40348400	-0.75699500	-2.67892500
Fe	4.11555000	1.11997100	-0.55719000
C	4.16902100	2.80316100	-1.78149600
C	4.77604900	3.09497700	-0.52530500
C	2.82733600	2.39330200	-1.53011600
H	4.65029700	2.84969200	-2.75886700
C	3.80283100	2.87943700	0.49685600
H	5.80932200	3.40379600	-0.36271200
C	2.57160300	2.44137600	-0.11012400
H	2.11946100	2.08596100	-2.29377200
H	3.99643300	3.00891100	1.55854600
P	0.89554300	2.08703700	0.59499800
P	1.79290000	-1.60762500	-0.72244000

Pd	-0.05333000	-0.27584400	0.25116600
C	-0.09714100	3.59032200	-0.16707100
C	-1.30926100	3.98296300	0.69579500
H	-1.91102100	4.72165400	0.13211700
H	-1.97074900	3.13320200	0.91967900
H	-1.01458600	4.46674200	1.64016900
C	0.77309100	4.84399600	-0.38310000
H	1.21829800	5.21084000	0.55607600
H	1.58818400	4.67371000	-1.10347100
H	0.13585700	5.65433600	-0.78714700
C	-0.63471800	3.10003500	-1.52911300
H	-1.23527800	3.90370200	-1.99668500
H	0.17037000	2.84362800	-2.23619700
H	-1.28078400	2.21262500	-1.41236000
C	1.05904600	2.33203800	2.50820400
C	1.48682200	3.74308800	2.95599000
H	0.71783700	4.50035400	2.73692200
H	1.63691700	3.74178600	4.05283800
H	2.42927400	4.07730200	2.49547000
C	2.07526800	1.29150600	3.02645500
H	1.77357700	0.26896900	2.73989000
H	3.09935600	1.46358500	2.66559300
H	2.09890200	1.33690500	4.13163100
C	-0.29147700	1.97756500	3.16958600
H	-0.16116700	1.99950900	4.26830400
H	-1.09613600	2.68255200	2.91944000
H	-0.62588100	0.96649900	2.88372900
C	1.41637300	-1.80019300	-2.61615600
C	1.48696900	-0.40033000	-3.26000400
H	0.82276200	0.30809500	-2.73631000
H	2.50194700	0.02108700	-3.27623700
H	1.13826700	-0.47388400	-4.30741800
C	-0.04106900	-2.27615200	-2.78084500
H	-0.74798400	-1.57269900	-2.31231800
H	-0.27585900	-2.33153900	-3.86087400
H	-0.22477100	-3.27114200	-2.35253800
C	2.33720800	-2.76707600	-3.38531300
H	3.40839600	-2.54786300	-3.25775500
H	2.16712100	-3.81669100	-3.09722000
H	2.10988100	-2.68936100	-4.46578600
C	2.19230700	-3.36126900	0.03586900
C	3.53424100	-3.95747700	-0.43135500
H	4.38413800	-3.29556300	-0.19834000

H	3.70148100	-4.91192900	0.10448300
H	3.55602800	-4.17985300	-1.50826300
C	1.05531300	-4.34889500	-0.27865000
H	1.02768000	-4.63805000	-1.34130700
H	1.21097100	-5.27512900	0.30598700
H	0.07136800	-3.94122200	0.00234700
C	2.26077900	-3.18413000	1.56835800
H	2.32538600	-4.18281600	2.04078400
H	3.15397300	-2.62246700	1.88160100
H	1.36699600	-2.68012200	1.96963500
C	-3.43157700	-1.10109100	-0.90289500
C	-2.62171400	-2.11266900	-0.34101900
C	-2.72913100	-3.43238400	-0.79236700
C	-3.61539500	-3.71932100	-1.83246900
C	-4.38176200	-2.69579500	-2.41748700
C	-4.30567000	-1.37531800	-1.96410100
C	-1.80237000	-1.44097200	0.67419300
H	-2.13805900	-4.22637900	-0.33014000
H	-3.71279300	-4.74628900	-2.19660100
H	-5.06355000	-2.93464400	-3.23956700
H	-4.91412900	-0.59286600	-2.41195300
N	-2.20134400	-0.15606200	0.80606000
N	-3.16880700	0.07971200	-0.18068600
C	-3.98687200	1.20359800	-0.02409300
O	-4.84303000	1.29489000	-1.04349100
O	-3.88982600	1.97010300	0.90850400
C	-5.87751600	2.34777300	-1.12141100
C	-6.61934200	1.99997000	-2.41405900
H	-7.07463100	0.99696200	-2.34698700
H	-7.42210100	2.73453700	-2.59594600
H	-5.93018800	2.01608700	-3.27584800
C	-6.81576100	2.24883000	0.08542000
H	-6.29438300	2.49363100	1.02284900
H	-7.65404200	2.95517400	-0.04473300
H	-7.23495800	1.23046600	0.16510800
C	-5.20759200	3.72064600	-1.23314300
H	-4.49874400	3.73525000	-2.07966300
H	-5.97713900	4.49059000	-1.41656300
H	-4.66473300	3.97888800	-0.31169900
I	-1.56589500	-2.55641100	2.63309000

TS-1



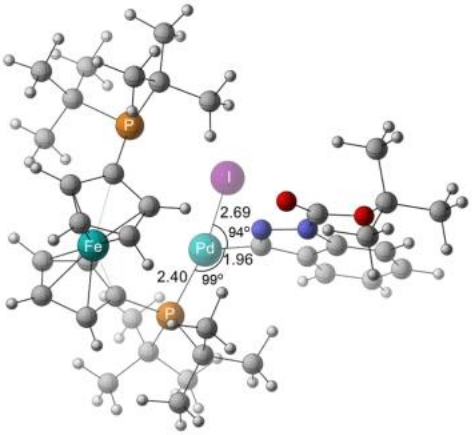
E(RB3LYP) = -4112.83362087
Zero-point correction= .875525 (Hartree/Particle)
Thermal correction to Energy= 0.929136
Thermal correction to Enthalpy= 0.930080
Thermal correction to Gibbs Free Energy= 0.791421
Sum of electronic and zero-point Energies= -4111.958096
Sum of electronic and thermal Energies= -4111.904485
Sum of electronic and thermal Enthalpies= -4111.903541
Sum of electronic and thermal Free Energies= -4112.042200

C	-4.08986200	-0.51520100	-0.90308100
C	-5.46425400	-0.15756900	-0.78129800
C	-5.82428000	-0.27227000	0.59329000
C	-4.67621800	-0.71216100	1.31708600
C	-3.57688900	-0.87545600	0.39761400
H	-3.52015600	-0.49709600	-1.82723400
H	-6.11020500	0.17994800	-1.59228400
H	-6.79668400	-0.03848000	1.02811100
H	-4.65694500	-0.87399400	2.39185300
F	-4.25680600	1.08595600	0.36855100
C	-4.45758200	2.73096000	1.63324000
C	-4.95020800	3.05303800	0.33553600
C	-3.09242900	2.34694000	1.49733900
H	-5.02759900	2.74176500	2.56266400
C	-3.88475900	2.88122600	-0.59811800
H	-5.96850800	3.35334800	0.08644400
C	-2.70881600	2.43698600	0.10785000
H	-2.45474200	2.03024200	2.31653400
H	-3.98266400	3.04210400	-1.66830900
P	-0.98379200	2.09902500	-0.46602000
P	-1.88778900	-1.59080700	0.62634300
P	-0.01406300	-0.22284600	-0.15761800
C	-0.02289800	3.51332300	0.47501100

C	1.27133700	3.91419400	-0.25327600
H	1.84809600	4.58691500	0.40980700
H	1.91692400	3.05540600	-0.48855100
H	1.07653500	4.47313700	-1.18223600
C	-0.87806300	4.77804900	0.68742300
H	-1.22936800	5.21043800	-0.26350200
H	-1.75701200	4.59258000	1.32399700
H	-0.25802600	5.54408800	1.19136900
C	0.38014300	2.92923100	1.84652100
H	0.95189700	3.69023100	2.41080700
H	-0.48824600	2.65323200	2.46524300
H	1.01795900	2.03533400	1.73282500
C	-0.97190400	2.44288100	-2.36961100
C	-1.35073200	3.88466600	-2.76071500
H	-0.59084300	4.61429900	-2.43929800
H	-1.41745700	3.95055300	-3.86348200
H	-2.32120500	4.20573600	-2.35193400
C	-1.94392200	1.44280800	-3.03317000
H	-1.66992600	0.40329100	-2.78311000
H	-2.99588600	1.59968000	-2.75691700
H	-1.86862900	1.55301100	-4.13111500
C	0.42585100	2.11451500	-2.93999100
H	0.38555100	2.22373400	-4.04016400
H	1.21781100	2.77937700	-2.57087000
H	0.72322200	1.07783200	-2.71154000
C	-1.65651000	-1.83754900	2.53591000
C	-1.82248000	-0.46586200	3.22018200
H	-1.13306000	0.27669500	2.78491800
H	-2.84569200	-0.06955200	3.16193000
H	-1.56538200	-0.57243100	4.29068200
C	-0.20691300	-2.28327600	2.81054400
H	0.51963500	-1.54405100	2.43809100
H	-0.06934400	-2.37834500	3.90417500
H	0.04016500	-3.25539200	2.36284600
C	-2.61303300	-2.85836700	3.18317300
H	-3.67492700	-2.66514300	2.96810100
H	-2.38436900	-3.89093800	2.87545400
H	-2.48419800	-2.81343200	4.28126400
C	-2.16211500	-3.31515800	-0.23387200
C	-3.52206700	-3.96020600	0.09896100
H	-4.36851200	-3.30867200	-0.17204900
H	-3.61902500	-4.89156800	-0.49138100
H	-3.62241400	-4.23438000	1.15925200

C	-1.02941000	-4.28702900	0.14040300
H	-1.08075200	-4.60992200	1.19244800
H	-1.11995400	-5.19622800	-0.48290900
H	-0.03659600	-3.85267400	-0.05597500
C	-2.11195300	-3.07231000	-1.75815900
H	-2.09611900	-4.05154300	-2.27272700
H	-3.00056000	-2.53341800	-2.12050600
H	-1.20833900	-2.52163300	-2.06402100
C	3.54703000	-0.97681800	1.05348700
C	2.62726300	-1.98086200	0.67164900
C	2.70785000	-3.25980300	1.23622300
C	3.68762200	-3.51128600	2.19594400
C	4.57776600	-2.49428400	2.59079200
C	4.52643400	-1.21688700	2.02877700
C	1.74578500	-1.34692700	-0.31045200
H	2.02511600	-4.04973800	0.91654600
H	3.76689300	-4.50508900	2.64613100
H	5.33504600	-2.70732100	3.35161200
H	5.22553000	-0.44093400	2.33270700
N	2.16706000	-0.11417300	-0.55667400
N	3.25120700	0.16227500	0.27885800
C	4.07169300	1.25135100	-0.04023200
O	5.06001600	1.35603000	0.84786700
O	3.86597700	1.97973900	-0.98516900
C	6.12413300	2.37806600	0.73838100
C	7.02324200	2.06000300	1.93507100
H	7.43552400	1.03951700	1.85525700
H	7.86445700	2.77267000	1.97257600
H	6.45800700	2.13803200	2.87969600
C	6.88607300	2.19588700	-0.57768800
H	6.24749800	2.41402600	-1.44675000
H	7.75082700	2.88169800	-0.59677600
H	7.26583700	1.16272800	-0.66357400
C	5.51284900	3.77566800	0.87466400
H	4.92341900	3.84928500	1.80539400
H	6.32150400	4.52575700	0.92077500
H	4.86123400	4.01487300	0.02106800
I	1.78716500	-2.75816400	-2.46357400

Int-2



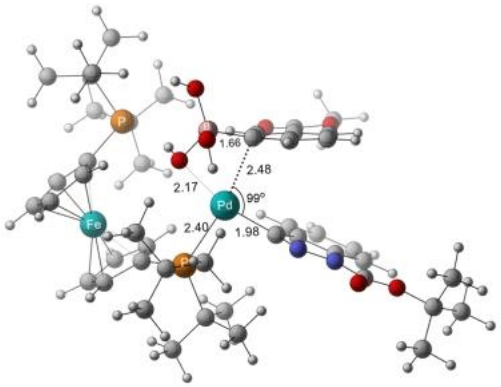
E(RB3LYP) = -4112.87675896
Zero-point correction= 0.874965 (Hartree/Particle)
Thermal correction to Energy= 0.929964
Thermal correction to Enthalpy= 0.930908
Thermal correction to Gibbs Free Energy= 0.785585
Sum of electronic and zero-point Energies= -4112.001794
Sum of electronic and thermal Energies= -4111.946795
Sum of electronic and thermal Enthalpies= -4111.945851
Sum of electronic and thermal Free Energies= -4112.091174

C	3.00177200	-1.57731600	-0.60714200
C	4.19757000	-1.35397800	-1.35072300
C	3.89414000	-1.52028400	-2.73359900
C	2.51402300	-1.85634900	-2.84816900
C	1.94015500	-1.91938100	-1.52590400
H	2.91279500	-1.50473600	0.47678700
H	5.16743800	-1.08286900	-0.93637300
H	4.58599300	-1.38532800	-3.56564700
H	1.99727200	-2.03528400	-3.78866000
F	2.71901800	-0.00129100	-1.92648000
C	1.59923300	1.37728800	-3.00236700
C	2.99156900	1.61404300	-3.20060600
C	1.32736900	1.50533100	-1.60589700
H	0.87686900	1.12346700	-3.77728300
C	3.57321100	1.90468100	-1.92951300
H	3.52696400	1.55772100	-4.14942200
C	2.54503200	1.86867900	-0.92371700
H	0.35642100	1.34956600	-1.13331900
H	4.62829300	2.11863600	-1.76668800
P	2.49250600	2.36735700	0.85936700
P	0.35163200	-2.64565200	-0.95300000
P	-0.15613800	-1.61880600	1.15857300

C	1.79910500	4.17633600	0.67176400
C	2.00789700	4.95710700	1.98382100
H	1.43654600	5.90405900	1.93607800
H	1.64069100	4.39517000	2.86124900
H	3.06253500	5.22413000	2.15897400
C	2.37163400	4.97688200	-0.51080100
H	3.45675200	5.14489400	-0.42423900
H	2.18040300	4.47344900	-1.47334200
H	1.88454100	5.97130000	-0.55352200
C	0.27666000	4.01681300	0.46899300
H	-0.19374400	5.01892400	0.43482800
H	0.02210600	3.50557100	-0.47258300
H	-0.18854000	3.45393300	1.29748400
C	4.31778500	2.44596500	1.48548000
C	5.22100400	3.55017800	0.90767800
H	4.88331900	4.55913800	1.19417400
H	6.24900000	3.42790500	1.30224500
H	5.28451700	3.51377700	-0.19224500
C	4.95551600	1.07262100	1.19653800
H	4.32705300	0.24297500	1.56644600
H	5.13425900	0.91314400	0.12343900
H	5.93143300	1.00748500	1.71483100
C	4.24953000	2.59375000	3.02354700
H	5.27125600	2.52226000	3.44364000
H	3.82929900	3.55907200	3.34454300
H	3.64138600	1.79138700	3.47730800
C	-0.89500200	-2.64813600	-2.42067700
C	-0.93889100	-1.22110000	-3.00404100
H	-1.14449900	-0.46254600	-2.23244800
H	-0.00170700	-0.95389700	-3.51254200
H	-1.75193200	-1.17656900	-3.75277800
C	-2.30297700	-2.99967400	-1.89491500
H	-2.65683900	-2.27867500	-1.14484100
H	-3.00719100	-2.97130400	-2.74695800
H	-2.36012400	-4.00676900	-1.45610600
C	-0.53759200	-3.63959800	-3.54718100
H	0.48048200	-3.50383400	-3.94277500
H	-0.65143300	-4.68954200	-3.23580000
H	-1.24036400	-3.47288000	-4.38472900
C	0.88508400	-4.46292800	-0.50893600
C	1.81440200	-5.08500900	-1.56882500
H	2.74319200	-4.50372900	-1.68986300
H	2.09866900	-6.10003500	-1.23220800

H	1.34078700	-5.18849500	-2.55541300
C	-0.35944900	-5.34603500	-0.29817800
H	-0.89171000	-5.56440200	-1.23718300
H	-0.03825300	-6.31549400	0.12596000
H	-1.07104700	-4.89226700	0.41422500
C	1.66059800	-4.41613400	0.82531200
H	1.99698800	-5.43990400	1.07370600
H	2.55944000	-3.78146300	0.77283600
H	1.03087500	-4.07394400	1.66684600
C	-3.96242700	-0.01096800	0.50828300
C	-3.14285100	-1.02073900	1.06946200
C	-3.70532400	-2.05548900	1.83364700
C	-5.08363100	-2.06297600	2.02550700
C	-5.89148800	-1.04945100	1.46471000
C	-5.35382000	-0.01279700	0.70271400
C	-1.79548400	-0.68112300	0.65113600
H	-3.06648100	-2.83073900	2.26481200
H	-5.54891700	-2.85658400	2.61726200
H	-6.97278800	-1.07488700	1.63181800
H	-5.98828600	0.76240200	0.27814700
N	-1.78863200	0.40328800	-0.06814900
N	-3.09579500	0.84223800	-0.18158900
C	-3.34337300	1.98592200	-0.96182600
O	-4.64590900	2.25424700	-0.97027300
O	-2.46621300	2.59719700	-1.52461400
C	-5.21956300	3.39339300	-1.72319500
C	-6.71651900	3.27105600	-1.43236400
H	-6.91202500	3.34998400	-0.34919600
H	-7.26544100	4.07906900	-1.94492500
H	-7.10701200	2.30313100	-1.79075400
C	-4.66225200	4.70832900	-1.17098300
H	-3.58317100	4.80138200	-1.36491900
H	-5.17990400	5.55530000	-1.65382600
H	-4.83714600	4.77442100	-0.08291100
C	-4.93831200	3.21656500	-3.21818200
H	-5.30476800	2.23488800	-3.56623800
H	-5.46948400	4.00105200	-3.78461700
H	-3.86294200	3.29425900	-3.43782500
I	-0.24705700	-0.73240900	3.69953400

Int-3



E(RB3LYP) = -4526.46989970
Zero-point correction= 1.056604 (Hartree/Particle)
Thermal correction to Energy= 1.124397
Thermal correction to Enthalpy= 1.125341
Thermal correction to Gibbs Free Energy= 0.954410
Sum of electronic and zero-point Energies= -4525.413295
Sum of electronic and thermal Energies= -4525.345503
Sum of electronic and thermal Enthalpies= -4525.344559
Sum of electronic and thermal Free Energies= -4525.515489

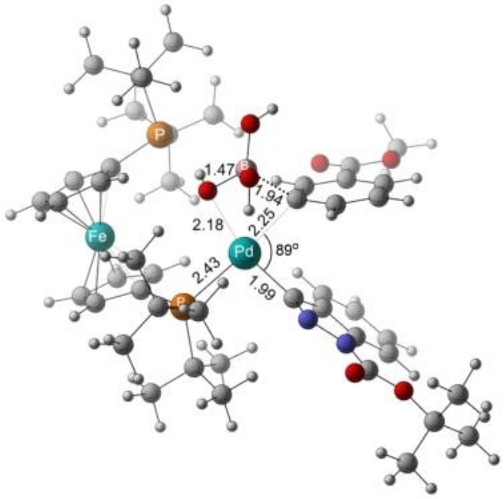
C	-4.26765000	-1.33797600	0.88055500
C	-4.88021500	-2.58571800	0.56236100
C	-5.61421000	-2.41054400	-0.64944300
C	-5.46366900	-1.05309500	-1.06651900
C	-4.64286300	-0.35947500	-0.11085200
H	-3.60365700	-1.15077900	1.72183400
H	-4.78232500	-3.51384300	1.12595300
H	-6.16825500	-3.18333700	-1.18380300
H	-5.90330700	-0.62851400	-1.96794000
F	-3.60935600	-2.00226500	-0.97046400
C	-2.84827400	-1.98432700	-2.90802000
C	-3.16219800	-3.31712400	-2.50329900
C	-1.87026300	-1.47197900	-2.00669600
H	-3.29379200	-1.44817600	-3.74557400
C	-2.38296600	-3.62593500	-1.34953900
H	-3.89818500	-3.97391700	-2.96810800
C	-1.54501200	-2.49180800	-1.04266700
H	-1.41400300	-0.48327100	-2.04260800
H	-2.40925800	-4.57314200	-0.81369400
P	0.02932000	-2.43897600	-0.10178400
P	-4.21635300	1.41684300	0.15763400
P	0.42234300	-0.20066000	0.66856200
C	1.22389300	-3.26427400	-1.40043500

C	2.57826500	-3.61842900	-0.75364100
H	3.28097700	-3.91062000	-1.55629000
H	3.02064200	-2.77177700	-0.20752200
H	2.50110300	-4.47719100	-0.06765500
C	0.61942800	-4.53544700	-2.03677500
H	0.34246000	-5.30927700	-1.30807400
H	-0.26185200	-4.30962100	-2.65615200
H	1.38713800	-4.97303500	-2.70214400
C	1.45213700	-2.25772700	-2.54432400
H	2.08040700	-2.74271500	-3.31460800
H	0.50803400	-1.96065400	-3.03040200
H	1.97294700	-1.35182500	-2.21029300
C	-0.10104200	-3.53844900	1.48141000
C	-0.13052200	-5.05738400	1.21848500
H	0.80504300	-5.43802500	0.78199300
H	-0.26382100	-5.56670800	2.19101800
H	-0.97047400	-5.36497300	0.57600800
C	-1.39442200	-3.15206800	2.22513400
H	-1.43417700	-2.07989200	2.46806400
H	-2.29082100	-3.40438200	1.63714200
H	-1.43543000	-3.72647700	3.16968200
C	1.10987300	-3.22006300	2.38495500
H	0.99908400	-3.77493300	3.33481100
H	2.06930100	-3.51591600	1.93435500
H	1.17511300	-2.14500500	2.62158900
C	-4.44571000	2.34880700	-1.51357300
C	-3.59678300	1.60993100	-2.56591700
H	-2.55008200	1.49925800	-2.23347400
H	-3.99142800	0.60998100	-2.79902700
H	-3.58673000	2.19963300	-3.50237700
C	-3.81990500	3.75243700	-1.33889100
H	-2.75731400	3.69228600	-1.04601800
H	-3.86775700	4.28966800	-2.30573400
H	-4.34803200	4.36954000	-0.59607600
C	-5.88545600	2.49597200	-2.03727500
H	-6.40350400	1.52811700	-2.13846900
H	-6.49874100	3.14535500	-1.39189300
H	-5.86220400	2.96543900	-3.04008600
C	-5.62986400	1.91955900	1.39253000
C	-7.03663400	1.42016700	1.02027900
H	-7.06436400	0.32276500	0.91149100
H	-7.74565700	1.69144500	1.82718300
H	-7.41564400	1.86533100	0.08764600

C	-5.64077800	3.45096300	1.56327300
H	-6.02406900	3.97427700	0.67228000
H	-6.30481500	3.71747100	2.40766000
H	-4.63538200	3.84583100	1.79501400
C	-5.23603000	1.30037200	2.75148000
H	-5.93651200	1.65746900	3.53077400
H	-5.29646300	0.19956100	2.73787600
H	-4.21322900	1.58765000	3.04632100
C	4.16375500	0.65177500	-1.08028300
C	2.75075200	0.70767300	-1.15118900
C	2.12032900	1.42576800	-2.18096500
C	2.91322000	2.08093000	-3.11826900
C	4.32180400	2.02347300	-3.03246100
C	4.96967000	1.31474300	-2.02178900
C	2.27393300	-0.08842900	-0.03036200
H	1.02950800	1.46961500	-2.23652800
H	2.44586900	2.64593500	-3.93018400
H	4.92485700	2.54806500	-3.78007600
H	6.05569900	1.27686300	-1.96741000
N	3.28680600	-0.57399900	0.63855600
N	4.45350700	-0.14377500	0.02976300
C	5.67776400	-0.56302000	0.57878300
O	6.68803500	-0.05734900	-0.12527600
O	5.74883700	-1.27928800	1.54884200
C	8.10387700	-0.32793000	0.21011800
C	8.86203400	0.45155200	-0.86618200
H	8.62211000	1.52732400	-0.81180900
H	9.94903800	0.32971200	-0.72267600
H	8.60039600	0.08344600	-1.87309900
C	8.41691800	0.22300600	1.60435300
H	7.86612900	-0.32238400	2.38525500
H	9.49826600	0.12352200	1.80257200
H	8.15445600	1.29382600	1.66339200
C	8.38345600	-1.82926200	0.09448800
H	8.09879700	-2.19848800	-0.90638500
H	9.46327600	-2.01177300	0.23293300
H	7.83139500	-2.40079600	0.85551100
C	1.26732400	3.38971700	0.55590300
C	0.28238500	2.50752200	1.04805400
C	0.48162400	1.73558100	2.21520000
C	1.74748500	1.85206800	2.84565800
C	2.73428000	2.70832600	2.36344800
C	2.49424000	3.48759200	1.22153400

H	-0.68881900	2.49935100	0.54416700
H	1.93179800	1.26507000	3.75133700
H	3.69733500	2.78635800	2.87744400
H	3.26040100	4.17042500	0.84906100
C	0.94844800	4.20406200	-0.65154200
O	1.92966200	5.05831900	-0.97881600
O	-0.08752200	4.12039300	-1.28207900
C	1.71305600	5.88871700	-2.12163700
H	0.81722300	6.51608800	-1.98218400
H	2.60938100	6.51853800	-2.21139500
H	1.58602500	5.27488300	-3.02876100
B	-0.78760100	0.94753200	2.93223200
O	-1.73104300	1.93192700	3.41777900
H	-2.26333200	1.51166200	4.11291600
O	-0.40717500	0.06247800	4.01545300
H	0.15947600	-0.66008300	3.70819600
O	-1.41550600	0.09893800	1.79206000
H	-2.07867700	0.63293800	1.30169100

TS-2



E(RB3LYP) = -4526.46245469
Zero-point correction= .054833 (Hartree/Particle)
Thermal correction to Energy= 1.122349
Thermal correction to Enthalpy= 1.123293
Thermal correction to Gibbs Free Energy= 0.953228
Sum of electronic and zero-point Energies= -4525.407621
Sum of electronic and thermal Energies= -4525.340106
Sum of electronic and thermal Enthalpies= -4525.339161
Sum of electronic and thermal Free Energies= -4525.509227

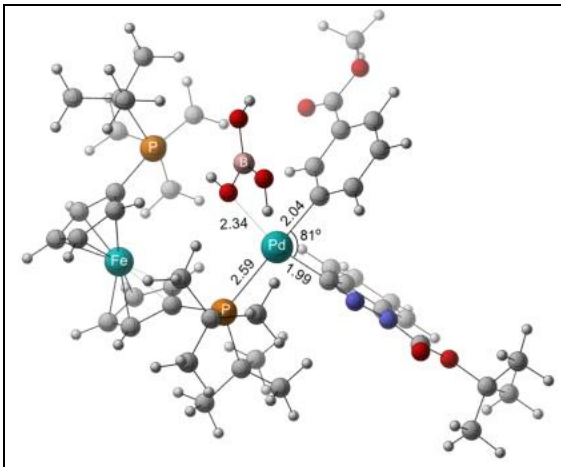
C	4.15810400	-1.56336400	-1.03699800

C	4.73057600	-2.84155900	-0.76782500
C	5.54936800	-2.71270300	0.39397200
C	5.49175600	-1.35368400	0.82862700
C	4.64320200	-0.61321800	-0.06570800
H	3.45335000	-1.33703000	-1.83398200
H	4.55393200	-3.75826400	-1.33077900
H	6.10044000	-3.51552700	0.88536000
H	6.00936100	-0.96019900	1.70216100
F	3.58992700	-2.21168100	0.84841600
C	2.93965700	-2.14514200	2.82447000
C	3.17407300	-3.49340300	2.41787200
C	1.93392800	-1.60045700	1.97310400
H	3.45311700	-1.62162200	3.63038500
C	2.31674200	-3.77856100	1.31434700
H	3.90683700	-4.17687100	2.84817200
C	1.50979500	-2.61425800	1.04194500
H	1.52365500	-0.59207300	2.02257200
H	2.27351100	-4.73111900	0.78931300
P	-0.10732300	-2.48670100	0.17350300
P	4.25756600	1.17956500	-0.27251700
P	-0.48538500	-0.21570300	-0.60687600
C	-1.27145200	-3.24971600	1.53097800
C	-2.66165500	-3.56695300	0.94400700
H	-3.34381300	-3.82124500	1.77701700
H	-3.09399700	-2.71555200	0.39776000
H	-2.63906500	-4.43854700	0.26988100
C	-0.69724700	-4.52741800	2.17821300
H	-0.49431200	-5.33174400	1.45657100
H	0.22571500	-4.32808600	2.74400500
H	-1.44762800	-4.91186200	2.89472200
C	-1.41805800	-2.19519800	2.64582800
H	-2.06077300	-2.61161100	3.44423900
H	-0.44728100	-1.94191700	3.10399800
H	-1.88581700	-1.26873700	2.28583200
C	-0.07875900	-3.60380400	-1.39901100
C	-0.08473400	-5.12148700	-1.13281900
H	-1.01604800	-5.46912600	-0.66001400
H	-0.00136700	-5.64207700	-2.10534300
H	0.76547900	-5.45211000	-0.51579800
C	1.19177700	-3.24949500	-2.19601700
H	1.26073100	-2.17101100	-2.40843600
H	2.10488600	-3.55268800	-1.66115300
H	1.16529400	-3.79156900	-3.16007800

C	-1.30941700	-3.24660700	-2.25994800
H	-1.27681200	-3.84235700	-3.19113400
H	-2.26393100	-3.46017300	-1.75603900
H	-1.31346800	-2.17924100	-2.53672300
C	4.69818700	2.07810800	1.37382000
C	3.93026400	1.36140800	2.50166100
H	2.85028700	1.30229300	2.28103300
H	4.29977500	0.34145100	2.68177800
H	4.04629400	1.93647400	3.44000500
C	4.12612200	3.51185900	1.28446200
H	3.03869100	3.51164200	1.09528300
H	4.29275000	4.02409400	2.25160500
H	4.61005800	4.12069600	0.50595100
C	6.19119000	2.14908800	1.74150000
H	6.66975400	1.15664600	1.77410100
H	6.76240200	2.77989500	1.04134800
H	6.29776900	2.60186800	2.74652000
C	5.53380400	1.65804500	-1.65524900
C	6.94721900	1.08351500	-1.45749400
H	6.93339400	-0.01770700	-1.39202000
H	7.57759100	1.35633400	-2.32666700
H	7.44469900	1.47274600	-0.55576700
C	5.59790300	3.19186600	-1.78798500
H	6.11045800	3.67159600	-0.93846300
H	6.16700100	3.45281600	-2.70062600
H	4.59134000	3.63620800	-1.88675200
C	4.95648100	1.10259200	-2.97648700
H	5.60019600	1.43098300	-3.81550800
H	4.94320900	0.00029800	-2.99176900
H	3.93195900	1.46809000	-3.16233900
C	-4.30541600	0.62778300	1.00256500
C	-2.89564000	0.72006700	1.09766300
C	-2.30374900	1.48313900	2.11787900
C	-3.12975300	2.13865800	3.02690000
C	-4.53397800	2.03826100	2.92028100
C	-5.14495500	1.28821900	1.91564900
C	-2.37276800	-0.08718500	0.00455400
H	-1.21539900	1.55585400	2.19135100
H	-2.69190700	2.73819300	3.83046800
H	-5.16428100	2.56266000	3.64543000
H	-6.22854500	1.21923800	1.84433900
N	-3.36109800	-0.60399300	-0.67971600
N	-4.55390800	-0.19151700	-0.09996600

C	-5.75407300	-0.63891200	-0.67206200
O	-6.79277200	-0.14796500	0.00359500
O	-5.79134500	-1.36403000	-1.63844600
C	-8.19270600	-0.44136600	-0.37122800
C	-8.99425100	0.32962800	0.67969000
H	-8.77036300	1.40899300	0.62785100
H	-10.07464500	0.18936600	0.50602200
H	-8.75520600	-0.03029100	1.69517200
C	-8.47467700	0.10011100	-1.77601900
H	-7.89278400	-0.43897000	-2.53854300
H	-9.54815400	-0.01693500	-2.00515800
H	-8.22732200	1.17475800	-1.83136200
C	-8.45424500	-1.94637100	-0.25845700
H	-8.19223300	-2.30845100	0.75120000
H	-9.52710400	-2.14493600	-0.42618600
H	-7.87267100	-2.51189500	-1.00170600
C	-0.92109000	3.94864400	-0.25231100
C	-0.24018600	2.75445800	-0.53395800
C	-0.69092100	1.83695200	-1.50765300
C	-1.88418400	2.17746100	-2.18736300
C	-2.56727000	3.37132600	-1.93850000
C	-2.09080600	4.25844300	-0.96871600
H	0.68721100	2.55834500	0.01298200
H	-2.27288800	1.49582700	-2.95063100
H	-3.47669700	3.61393200	-2.49716100
H	-2.62208600	5.18979200	-0.76171400
C	-0.37857400	4.84492800	0.80830000
O	-1.09327700	5.97220800	0.95453700
O	0.60194500	4.59849500	1.48270600
C	-0.65263500	6.89319200	1.95447700
H	0.37229100	7.23906900	1.74054900
H	-1.35490300	7.73802100	1.91801100
H	-0.67222000	6.42347400	2.95196300
B	0.69273400	1.04781700	-2.60737700
O	1.52794000	2.13222500	-2.97494600
H	1.11872700	2.62331300	-3.70550100
O	0.06182100	0.42188000	-3.71738100
H	-0.56177000	-0.26951300	-3.44713000
O	1.37889200	0.13530300	-1.68443700
H	2.09332000	0.60240700	-1.18389100

Int-4



E(RB3LYP) = -4526.49721381
Zero-point correction= 1.055916 (Hartree/Particle)
Thermal correction to Energy= 1.124276
Thermal correction to Enthalpy= 1.125220
Thermal correction to Gibbs Free Energy= 0.951368
Sum of electronic and zero-point Energies= -4525.441298
Sum of electronic and thermal Energies= -4525.372938
Sum of electronic and thermal Enthalpies= -4525.371993
Sum of electronic and thermal Free Energies= -4525.545846

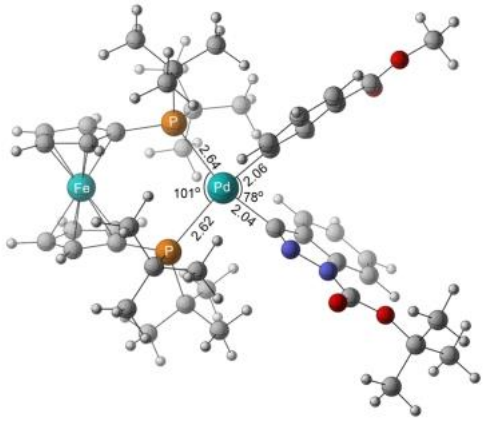
C	-4.13487200	-1.71899000	0.94086200
C	-4.64647800	-3.03959700	0.77609900
C	-5.32900000	-3.08442200	-0.47729000
C	-5.24680300	-1.78993700	-1.07472000
C	-4.52317700	-0.91534100	-0.19184800
H	-3.54525400	-1.36503300	1.78362900
H	-4.51710600	-3.87220200	1.46794800
H	-5.80299100	-3.96133000	-0.91996300
H	-5.66712900	-1.52451900	-2.04379100
F	-3.34211300	-2.58193500	-0.77196000
C	-2.50690000	-2.81091500	-2.66083300
C	-2.73733700	-4.08353500	-2.05483500
C	-1.60326500	-2.09010500	-1.82568600
H	-2.95786300	-2.44978200	-3.58515400
C	-1.97792000	-4.14295100	-0.84795600
H	-3.40564800	-4.86113400	-2.42649800
C	-1.23833100	-2.91497000	-0.70349900
H	-1.21886000	-1.08710600	-2.00692600
H	-1.95551300	-4.99225700	-0.16685400
P	0.27530400	-2.52098700	0.27176400
P	-4.26196200	0.90760100	-0.12613400
P	0.63680000	0.02350700	0.59617700

C	1.58906700	-3.47509800	-0.80425400
C	2.93379100	-3.55142000	-0.05323100
H	3.71036600	-3.91414600	-0.75343600
H	3.25739900	-2.57095100	0.33063900
H	2.90205400	-4.26509800	0.78629000
C	1.16284900	-4.89570000	-1.22540500
H	0.96077300	-5.56310800	-0.37551700
H	0.27412000	-4.88599800	-1.87563200
H	1.99050000	-5.34648300	-1.80605900
C	1.78338100	-2.65425400	-2.09549100
H	2.54041200	-3.15686600	-2.72718100
H	0.85396400	-2.58906700	-2.68594100
H	2.13738800	-1.63372900	-1.89246800
C	0.13851400	-3.35527500	2.00850900
C	0.23644100	-4.89206900	2.04465400
H	1.22195500	-5.26419400	1.72543100
H	0.08599400	-5.22882800	3.08808700
H	-0.53681800	-5.38201100	1.43135100
C	-1.21789800	-2.94818000	2.61529300
H	-1.35302500	-1.85584700	2.63876200
H	-2.06090200	-3.38211400	2.05612700
H	-1.27064700	-3.31937100	3.65621700
C	1.26251200	-2.76766800	2.89057600
H	1.13735800	-3.12752700	3.92894300
H	2.26766500	-3.06391700	2.55327100
H	1.23797400	-1.66336600	2.90240000
C	-4.38083600	1.61179300	-1.91285900
C	-3.35575800	0.83608500	-2.76227000
H	-2.34672600	0.88202800	-2.31603900
H	-3.62918100	-0.22252000	-2.88558300
H	-3.29649000	1.29472400	-3.76756800
C	-3.90926900	3.08262000	-1.86174900
H	-2.90748100	3.18448400	-1.41118000
H	-3.84806100	3.47608300	-2.89448400
H	-4.59989600	3.73476200	-1.30575600
C	-5.75859500	1.54817800	-2.59579000
H	-6.17377700	0.52761300	-2.62766100
H	-6.49639500	2.20284500	-2.10453600
H	-5.66103800	1.89831500	-3.64176200
C	-5.81469000	1.44031300	0.91139800
C	-7.14105900	0.80024800	0.46506100
H	-7.09200000	-0.30136000	0.49208300
H	-7.94663500	1.11366000	1.15770200

H	-7.44369000	1.10401400	-0.54857200
C	-5.93773400	2.97623000	0.89687300
H	-6.27307400	3.36431100	-0.07864200
H	-6.69022700	3.28708700	1.64646400
H	-4.98402200	3.46770600	1.15993200
C	-5.53114300	1.00428800	2.36596700
H	-6.35245700	1.36488900	3.01487900
H	-5.49363500	-0.09291700	2.46918800
H	-4.58461900	1.42456700	2.74479500
C	4.37754200	0.63104200	-1.31498200
C	2.96472900	0.71240900	-1.34343100
C	2.30830700	1.24486500	-2.46449100
C	3.07390400	1.68721200	-3.54065300
C	4.48220200	1.59946300	-3.49975500
C	5.15672900	1.07414000	-2.39704800
C	2.50439800	0.16273100	-0.07611800
H	1.21648200	1.30429600	-2.48340200
H	2.58548000	2.10709800	-4.42506400
H	5.06524700	1.95301200	-4.35612100
H	6.24303100	1.01269100	-2.37906100
N	3.53520900	-0.19453100	0.65010100
N	4.69352600	0.06753900	-0.07760300
C	5.92525600	-0.26162200	0.50144300
O	6.92139800	0.06344500	-0.32462700
O	6.02583700	-0.76783000	1.59508000
C	8.34030700	-0.16679300	0.01662500
C	9.07661200	0.35931500	-1.21740500
H	8.85853200	1.42945100	-1.37586900
H	10.16546900	0.24170900	-1.08434500
H	8.77384100	-0.19812800	-2.12046300
C	8.71258600	0.64790100	1.25932400
H	8.18139300	0.28447000	2.15165300
H	9.79879000	0.56718000	1.43890100
H	8.46847500	1.71402800	1.10778200
C	8.59200000	-1.66666000	0.20055700
H	8.26461800	-2.22444800	-0.69440100
H	9.67311700	-1.84294600	0.33761000
H	8.05850600	-2.05870200	1.07932700
C	0.41691000	4.36387800	0.48652300
C	0.30634100	2.99262700	0.18296400
C	0.94910400	2.01179400	0.95486800
C	1.72736100	2.45316200	2.04228600
C	1.83667100	3.81435000	2.36262100

C	1.18615500	4.77608700	1.58819100
H	-0.30215300	2.71548600	-0.68235800
H	2.26964000	1.72505300	2.65419400
H	2.44295300	4.12468400	3.22026700
H	1.27400500	5.83769800	1.82686600
C	-0.28765800	5.34052700	-0.39187600
O	-0.10542900	6.61656400	-0.00757500
O	-0.96107500	5.04252600	-1.35913200
C	-0.74366900	7.62483100	-0.79186200
H	-1.83775000	7.48607500	-0.79112800
H	-0.48209800	8.58418700	-0.32296700
H	-0.38057000	7.59833200	-1.83293800
B	-1.42812600	1.08083800	2.80778600
O	-2.26906800	2.14016300	2.99493300
H	-2.20090700	2.50539000	3.89314300
O	-0.61625300	0.66883800	3.82522300
H	-0.02703200	-0.06000300	3.57170000
O	-1.44415200	0.41020100	1.59509900
H	-2.17207000	0.72883600	0.99152100

Int-5



E(RB3LYP) = -4274.20137876
Zero-point correction= 1.009596 (Hartree/Particle)
Thermal correction to Energy= 1.071424
Thermal correction to Enthalpy= 1.072368
Thermal correction to Gibbs Free Energy= 0.916040
Sum of electronic and zero-point Energies= -4273.191783
Sum of electronic and thermal Energies= -4273.129955
Sum of electronic and thermal Enthalpies= -4273.129011
Sum of electronic and thermal Free Energies= -4273.285339

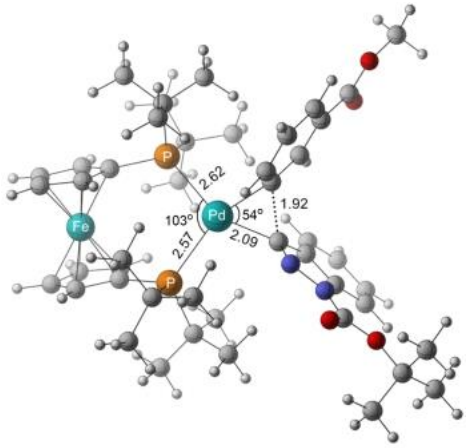
C	4.47724000	-0.15282400	1.40568300

C	5.82887300	0.28521400	1.29615900
C	6.29767300	-0.07264500	-0.00134000
C	5.23903500	-0.74176100	-0.68534900
C	4.08683900	-0.80670900	0.17940200
H	3.84407100	0.00052400	2.27354100
H	6.38736000	0.82935200	2.05837200
H	7.28139200	0.14842500	-0.41703500
H	5.31255900	-1.11225900	-1.70416400
F	4.63292400	1.16999800	-0.15990200
C	4.84210600	2.50645300	-1.74157700
C	5.21592700	3.13760600	-0.51918200
C	3.49064300	2.07288900	-1.61121500
H	5.48304900	2.34819200	-2.60941300
C	4.09103300	3.10423400	0.35845500
H	6.19658900	3.54961200	-0.27838700
C	2.99599900	2.44413600	-0.30689200
H	2.93326500	1.53445600	-2.37190400
H	4.09506800	3.50089500	1.37045800
P	1.22480800	2.20203400	0.17095000
P	2.45556400	-1.66534800	-0.00524100
P	0.25348900	-0.22998900	0.18617900
C	0.40942700	3.54550600	-0.99084200
C	-0.98172300	3.97032100	-0.48137200
H	-1.46603100	4.58994400	-1.25976000
H	-1.63615200	3.10960600	-0.27898900
H	-0.92539400	4.58557800	0.43042200
C	1.28239500	4.80421500	-1.16574400
H	1.46737200	5.33234300	-0.21808200
H	2.25601800	4.57494300	-1.62732700
H	0.75413400	5.50745200	-1.83815000
C	0.22888600	2.88613000	-2.37386600
H	-0.27699900	3.60148200	-3.04993800
H	1.19035000	2.62521700	-2.84300400
H	-0.39038700	1.97816800	-2.31759000
C	1.08414700	2.79286800	2.01297500
C	1.40256900	4.28153500	2.25451100
H	1.40492600	4.46899400	3.34535100
H	2.38483900	4.59032900	1.86616300
H	0.64037900	4.94522500	1.81710900
C	2.03062700	1.92030200	2.86243700
H	1.81806600	0.84761700	2.71367900
H	3.09429800	2.09843600	2.65088400
H	1.85981600	2.14927800	3.93115200

C	-0.34143600	2.50453600	2.52609200
H	-0.38593000	2.77529300	3.59845900
H	-1.12017300	3.07669600	2.00473100
H	-0.59922700	1.43943400	2.42446400
C	2.44645600	-2.36136000	-1.81629100
C	2.55938500	-1.16095700	-2.77951500
H	1.77607600	-0.41230700	-2.56812900
H	3.53652900	-0.65983500	-2.74118800
H	2.40832200	-1.52026300	-3.81479000
C	1.07587600	-3.00656700	-2.10127000
H	0.26569300	-2.27330700	-1.97915300
H	1.06319200	-3.35811100	-3.15020200
H	0.85300200	-3.87000300	-1.45958700
C	3.54438600	-3.39437800	-2.13794700
H	4.56046600	-3.05087300	-1.89348800
H	3.37522400	-4.35091300	-1.61856600
H	3.51970100	-3.60869800	-3.22347700
C	2.75016200	-3.14533700	1.23915400
C	4.19941900	-3.67087000	1.22705800
H	4.92635100	-2.89432400	1.51359900
H	4.28116100	-4.49012700	1.96719600
H	4.49984500	-4.07982600	0.25098400
C	1.79051000	-4.31828100	0.95874400
H	2.04006300	-4.85232200	0.02822600
H	1.88142000	-5.05014900	1.78361400
H	0.73810000	-3.99841600	0.91084100
C	2.44616000	-2.61114600	2.65480300
H	2.53773400	-3.44351100	3.37825500
H	3.15618500	-1.83195500	2.97141900
H	1.42504700	-2.20921500	2.73191600
C	-3.63294800	0.76445400	-1.30872400
C	-2.31723400	0.27291100	-1.48947600
C	-1.92003800	-0.21195900	-2.74672200
C	-2.83515000	-0.19727600	-3.79691300
C	-4.14097900	0.29926400	-3.60009800
C	-4.56171900	0.78704700	-2.36265700
C	-1.64889500	0.40819800	-0.19670500
H	-0.90532700	-0.58902100	-2.89531300
H	-2.54310800	-0.57255000	-4.78227200
H	-4.84528400	0.30314400	-4.43806500
H	-5.57143800	1.16767700	-2.22188500
N	-2.49030800	0.91308700	0.67126200
N	-3.70233500	1.15207500	0.02914800

C	-4.74455600	1.71123700	0.77836900
O	-5.83218800	1.85367600	0.01788000
O	-4.63324100	2.00805000	1.94563500
C	-7.09587600	2.41301300	0.53921800
C	-8.01650500	2.37077300	-0.68258000
H	-8.14063000	1.33507200	-1.04283300
H	-9.01080800	2.76938800	-0.41855600
H	-7.60367000	2.98104200	-1.50423600
C	-7.63619700	1.51593300	1.65736600
H	-6.97581400	1.52935100	2.53730300
H	-8.63599200	1.87105500	1.96221900
H	-7.73563100	0.47540300	1.30154900
C	-6.87316500	3.85672700	1.00064600
H	-6.43421400	4.45794400	0.18508900
H	-7.84270000	4.30764800	1.27512700
H	-6.20578900	3.90071800	1.87418200
C	-1.05446800	-1.88336300	2.26240800
C	-0.88013000	-1.81633700	0.86373800
C	-1.55860300	-2.77866000	0.10154100
C	-2.32891400	-3.79778900	0.69547300
C	-2.45370300	-3.86088300	2.09304400
C	-1.81812400	-2.89044300	2.86942700
H	-0.59433400	-1.12660900	2.90629300
H	-1.51993900	-2.76580100	-0.98823900
H	-3.04839300	-4.64969700	2.55749600
H	-1.91883400	-2.91140500	3.95978300
C	-2.99309800	-4.78459700	-0.20330100
O	-3.72163000	-5.69581200	0.46746400
O	-2.90230400	-4.78898800	-1.41540500
C	-4.39357800	-6.68513100	-0.31218800
H	-5.11195500	-6.21558700	-1.00495200
H	-3.67128500	-7.28027000	-0.89581500
H	-4.92331300	-7.32824800	0.40512400

TS-3



E(RB3LYP) = -4274.18602366
Zero-point correction= 1.007092 (Hartree/Particle)
Thermal correction to Energy= 1.068862
Thermal correction to Enthalpy= 1.069806
Thermal correction to Gibbs Free Energy= 0.913659
Sum of electronic and zero-point Energies= -4273.178932
Sum of electronic and thermal Energies= -4273.117162
Sum of electronic and thermal Enthalpies= -4273.116218
Sum of electronic and thermal Free Energies= -4273.272364

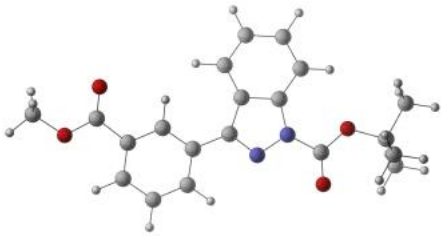
C	4.37298600	0.36747500	1.42864300
C	5.65656200	0.97943600	1.33083700
C	6.20710300	0.63062500	0.06331400
C	5.26790600	-0.20655400	-0.61104500
C	4.10983200	-0.38900700	0.22808300
H	3.69887300	0.47417000	2.27202700
H	6.11522500	1.62522100	2.08027000
H	7.16536200	0.96154900	-0.33888300
H	5.42175000	-0.61012600	-1.60822900
F	4.39902400	1.63323500	-0.19337700
C	4.42946700	2.87229200	-1.86326000
C	4.74194300	3.62592500	-0.69380100
C	3.13813500	2.29749100	-1.67634200
H	5.07396900	2.72862700	-2.73105900
C	3.63730400	3.52608800	0.20505800
H	5.67053200	4.16480500	-0.50160300
C	2.61711400	2.70267400	-0.39302000
H	2.63892900	1.64148200	-2.38325000
H	3.60521000	3.99242400	1.18668200
P	0.89521500	2.26818000	0.13422500
P	2.58259700	-1.42321100	0.02964500
P	0.26336100	-0.21736100	0.17444300

C	-0.10581300	3.40402800	-1.09689500
C	-1.54179800	3.62957200	-0.58670000
H	-2.13850700	4.09408900	-1.39456600
H	-2.03502800	2.68687000	-0.30337800
H	-1.57900800	4.31366500	0.27585800
C	0.55919500	4.76711200	-1.36725700
H	0.65416500	5.38444800	-0.46106500
H	1.56076800	4.65677100	-1.81374500
H	-0.06497400	5.33128600	-2.08737000
C	-0.19627600	2.63519800	-2.43196900
H	-0.82463200	3.21102600	-3.13811500
H	0.78791500	2.50585500	-2.90871300
H	-0.65397200	1.64207400	-2.30091500
C	0.69970400	2.96864500	1.93350500
C	0.82433800	4.49848400	2.06821200
H	0.81396500	4.76371400	3.14298800
H	1.75422200	4.90183600	1.63886200
H	-0.02213800	5.02520700	1.59996600
C	1.75991900	2.28419900	2.82070100
H	1.66842000	1.18572500	2.76473900
H	2.79148500	2.56078800	2.56110400
H	1.58821600	2.58012800	3.87284200
C	-0.66939300	2.53265500	2.49579300
H	-0.72902000	2.84730300	3.55537400
H	-1.52328700	2.97968800	1.96928500
H	-0.79332400	1.43967400	2.45093800
C	2.74905700	-2.23393000	-1.72444700
C	2.77428300	-1.09255500	-2.76431100
H	1.89257200	-0.43799300	-2.65021100
H	3.67534900	-0.46629100	-2.70884500
H	2.73494800	-1.53301200	-3.77842100
C	1.47185100	-3.04449600	-2.02438000
H	0.57862000	-2.40655700	-1.95117500
H	1.53100300	-3.43105100	-3.05941100
H	1.32665200	-3.90562800	-1.35813200
C	3.97019600	-3.15266500	-1.92227900
H	4.92585500	-2.67605100	-1.65600200
H	3.88241900	-4.08356500	-1.33946900
H	4.03040300	-3.44434000	-2.98853300
C	2.93664800	-2.77752100	1.39169600
C	4.42234500	-3.16496400	1.51660300
H	5.05542600	-2.30204800	1.77928400
H	4.52864500	-3.91317600	2.32613900

H	4.82399000	-3.61726400	0.59693300
C	2.10237900	-4.04661900	1.13503500
H	2.46906200	-4.62385600	0.27133300
H	2.18033300	-4.70677500	2.01967800
H	1.03496100	-3.82121800	0.98165000
C	2.47233700	-2.17892800	2.73722000
H	2.56893900	-2.94847700	3.52685700
H	3.08578900	-1.32017300	3.05000100
H	1.41791300	-1.86126700	2.69961100
C	-3.70743300	0.35511700	-1.21836300
C	-2.43201200	-0.24167100	-1.34832300
C	-2.01163700	-0.72257500	-2.59854800
C	-2.87047700	-0.60997000	-3.69012600
C	-4.13999300	-0.01462800	-3.54217700
C	-4.57868200	0.47858900	-2.31343300
C	-1.81522500	-0.17636700	-0.01765200
H	-1.02127200	-1.16794000	-2.71586900
H	-2.55837200	-0.98192000	-4.67038900
H	-4.79956600	0.06697700	-4.41179100
H	-5.55806700	0.94076400	-2.20980400
N	-2.66362900	0.39851600	0.81766200
N	-3.81079700	0.73128500	0.12334100
C	-4.84640100	1.36058200	0.82886000
O	-5.88370600	1.58412500	0.02062500
O	-4.76509400	1.64416000	2.00194900
C	-7.12251900	2.24224400	0.48562500
C	-7.98842500	2.26719700	-0.77584800
H	-8.17453000	1.24301900	-1.14224900
H	-8.96034700	2.74030900	-0.55531900
H	-7.49503300	2.84289400	-1.57775800
C	-7.78032100	1.39427600	1.57871000
H	-7.16210400	1.36135700	2.48823800
H	-8.76282200	1.82678400	1.83618200
H	-7.94310600	0.36279300	1.21995600
C	-6.80735500	3.66545200	0.95638900
H	-6.28927800	4.22846300	0.16026000
H	-7.74954700	4.19096000	1.19024700
H	-6.17600300	3.66028400	1.85744700
C	-1.19758900	-1.86515900	2.15517100
C	-1.08099000	-1.77235200	0.74418700
C	-1.39478400	-2.93089600	0.00954300
C	-1.76806100	-4.13237700	0.63675500
C	-1.84299100	-4.20361000	2.03694300

C	-1.55298100	-3.05784000	2.78662700
H	-1.02455000	-0.97499200	2.76646000
H	-1.37400100	-2.92620600	-1.08003900
H	-2.13200200	-5.13521400	2.52631800
H	-1.61456500	-3.09231600	3.87922100
C	-2.06107400	-5.30697900	-0.23457100
O	-2.44615400	-6.39052400	0.46144700
O	-1.96517900	-5.30886500	-1.44619000
C	-2.74060800	-7.56930400	-0.28931000
H	-3.56858300	-7.38633200	-0.99439500
H	-1.85500100	-7.90263600	-0.85581100
H	-3.03021800	-8.33274200	0.44677300

Substrate 9



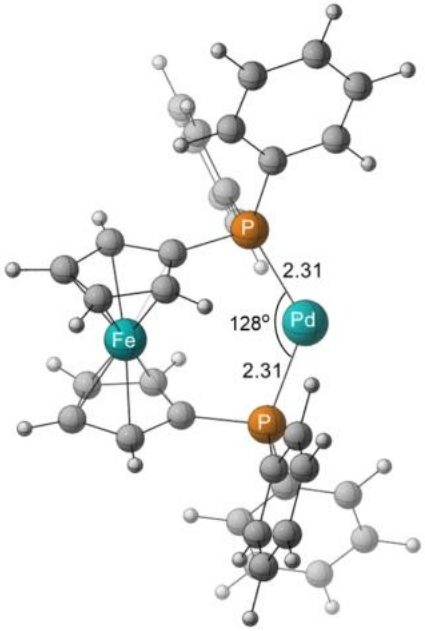
E(RB3LYP) = -1183.71833390
Zero-point correction= 0.367750 (Hartree/Particle)
Thermal correction to Energy= 0.391522
Thermal correction to Enthalpy= 0.392466
Thermal correction to Gibbs Free Energy= 0.312432
Sum of electronic and zero-point Energies= -1183.350584
Sum of electronic and thermal Energies= -1183.326812
Sum of electronic and thermal Enthalpies= -1183.325868
Sum of electronic and thermal Free Energies= -1183.405902

C	1.48214400	1.06241100	-0.19070300
C	0.07288700	1.13076600	-0.32467000
C	-0.55332400	2.37500700	-0.53436300
C	0.23765000	3.51788300	-0.58008400
C	1.63854400	3.43409000	-0.42452300
C	2.28425100	2.21517400	-0.23326700
C	-0.37336100	-0.24705500	-0.23876100
H	-1.63365800	2.44900800	-0.67195300
H	-0.22858800	4.49392000	-0.74194400
H	2.23667400	4.34956600	-0.46257000

H	3.36517500	2.15931300	-0.12638600
N	0.65288300	-1.05473700	-0.08125000
N	1.78125200	-0.29471200	-0.04596600
C	3.01749700	-0.96535600	0.12613300
O	4.00636600	-0.08231400	0.15650300
O	3.09246700	-2.16415500	0.22344200
C	5.42550200	-0.48223300	0.32269800
C	6.15987900	0.85903900	0.29361000
H	5.81534300	1.51172500	1.11394800
H	7.24418400	0.69447300	0.41200400
H	5.98944400	1.37815300	-0.66514100
C	5.60626400	-1.17602500	1.67544800
H	5.07075500	-2.13664000	1.71078500
H	6.67995200	-1.36698000	1.84586000
H	5.23874100	-0.53082900	2.49246800
C	5.84988200	-1.36437400	-0.85445100
H	5.65327900	-0.85123700	-1.81198000
H	6.93356200	-1.56301100	-0.78809000
H	5.31756600	-2.32740100	-0.84955300
C	-1.93724600	-2.11666800	-0.78746400
C	-1.74005200	-0.79976800	-0.32362700
C	-2.86148400	-0.05526900	0.07018100
C	-4.15210300	-0.60070100	-0.00428200
C	-4.33220300	-1.91036900	-0.47489000
C	-3.21909400	-2.66317800	-0.86120400
H	-1.06913800	-2.70454700	-1.09436100
H	-2.75619900	0.95478000	0.46762200
H	-5.33653600	-2.33325300	-0.53536600
H	-3.35330800	-3.68493600	-1.22799300
C	-5.29484900	0.25524400	0.43809200
O	-6.47877500	-0.36202800	0.32122600
O	-5.17591900	1.38745200	0.85889900
C	-7.63650900	0.37612100	0.72084700
H	-7.57044000	0.65481500	1.78553800
H	-7.74156600	1.29123200	0.11484200
H	-8.49295600	-0.29206800	0.55389600

(2) **L = dppf**

Precatalyst



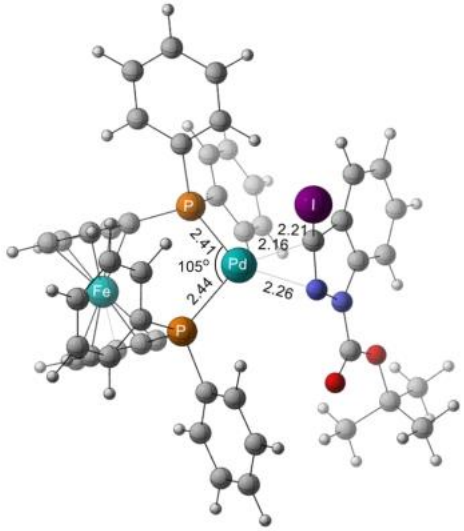
E(RB3LYP) = -3385.59363594
Zero-point correction= 0.516500 (Hartree/Particle)
Thermal correction to Energy= 0.550307
Thermal correction to Enthalpy= 0.551251
Thermal correction to Gibbs Free Energy= 0.446702
Sum of electronic and zero-point Energies= -3385.077136
Sum of electronic and thermal Energies= -3385.043329
Sum of electronic and thermal Enthalpies= -3385.042385
Sum of electronic and thermal Free Energies= -3385.146934

C	1.00617200	-1.66572400	1.58216300
C	0.93894600	-1.72266600	3.00620400
C	1.59063600	-0.56157300	3.52413500
C	2.07370300	0.20531100	2.41970100
C	1.72567200	-0.47722500	1.20583000
H	0.58278300	-2.39560300	0.89212300
H	0.44736500	-2.49944000	3.59302400
H	1.68314800	-0.29273600	4.57715900
H	2.60380600	1.15475400	2.48517400
F	-0.00003600	-0.00066300	2.30761300
C	-0.93965900	1.72050100	3.00759200
C	-1.59081100	0.55869300	3.52459800
C	-1.00690400	1.66468400	1.58350900
H	-0.44853300	2.49710500	3.59501800
C	-2.07355400	-0.20752000	2.41954800
H	-1.68320800	0.28898300	4.57740900
C	-1.72588200	0.47617800	1.20622400

H	-0.58383600	2.39531500	0.89406600
H	-2.60318500	-1.15727700	2.48425000
P	-2.07229400	0.00705900	-0.54124800
P	2.07245000	-0.00696800	-0.54125000
P	-0.00000300	0.00020500	-1.55370800
C	3.47585000	-1.14027100	-0.98712600
C	4.19788800	-1.90317000	-0.05314200
C	3.80914600	-1.24957800	-2.34989000
C	5.23396100	-2.74713300	-0.47235900
H	3.95225700	-1.84286200	1.01056900
C	4.85077200	-2.08295900	-2.76778100
H	3.24094200	-0.67893700	-3.09311500
C	5.56541300	-2.83691300	-1.82845400
H	5.78519600	-3.33645700	0.26733900
H	5.09853700	-2.15232700	-3.83168500
H	6.37477200	-3.49759800	-2.15439600
C	2.93581800	1.62785500	-0.35606100
C	2.24453800	2.79256000	-0.73192900
C	4.24817800	1.74928900	0.13463000
C	2.84339400	4.05173700	-0.60882100
H	1.22820600	2.70351400	-1.13188900
C	4.84957600	3.00676600	0.25365500
H	4.81124300	0.85709400	0.42382300
C	4.14814000	4.16104200	-0.11589500
H	2.29067800	4.94837000	-0.90617400
H	5.87250700	3.08489200	0.63531400
H	4.62120900	5.14379800	-0.02463000
C	-2.93617700	-1.62763200	-0.35722700
C	-4.24845200	-1.74909100	0.13367100
C	-2.24532400	-2.79222700	-0.73422700
C	-4.85019400	-3.00649200	0.25178500
H	-4.81120900	-0.85698000	0.42372200
C	-2.84451900	-4.05133000	-0.61203900
H	-1.22905900	-2.70311600	-1.13434100
C	-4.14917900	-4.16066300	-0.11888700
H	-5.87306000	-3.08463300	0.63361300
H	-2.29213900	-4.94788100	-0.91026300
H	-4.62250300	-5.14335900	-0.02831300
C	-3.47521400	1.14112300	-0.98674900
C	-3.80713300	1.25261200	-2.34966600
C	-4.19829800	1.90241900	-0.05225700
C	-4.84844700	2.08654200	-2.76725900
H	-3.23805600	0.68327800	-3.09322400

C	-5.23406000	2.74691900	-0.47114400
H	-3.95370100	1.84046200	1.01160100
C	-5.56414800	2.83885600	-1.82743300
H	-5.09512900	2.15763000	-3.83130200
H	-5.78611600	3.33497500	0.26894900
H	-6.37326600	3.49996200	-2.15312000

Int-1



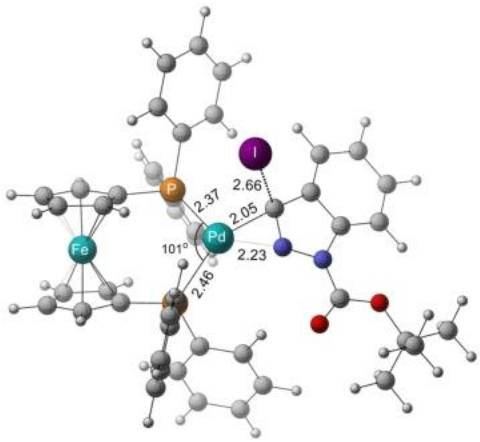
E(RB3LYP) = -4407.90690466
Zero-point correction= 0.750578 (Hartree/Particle)
Thermal correction to Energy 0.802186
Thermal correction to Enthalpy= 0.803130
Thermal correction to Gibbs Free Energy 0.659733
Sum of electronic and zero-point Energies= -4407.156327
Sum of electronic and thermal Energies= -4407.104719
Sum of electronic and thermal Enthalpies= -4407.103774
Sum of electronic and thermal Free Energies= -4407.247172

C	3.89260500	0.47715400	-0.95152700
C	4.71136800	0.99398600	-1.99963100
C	4.24760900	0.44685600	-3.23462100
C	3.14999200	-0.42009500	-2.95050700
C	2.92009900	-0.41330900	-1.53128200
H	3.98884300	0.71644100	0.10698400
H	5.52616700	1.70861900	-1.87868200
H	4.64498900	0.66946400	-4.22550200
H	2.57205700	-0.97935200	-3.68461700
F	2.71607700	1.50655100	-2.29846900
C	1.49137200	2.53438600	-3.64458400
C	2.50465500	3.40536300	-3.13921400

C	0.73681800	2.04739400	-2.53745700
H	1.33993100	2.26386100	-4.69000000
C	2.37474100	3.46504100	-1.71939000
H	3.26648100	3.91434600	-3.73085500
C	1.27587400	2.62186500	-1.33044700
H	-0.09593100	1.34590200	-2.58619600
H	3.02129600	4.02565600	-1.04589200
P	0.62826700	2.20867700	0.32719400
P	1.66837400	-1.37404700	-0.58432800
P	-0.04070800	-0.12549300	0.57409500
C	-3.18078400	-1.91043000	0.01256700
C	-2.15970200	-2.52143300	0.77569500
C	-1.95517800	-3.90415300	0.71801900
C	-2.77228000	-4.66586600	-0.11889400
C	-3.77626500	-4.04904600	-0.88758800
C	-3.99723400	-2.66942100	-0.83853000
C	-1.50962600	-1.42547400	1.48884100
H	-1.17754200	-4.37641900	1.32419000
H	-2.63398000	-5.74941300	-0.17604200
H	-4.40806600	-4.66158100	-1.53810100
H	-4.78226000	-2.20593500	-1.43145200
N	-2.17562300	-0.26808000	1.28712100
N	-3.15171900	-0.54056800	0.32516800
C	-3.99178800	0.50592800	-0.07064600
O	-4.90220700	0.05980700	-0.93791300
O	-3.86548300	1.63947800	0.33155900
C	-5.92130600	0.94460900	-1.54100600
C	-6.70883800	-0.00944800	-2.44168100
H	-7.16589200	-0.81973600	-1.84809300
H	-7.51374000	0.54011800	-2.95853700
H	-6.05048900	-0.46066700	-3.20387200
C	-6.82057200	1.52220000	-0.44377200
H	-6.26284000	2.20424800	0.21520000
H	-7.65084700	2.08219200	-0.90815700
H	-7.25358800	0.71012500	0.16627900
C	-5.23483400	2.03347700	-2.37129300
H	-4.55610900	1.58002000	-3.11494600
H	-5.99913800	2.61567500	-2.91489500
H	-4.65767300	2.72078100	-1.73490100
I	-0.73656200	-1.73606000	3.53668100
C	2.74098400	-2.61700200	0.28323700
C	4.10185200	-2.81174800	-0.01435900
C	2.15453700	-3.40241200	1.29106300

C	4.85168100	-3.77108200	0.67659100
H	4.58612300	-2.21571200	-0.79130700
C	2.90065000	-4.36632400	1.97566500
H	1.10381400	-3.25235500	1.55131400
C	4.25418900	-4.55201900	1.67160400
H	5.90977200	-3.90814100	0.43228900
H	2.42381400	-4.96698500	2.75641000
H	4.84250800	-5.30054900	2.21133000
C	0.90424300	-2.37854900	-1.94777000
C	1.51040500	-3.53518700	-2.46891100
C	-0.31425300	-1.94694000	-2.49924400
C	0.91418400	-4.23751400	-3.52176000
H	2.45607600	-3.89465500	-2.05430700
C	-0.90510000	-2.64253000	-3.55988200
H	-0.81010400	-1.06289100	-2.08476900
C	-0.29262900	-3.79102700	-4.07279800
H	1.39715000	-5.13807200	-3.91388300
H	-1.85301900	-2.29066900	-3.97818300
H	-0.75751700	-4.34106000	-4.89688800
C	1.97776900	2.70729000	1.49748800
C	2.37297600	4.04916200	1.65264800
C	2.60371600	1.72397300	2.28171600
C	3.38666100	4.39302800	2.55202700
H	1.87961300	4.83694100	1.07618300
C	3.61617900	2.06813800	3.18598800
H	2.28962600	0.67941400	2.18771300
C	4.01253700	3.40247400	3.31934800
H	3.68508900	5.44061100	2.65850900
H	4.09110500	1.28973600	3.79094900
H	4.80239700	3.67359100	4.02669200
C	-0.61476400	3.54649700	0.64515700
C	-1.15153900	3.65895100	1.94187100
C	-1.07974500	4.41376100	-0.35648800
C	-2.11806600	4.62449500	2.23196100
H	-0.81019800	2.98578100	2.73541600
C	-2.05605200	5.37613200	-0.06653800
H	-0.67859800	4.34612400	-1.37123800
C	-2.57575700	5.48652700	1.22669500
H	-2.52030000	4.70160700	3.24700100
H	-2.40577100	6.04642700	-0.85820400
H	-3.33589800	6.24080600	1.45244000

TS-1



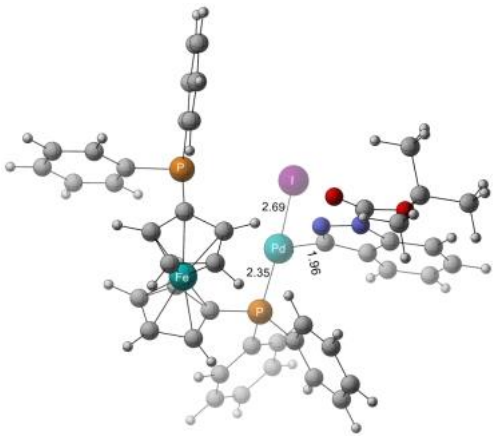
Zero-point correction= 0.751637 (Hartree/Particle)
Thermal correction to Energy= 0.802423
Thermal correction to Enthalpy= 0.803367
Thermal correction to Gibbs Free Energy= 0.661776
Sum of electronic and zero-point Energies= -4407.156690
Sum of electronic and thermal Energies= -4407.105903
Sum of electronic and thermal Enthalpies= -4407.104959
Sum of electronic and thermal Free Energies= -4407.246550

C	-3.42403900	-0.07054100	1.67800100
C	-4.72588300	-0.55555400	1.99655500
C	-5.56477200	-0.35420300	0.85863700
C	-4.78724000	0.25914700	-0.16762900
C	-3.44723400	0.43938300	0.32954600
H	-2.55295900	-0.09202400	2.33246500
H	-5.01886700	-1.02645100	2.93525600
H	-6.61140900	-0.64809000	0.77285300
H	-5.14302300	0.51224200	-1.16492900
F	-3.93420700	-1.55365100	0.33830000
C	-4.42104200	-3.02938500	-1.05219700
C	-4.44354700	-3.57945700	0.26518200
C	-3.11667200	-2.50478200	-1.29292000
H	-5.26169700	-2.98690400	-1.74529800
C	-3.14985900	-3.40886700	0.84105200
H	-5.30511600	-4.03118400	0.75764800
C	-2.31272800	-2.74128900	-0.11957300
H	-2.78935100	-2.00610600	-2.20458400
H	-2.85134600	-3.71047100	1.84378900
P	-0.57951100	-2.20407000	0.11039700
P	-1.99450900	1.18978500	-0.48547300
P	0.05262300	0.17096000	0.12179000
C	3.46322800	1.81272500	-0.76693500

C	2.25773700	2.50564300	-0.49158500
C	2.03190600	3.77649200	-1.03653000
C	3.00766900	4.33243700	-1.86242200
C	4.19687400	3.62908700	-2.13923200
C	4.44785700	2.36644300	-1.59890300
C	1.49081300	1.61130200	0.36770800
H	1.11531700	4.32138400	-0.80167000
H	2.85378400	5.32472200	-2.29628500
H	4.94976900	4.08344200	-2.79068200
H	5.37343800	1.83615500	-1.81300200
N	2.19454300	0.52339000	0.62272900
N	3.39374000	0.59192100	-0.07468600
C	4.34866100	-0.40606600	0.14601000
O	5.47750200	-0.11353500	-0.49592600
O	4.12212800	-1.38566200	0.82141700
C	6.67860400	-0.97682000	-0.43191500
C	7.68746700	-0.21683200	-1.29516900
H	7.87230900	0.79049200	-0.88444800
H	8.64527500	-0.76349900	-1.32186500
H	7.31751000	-0.11246900	-2.32970400
C	7.16517800	-1.07437500	1.01685300
H	6.44024700	-1.60772800	1.64991800
H	8.12367100	-1.62118500	1.04401500
H	7.33275000	-0.06683800	1.43601500
C	6.36424200	-2.34668500	-1.03954000
H	5.96320500	-2.23160700	-2.06189100
H	7.29241500	-2.94094300	-1.10111000
H	5.63453500	-2.89987900	-0.42952900
I	0.81473500	2.88324700	2.60421500
C	-2.25078600	2.99381800	-0.17470000
C	-1.65818700	3.93722700	-1.03299100
C	-2.99322500	3.45129900	0.92633400
C	-1.81023300	5.30650500	-0.79850700
H	-1.08025300	3.60404100	-1.89977800
C	-3.14234700	4.82271100	1.16137700
H	-3.46321200	2.73907400	1.60870000
C	-2.55207900	5.75397700	0.30162200
H	-1.34808400	6.02722700	-1.48018200
H	-3.72613400	5.16205000	2.02253800
H	-2.67124000	6.82609500	0.48524300
C	-2.31015600	1.05765400	-2.30225500
C	-3.39045800	1.72425900	-2.91116000
C	-1.44244700	0.29903100	-3.10561600

C	-3.60963400	1.61053200	-4.28686800
H	-4.05958300	2.35008100	-2.31459400
C	-1.66071900	0.18832900	-4.48411600
H	-0.58468800	-0.20636200	-2.65079900
C	-2.74697600	0.83979000	-5.07607700
H	-4.45524500	2.13221300	-4.74519700
H	-0.97431100	-0.40524500	-5.09521800
H	-2.91764300	0.75579700	-6.15366500
C	-0.14107100	-2.95676800	1.74170700
C	0.06344200	-4.34135900	1.88157700
C	-0.02035300	-2.13116000	2.87192900
C	0.37620700	-4.88721700	3.12977600
H	-0.01868500	-5.00001900	1.01220600
C	0.28945800	-2.67969900	4.12206100
H	-0.15742600	-1.04944300	2.77594100
C	0.48829600	-4.05767100	4.25268500
H	0.53525800	-5.96570600	3.22522700
H	0.38193000	-2.02437900	4.99324000
H	0.73601600	-4.48664000	5.22848900
C	0.36591800	-3.22781800	-1.10597200
C	1.75111200	-3.00118400	-1.21149000
C	-0.22911100	-4.19884500	-1.92894300
C	2.52251600	-3.73476300	-2.11689000
H	2.23649400	-2.25883700	-0.57077000
C	0.54560400	-4.92580500	-2.84147300
H	-1.30119700	-4.39737900	-1.86299300
C	1.92121400	-4.69605600	-2.93877500
H	3.59918100	-3.55098500	-2.18152000
H	0.06718800	-5.67800800	-3.47628900
H	2.52494800	-5.26484000	-3.65254700

Int-2



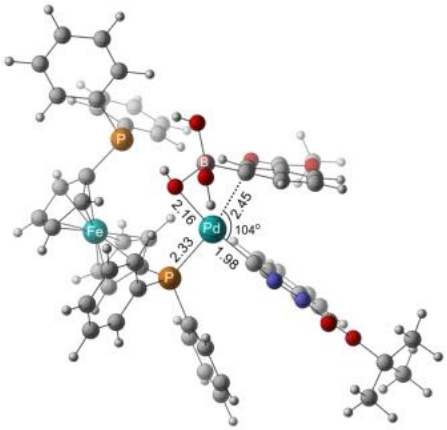
E(RB3LYP) = -4407.94178867
Zero-point correction= 0.750800 (Hartree/Particle)
Thermal correction to Energy= 0.802304
Thermal correction to Enthalpy= 0.803248
Thermal correction to Gibbs Free Energy= 0.654862
Sum of electronic and zero-point Energies= -4407.190989
Sum of electronic and thermal Energies= -4407.139485
Sum of electronic and thermal Enthalpies= -4407.138541
Sum of electronic and thermal Free Energies= -4407.286927

C	1.84393100	-2.49242800	-0.97379200
C	2.80310300	-2.72818800	-2.00071500
C	2.13112200	-2.65716300	-3.26031900
C	0.75319600	-2.38132300	-3.01849800
C	0.56130700	-2.28561400	-1.59373500
H	2.03682600	-2.47779300	0.09874800
H	3.86894500	-2.90000500	-1.85023200
H	2.59557800	-2.76367800	-4.24117200
H	-0.02161200	-2.26503400	-3.77568500
F	1.93227900	-0.85224200	-2.24541700
C	1.34573100	0.97135900	-3.07556600
C	2.62742200	0.58460800	-3.57318200
C	1.43598400	1.08428900	-1.65498200
H	0.45160800	1.13318500	-3.67809600
C	3.51528300	0.46518100	-2.46209000
H	2.87864600	0.38639200	-4.61592200
C	2.78657900	0.77930100	-1.26272600
H	0.62065800	1.35893100	-0.98178900
H	4.56159200	0.16530500	-2.51106000
P	3.34776300	0.84394000	0.48406000
P	-0.99895200	-2.25348800	-0.66556200
P	-0.77661600	-1.29712400	1.46451100
C	-3.68285600	1.62513600	0.73167000
C	-3.33900300	0.34971500	1.24479800
C	-4.30918100	-0.45826000	1.85948400
C	-5.61219300	0.02246200	1.94797900
C	-5.94400200	1.29483000	1.43297600
C	-4.99640100	2.11489300	0.82151100
C	-1.92181200	0.21266900	0.97417200
H	-4.03845000	-1.43875300	2.26032400
H	-6.38813500	-0.58552300	2.42201500
H	-6.97511600	1.65208000	1.51633000
H	-5.26569200	3.09453600	0.43197600

N	-1.45440600	1.26619000	0.37028600
N	-2.50156100	2.15333800	0.20409000
C	-2.23826600	3.36335600	-0.46266700
O	-3.34900900	4.09084800	-0.53626100
O	-1.14483000	3.64813600	-0.88935200
C	-3.38778100	5.41816500	-1.19190000
C	-4.85102300	5.83356400	-1.02845900
H	-5.12464100	5.88913000	0.03913100
H	-5.01188200	6.82658500	-1.48118600
H	-5.52070200	5.11131600	-1.52617300
C	-2.45968100	6.38422400	-0.45030500
H	-1.40564600	6.08352600	-0.54679500
H	-2.57554400	7.39792300	-0.87151500
H	-2.72283200	6.42556300	0.62109600
C	-3.02463700	5.27204600	-2.67256700
H	-3.67556500	4.52289800	-3.15671200
H	-3.17638000	6.23895700	-3.18300000
H	-1.97482800	4.96912100	-2.80203700
I	-0.40329100	-0.51043400	4.01097700
C	3.90607100	2.60806200	0.64904200
C	3.89144300	3.54698900	-0.39612700
C	4.31238000	3.03319900	1.92896000
C	4.28469400	4.87254300	-0.17035900
H	3.57172100	3.24651300	-1.39749800
C	4.71593000	4.35238600	2.15232300
H	4.31212600	2.32319900	2.76355600
C	4.70162400	5.27834600	1.10130100
H	4.26661200	5.59033500	-0.99676500
H	5.03354600	4.66168400	3.15320500
H	5.00934700	6.31405700	1.27588600
C	4.97525500	-0.05300000	0.41624900
C	5.03809200	-1.33667000	0.98684000
C	6.14366600	0.48910800	-0.15002500
C	6.22993600	-2.07125800	0.97374200
H	4.14644300	-1.76487500	1.45647600
C	7.33669500	-0.24128600	-0.16028800
H	6.12540900	1.49329700	-0.58372800
C	7.38202600	-1.52455500	0.39869600
H	6.25942400	-3.06889100	1.42298600
H	8.23667800	0.19503200	-0.60519600
H	8.31684700	-2.09373300	0.39262500
C	-1.37486000	-4.03643600	-0.37077500
C	-0.82589200	-5.05361200	-1.17158400

C	-2.23290900	-4.38648000	0.68806200
C	-1.13668400	-6.39364800	-0.91983400
H	-0.15270500	-4.80409500	-1.99537100
C	-2.54571100	-5.72729500	0.93356800
H	-2.65920800	-3.60753300	1.32776600
C	-1.99668200	-6.73316900	0.13091700
H	-0.70233500	-7.17636500	-1.54897800
H	-3.21513300	-5.98498200	1.75956400
H	-2.23555100	-7.78288400	0.32675500
C	-2.27686900	-1.67919700	-1.85622500
C	-2.16017600	-0.39883200	-2.42831700
C	-3.38514600	-2.47771800	-2.18628700
C	-3.12814300	0.06594900	-3.32255600
H	-1.31368400	0.23928700	-2.17112000
C	-4.35459500	-2.00562400	-3.07846600
H	-3.49797700	-3.47404000	-1.75299200
C	-4.22836500	-0.73573500	-3.64958700
H	-3.02241900	1.06210200	-3.76282100
H	-5.21104300	-2.63906600	-3.32819400
H	-4.98670200	-0.36941100	-4.34815000

Int-3



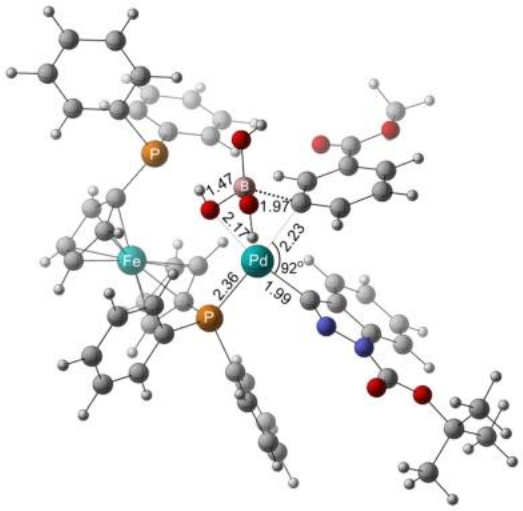
E(RB3LYP) = -4821.53981630
Zero-point correction= 0.933000 (Hartree/Particle)
Thermal correction to Energy= 0.997798
Thermal correction to Enthalpy= 0.998742
Thermal correction to Gibbs Free Energy= 0.825825
Sum of electronic and zero-point Energies= -4820.606816
Sum of electronic and thermal Energies= -4820.542018
Sum of electronic and thermal Enthalpies= -4820.541074
Sum of electronic and thermal Free Energies= -4820.713992

C	3.67577100	-2.08119600	-0.24847000
C	3.94787100	-3.26841000	0.49323200
C	4.69140100	-2.89833300	1.65626100
C	4.88649700	-1.48347700	1.62968200
C	4.26375400	-0.96384100	0.44310500
H	3.10282000	-2.01672400	-1.17316400
H	3.61976700	-4.27503300	0.23329500
H	5.02716700	-3.57318000	2.44453500
H	5.39872900	-0.89579300	2.39105000
F	2.86152300	-1.92005200	1.65263100
C	2.05444100	-0.92040000	3.29561400
C	2.01995600	-2.33305400	3.50936700
C	1.29622000	-0.63185500	2.12445400
H	2.58742600	-0.19114200	3.90569200
C	1.24903600	-2.92531400	2.46663500
H	2.52478400	-2.87283400	4.31113700
C	0.78346000	-1.87040500	1.59981500
H	1.13450800	0.35204700	1.68463300
H	1.04639900	-3.98950900	2.35154900
P	-0.42019900	-1.99981300	0.24014100
P	4.12845400	0.73889400	-0.21714300
P	-0.52243700	0.02202500	-0.91507500
C	-4.23829000	0.95562700	0.89512900
C	-2.82510700	0.92817800	0.99729200
C	-2.18566900	1.45525800	2.13123100
C	-2.96952100	1.99819700	3.14603000
C	-4.37667100	2.01857200	3.03249100
C	-5.03362800	1.50407500	1.91498100
C	-2.36353300	0.30227800	-0.22868100
H	-1.09609900	1.44446100	2.20785300
H	-2.49507600	2.41406200	4.03980300
H	-4.97217100	2.45125600	3.84246800
H	-6.11882400	1.52792200	1.83909400
N	-3.37872900	-0.02184500	-0.98343500
N	-4.53829100	0.36521300	-0.33454900
C	-5.76571200	0.12091500	-0.97373400
O	-6.76970200	0.53308300	-0.20224300
O	-5.84574800	-0.39101800	-2.06476300
C	-8.18595500	0.41499200	-0.61398000
C	-8.93685300	1.00660700	0.58059400
H	-8.64239000	2.05712600	0.74653600
H	-10.02368900	0.97515400	0.39399600
H	-8.72432200	0.43273500	1.49892900

C	-8.42639200	1.24850800	-1.87614700
H	-7.87916000	0.83917700	-2.73856300
H	-9.50447400	1.25078200	-2.11325600
H	-8.10873900	2.29349500	-1.71433800
C	-8.54684700	-1.06100000	-0.80664200
H	-8.30504600	-1.63845200	0.10285500
H	-9.63134900	-1.15096300	-0.99175900
H	-8.00821800	-1.49881000	-1.66028600
C	-0.95929200	3.48030600	-0.85742600
C	-0.03711800	2.51896600	-1.33114000
C	-0.22799400	1.82768600	-2.55100400
C	-1.41690600	2.12546600	-3.26706800
C	-2.33215000	3.07175400	-2.81297700
C	-2.10559600	3.75594000	-1.60767000
H	0.89105700	2.39146600	-0.76633600
H	-1.59798400	1.60567700	-4.21358900
H	-3.23324600	3.28987000	-3.39449200
H	-2.82203900	4.49933600	-1.25247200
C	-0.65859000	4.16689300	0.43188500
O	-1.55697800	5.11177800	0.74168500
O	0.29552800	3.90677200	1.13971900
C	-1.36332600	5.81475000	1.97151200
H	-0.38674500	6.32618100	1.97741500
H	-2.17904800	6.54897700	2.03073000
H	-1.41330300	5.11920500	2.82572000
B	0.96047500	0.84634800	-3.16464300
O	2.08494600	1.65506800	-3.56920200
H	2.68438500	1.10408400	-4.10006100
O	0.51764900	-0.00556400	-4.24998000
H	-0.22140200	-0.56864000	-3.97254000
O	1.35947200	-0.06799100	-1.96461300
H	2.08156600	0.35502500	-1.44872600
C	5.60502800	0.85529200	-1.33142900
C	6.75255800	0.05082700	-1.21521900
C	5.53937100	1.79456100	-2.37777400
C	7.81833200	0.19841000	-2.11033400
H	6.81666000	-0.70276000	-0.42492100
C	6.60835600	1.94705600	-3.26744000
H	4.63357100	2.39475400	-2.51055800
C	7.75137800	1.15027200	-3.13440300
H	8.70516500	-0.43490800	-2.00694300
H	6.54267200	2.68309600	-4.07496600
H	8.58533000	1.26399500	-3.83404100

C	4.58979800	1.81935700	1.21670800
C	5.88714200	1.89078000	1.75671900
C	3.58191500	2.62983800	1.76971500
C	6.16354500	2.73569600	2.83641800
H	6.69457200	1.28978700	1.32853000
C	3.85879600	3.47525300	2.85133100
H	2.57077100	2.62136100	1.34969600
C	5.14882400	3.52778200	3.38862200
H	7.17775000	2.77905500	3.24578800
H	3.06141400	4.10063700	3.26463300
H	5.36780200	4.19136400	4.23103800
C	-1.96414800	-2.58215500	1.05800000
C	-2.98996600	-3.13566200	0.27034600
C	-2.16392400	-2.43929100	2.44040300
C	-4.18588500	-3.55268600	0.85932000
H	-2.85726400	-3.24597700	-0.80946200
C	-3.36462100	-2.85616300	3.02717300
H	-1.38379500	-2.00446000	3.06920500
C	-4.37598900	-3.41475300	2.24017300
H	-4.97333600	-3.98654800	0.23580000
H	-3.50528400	-2.74355800	4.10634000
H	-5.31281600	-3.74292100	2.70064400
C	0.07745200	-3.43641700	-0.80346400
C	0.63563200	-3.23559400	-2.07729100
C	-0.08754100	-4.74997100	-0.32379800
C	1.02675700	-4.33315000	-2.85357500
H	0.77745500	-2.22333700	-2.46137500
C	0.31139300	-5.84107500	-1.10081600
H	-0.54128700	-4.93126600	0.65405600
C	0.86912000	-5.63493000	-2.36829700
H	1.45665000	-4.16464100	-3.84552000
H	0.17852000	-6.85648900	-0.71551700
H	1.17483000	-6.49028400	-2.97849300

TS-2



E(RB3LYP) = -4821.53025852
Zero-point correction= 0.931255 (Hartree/Particle)
Thermal correction to Energy= 0.995951
Thermal correction to Enthalpy= 0.996895
Thermal correction to Gibbs Free Energy= 0.822837
Sum of electronic and zero-point Energies= -4820.599003
Sum of electronic and thermal Energies= -4820.534307
Sum of electronic and thermal Enthalpies= -4820.533363
Sum of electronic and thermal Free Energies= -4820.707422

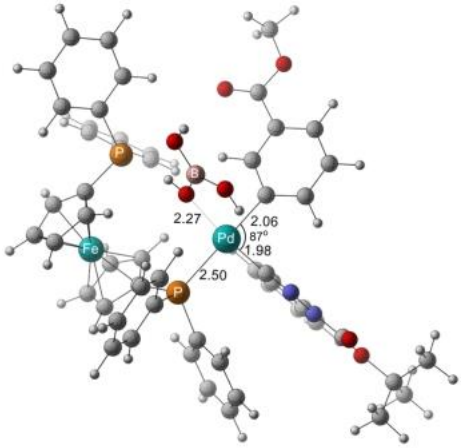
C	3.53136400	-2.36657100	-0.27897700
C	3.74456900	-3.55763700	0.47542100
C	4.51306900	-3.21369600	1.63007800
C	4.78202800	-1.81162900	1.58593200
C	4.18093200	-1.27391000	0.39616000
H	2.96417400	-2.28756400	-1.20605200
H	3.36324800	-4.54862400	0.22855400
H	4.81746100	-3.89613400	2.42449400
H	5.32928300	-1.24349100	2.33749000
F	2.73648100	-2.14149900	1.62565200
C	1.99058800	-1.09304100	3.26739400
C	1.89012800	-2.50125900	3.48989400
C	1.23608400	-0.77551200	2.10111100
H	2.56215700	-0.38675200	3.86962000
C	1.08172700	-3.06065600	2.45713700
H	2.37542100	-3.06017300	4.29066600
C	0.66015400	-1.99067300	1.58768300
H	1.11242000	0.21390000	1.66097900
H	0.82735300	-4.11455800	2.34962900
P	-0.55110800	-2.05809300	0.22583500

P	4.13699300	0.42434900	-0.28258100
P	-0.59312500	-0.00401600	-0.94018100
C	-4.30534700	1.06189900	0.79557000
C	-2.89026700	1.05545000	0.86349200
C	-2.22800500	1.67907100	1.93352700
C	-2.99119400	2.29584600	2.92170900
C	-4.40072900	2.29382400	2.84328500
C	-5.08034600	1.68402100	1.78854800
C	-2.44728100	0.33064700	-0.31476900
H	-1.13601100	1.68141400	1.98161000
H	-2.49925800	2.78851100	3.76562000
H	-4.98061400	2.78556000	3.63074800
H	-6.16739800	1.69197500	1.74003000
N	-3.47656100	-0.05939100	-1.01950700
N	-4.62795000	0.36992100	-0.37368200
C	-5.86607500	0.05159800	-0.95067800
O	-6.85651700	0.54223700	-0.20540300
O	-5.97101400	-0.57809500	-1.97682800
C	-8.27987000	0.36038300	-0.56095500
C	-9.00880500	1.08164400	0.57474000
H	-8.72269000	2.14694600	0.60831300
H	-10.09947100	1.01870700	0.42108500
H	-8.76708300	0.62218400	1.54857000
C	-8.56707200	1.03492700	-1.90588900
H	-8.03778200	0.53195900	-2.72897900
H	-9.65127400	0.99758300	-2.11007700
H	-8.25956100	2.09503900	-1.87842500
C	-8.62431700	-1.13211200	-0.56661400
H	-8.35079600	-1.59375800	0.39840300
H	-9.71159500	-1.25676700	-0.71076100
H	-8.10026900	-1.66220000	-1.37585100
C	-0.44980500	4.11594900	-0.61642300
C	0.06238300	2.83926800	-0.89272200
C	-0.47292700	2.00600300	-1.89850100
C	-1.56705300	2.52545200	-2.62760200
C	-2.07539300	3.80702500	-2.39071100
C	-1.52372700	4.60351900	-1.38281000
H	0.92142600	2.49969500	-0.30639900
H	-2.01796400	1.91508700	-3.41690500
H	-2.91125400	4.18741200	-2.98634300
H	-1.92482800	5.59929300	-1.18239500
C	0.15625500	4.89969100	0.49824600
O	-0.35005900	6.13802500	0.60072200

O	1.01301100	4.47578800	1.24974400
C	0.15425100	6.96139000	1.65471700
H	1.23955400	7.11865900	1.54016000
H	-0.37978700	7.91852800	1.57202900
H	-0.04071200	6.49899400	2.63662000
B	0.83847700	0.96935600	-2.94226700
O	1.85680000	1.89638100	-3.25547900
H	1.57047600	2.46526100	-3.98790000
O	0.14700800	0.45025100	-4.06437700
H	-0.57309100	-0.14600300	-3.80419000
O	1.30915500	-0.03618200	-1.98261000
H	2.07614300	0.29352700	-1.45322700
C	5.59956100	0.45139500	-1.41988800
C	6.66205700	-0.46744200	-1.36482300
C	5.61553200	1.44789500	-2.41391400
C	7.72564600	-0.37908200	-2.27067700
H	6.66147700	-1.26207900	-0.61321000
C	6.68274700	1.54092100	-3.31302900
H	4.77570800	2.14569900	-2.49625400
C	7.74155200	0.62775000	-3.24249900
H	8.54605400	-1.10166700	-2.21562600
H	6.68141700	2.32263300	-4.07921400
H	8.57376500	0.69533100	-3.95011000
C	4.69078100	1.49605000	1.12343000
C	5.99171900	1.46211600	1.65941200
C	3.76639300	2.41370200	1.65176600
C	6.34928900	2.30992300	2.71237400
H	6.73815800	0.77646900	1.24771300
C	4.12533100	3.26637500	2.70295600
H	2.75757500	2.48825100	1.23559500
C	5.41586200	3.21287400	3.23828400
H	7.36426600	2.27022000	3.12017600
H	3.39044000	3.97985000	3.08733300
H	5.70032900	3.88016100	4.05792600
C	-0.10348600	-3.51273700	-0.81778500
C	0.45602100	-3.30957500	-2.09085600
C	-0.30263500	-4.82828900	-0.35885800
C	0.81649000	-4.40357100	-2.88664800
H	0.62102800	-2.29418600	-2.45911800
C	0.06256100	-5.91783900	-1.15488300
H	-0.75747500	-5.01112100	0.61836700
C	0.62284000	-5.70775900	-2.42081300
H	1.24909100	-4.23176800	-3.87682800

H	-0.09753100	-6.93541400	-0.78577400
H	0.90285700	-6.56180900	-3.04503900
C	-2.11026500	-2.58889600	1.05373600
C	-3.14951800	-3.13640600	0.27997900
C	-2.31419700	-2.39429400	2.42962300
C	-4.36037200	-3.49891900	0.87551900
H	-3.01590600	-3.28581500	-0.79490000
C	-3.52966000	-2.75493000	3.02321900
H	-1.52407800	-1.96241800	3.04844500
C	-4.55361100	-3.30988200	2.24960900
H	-5.15746400	-3.92890400	0.26151000
H	-3.67210500	-2.60220300	4.09730400
H	-5.50193600	-3.59500500	2.71529700

Int-4



E(RB3LYP) = -4821.56835184

Zero-point correction= 0.932826 (Hartree/Particle)
Thermal correction to Energy= 0.998229
Thermal correction to Enthalpy= 0.999173
Thermal correction to Gibbs Free Energy= 0.821622
Sum of electronic and zero-point Energies= -4820.635526
Sum of electronic and thermal Energies= -4820.570123
Sum of electronic and thermal Enthalpies= -4820.569179
Sum of electronic and thermal Free Energies= -4820.746730

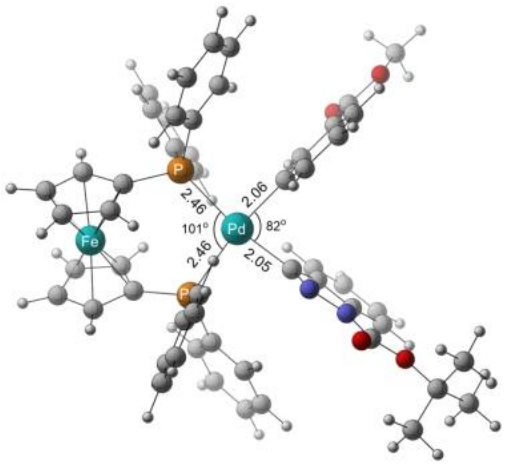
C	3.22548800	-2.51613800	-0.80803700
C	3.32985200	-3.90521700	-0.50655700
C	4.04795400	-4.03575100	0.72189300
C	4.39487200	-2.72854500	1.17822000
C	3.89299300	-1.77085500	0.22975200
H	2.71679100	-2.08811400	-1.67126700
H	2.91030400	-4.72077900	-1.09582000

H	4.26770100	-4.97009400	1.23967100
H	4.92715600	-2.49645900	2.10007500
F	2.33578500	-2.89646900	1.02644800
C	1.56353000	-2.43454800	2.90607300
C	1.35627700	-3.81701800	2.60962300
C	0.90094700	-1.66765200	1.90401700
H	2.14470100	-2.03507200	3.73723000
C	0.57271400	-3.90637400	1.42128500
H	1.75632600	-4.66084800	3.17281000
C	0.27514600	-2.56916800	0.97360800
H	0.86680900	-0.58063600	1.83931000
H	0.26052100	-4.83177700	0.93981300
P	-0.86865100	-2.00275200	-0.33766000
P	3.95666700	0.05439900	0.21267100
P	-0.71046900	0.46209600	-0.71828400
C	-4.33168900	1.14807700	1.36153900
C	-2.92152800	1.01600400	1.37837800
C	-2.21242300	1.13618100	2.58419500
C	-2.92360500	1.38011900	3.75683900
C	-4.32930800	1.50407400	3.72718400
C	-5.05523800	1.39273100	2.54062100
C	-2.52983200	0.76999100	0.00024300
H	-1.12313100	1.03941100	2.59354000
H	-2.39379900	1.47797400	4.70907700
H	-4.86903500	1.69539200	4.66012900
H	-6.13875200	1.49330200	2.53296400
N	-3.58759400	0.76491600	-0.77087100
N	-4.70553900	0.98911100	0.02592400
C	-5.96192900	1.02000000	-0.59283500
O	-6.91366300	1.24119900	0.31571300
O	-6.11604500	0.86505400	-1.78194400
C	-8.34422500	1.33113100	-0.04212400
C	-9.01747100	1.58396100	1.30865200
H	-8.64570300	2.51903200	1.76174100
H	-10.10900100	1.67183300	1.17452100
H	-8.81804500	0.75237800	2.00621300
C	-8.56692100	2.51363500	-0.99015900
H	-8.07478300	2.34843600	-1.96026100
H	-9.64907200	2.64681700	-1.16292900
H	-8.17377400	3.44401200	-0.54403200
C	-8.81313000	0.00163600	-0.64153300
H	-8.58382100	-0.83198700	0.04527600
H	-9.90645300	0.03221400	-0.79086300

H	-8.33173200	-0.19381500	-1.61131500
C	0.86649800	4.48515100	-0.73231000
C	0.62497300	3.11166000	-0.54347500
C	-0.58129600	2.50286900	-0.93468400
C	-1.55479200	3.33631100	-1.51961200
C	-1.32588100	4.70669300	-1.71927200
C	-0.12053200	5.29042600	-1.32612500
H	1.42836600	2.52677100	-0.08908700
H	-2.51642100	2.91346800	-1.82613200
H	-2.10086600	5.32387500	-2.18637400
H	0.06071800	6.35606400	-1.47959900
C	2.18997100	5.02764800	-0.31025200
O	2.28618800	6.35791900	-0.47448600
O	3.10337800	4.35773200	0.13337100
C	3.52594300	6.96781300	-0.11185600
H	4.35189400	6.56609500	-0.72247100
H	3.40135100	8.04319300	-0.30298900
H	3.75009000	6.79319900	0.95360200
B	1.56537700	0.76654000	-2.96966200
O	2.84740600	0.94850200	-3.39373700
H	2.88869500	1.26410000	-4.31206500
O	0.50433000	0.95923100	-3.80561700
H	-0.34234400	0.90406100	-3.32223100
O	1.34242400	0.33531300	-1.67299800
H	2.14025500	0.36675500	-1.07331500
C	5.57251800	0.45487800	-0.59063700
C	6.50868500	-0.51043200	-0.99481300
C	5.83611400	1.81389400	-0.85273200
C	7.69200200	-0.12487700	-1.63783900
H	6.31811800	-1.57100500	-0.80826500
C	7.02194500	2.19638400	-1.48547900
H	5.10803400	2.57925200	-0.56005500
C	7.95312500	1.22723800	-1.88126500
H	8.41350900	-0.88781300	-1.94691700
H	7.21677900	3.25609300	-1.67837200
H	8.87859100	1.52691400	-2.38275700
C	4.25594200	0.53653000	1.97295600
C	3.23527300	1.21377400	2.66188700
C	5.46830200	0.27829900	2.63884600
C	3.41031200	1.60367100	3.99509900
H	2.29802600	1.45146300	2.14928200
C	5.64343300	0.66676400	3.97056000
H	6.28721000	-0.22161400	2.11305300

C	4.61336700	1.32708400	4.65247400
H	2.60640600	2.13169800	4.51697100
H	6.59069500	0.45725500	4.47713800
H	4.75350400	1.63381100	5.69360500
C	-0.59855300	-3.13482800	-1.77658100
C	-0.11130600	-2.61500200	-2.98689600
C	-0.88532800	-4.51127100	-1.69820200
C	0.10728000	-3.45328700	-4.08732300
H	0.09157500	-1.54734400	-3.08304300
C	-0.66228600	-5.34832000	-2.79485400
H	-1.30388400	-4.93612100	-0.78200900
C	-0.16127600	-4.82155900	-3.99207300
H	0.48422800	-3.02953000	-5.02302400
H	-0.88829500	-6.41612800	-2.71602200
H	0.00866600	-5.47703100	-4.85171000
C	-2.51245500	-2.57225800	0.29388200
C	-3.58684700	-2.69445900	-0.60578800
C	-2.74178600	-2.81071800	1.65877700
C	-4.85593300	-3.06463800	-0.15248800
H	-3.43474600	-2.50473200	-1.67231900
C	-4.01467200	-3.17788100	2.11230600
H	-1.92585100	-2.71456700	2.37920600
C	-5.07400200	-3.30845500	1.20919300
H	-5.67876400	-3.16102300	-0.86754700
H	-4.17456900	-3.36477600	3.17870100
H	-6.06764600	-3.59924800	1.56382300

Int-5



E(RB3LYP) = -4569.28581024
Zero-point correction= 0.884201 (Hartree/Particle)
Thermal correction to Energy= 0.943498

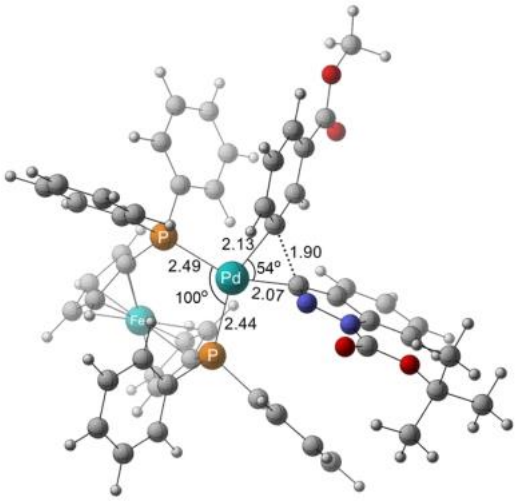
Thermal correction to Enthalpy= 0.944442
Thermal correction to Gibbs Free Energy= 0.782798
Sum of electronic and zero-point Energies= -4568.401609
Sum of electronic and thermal Energies= -4568.342312
Sum of electronic and thermal Enthalpies= -4568.341368
Sum of electronic and thermal Free Energies= -4568.503012

C	3.31910900	-2.16269500	-1.67935800
C	4.32362600	-3.17410000	-1.63068800
C	5.30864400	-2.77457000	-0.67810000
C	4.92258600	-1.51120800	-0.14004800
C	3.68154900	-1.11677000	-0.75469500
H	2.42078300	-2.19116600	-2.29525700
H	4.31862200	-4.10429000	-2.19948700
H	6.18994000	-3.34705600	-0.38710300
H	5.45895900	-0.95951800	0.62989000
F	3.43349400	-2.89794900	0.23739500
C	3.48094700	-3.53131600	2.22702700
C	3.23837400	-4.64541500	1.36817800
C	2.44606600	-2.57370000	2.01226800
H	4.32598700	-3.41453200	2.90604400
C	2.04870800	-4.38580700	0.62516900
H	3.86770200	-5.53072200	1.27182200
C	1.54383900	-3.09500100	1.01508000
H	2.36534600	-1.60495800	2.50438300
H	1.61953600	-5.03849800	-0.13297500
P	0.07079900	-2.20140800	0.39339300
P	2.68761000	0.39436100	-0.45497200
P	0.25901100	0.19034900	-0.15293600
C	-3.85213000	0.80698300	0.95324100
C	-2.47374000	0.85554000	1.27359000
C	-2.05768900	1.32293200	2.53051800
C	-3.02273500	1.73760100	3.44590100
C	-4.39266500	1.68772800	3.11098200
C	-4.83154600	1.22477800	1.86967100
C	-1.76573200	0.35837700	0.10294400
H	-0.99345800	1.35687300	2.78003500
H	-2.72143500	2.10639900	4.43097600
H	-5.13521700	2.02015500	3.84349800
H	-5.89151200	1.19038600	1.62547100
N	-2.63072400	0.04149200	-0.82996000
N	-3.91343000	0.29804500	-0.34475100
C	-5.00341600	0.01195800	-1.17461900

O	-6.14511000	0.32481800	-0.55693400
O	-4.88540200	-0.45274600	-2.28504300
C	-7.46624500	0.12918700	-1.18715300
C	-8.43388600	0.62355000	-0.10946500
H	-8.24220700	1.68338100	0.13114100
H	-9.47385700	0.52964600	-0.46557300
H	-8.32692400	0.02928200	0.81429800
C	-7.57219300	0.99243600	-2.44833800
H	-6.87222600	0.65376800	-3.22661600
H	-8.59931500	0.93312300	-2.84855500
H	-7.35730400	2.04906500	-2.21048700
C	-7.68859700	-1.35920800	-1.47403700
H	-7.55342400	-1.95292800	-0.55282600
H	-8.72122400	-1.51361200	-1.83248600
H	-6.99188100	-1.72899100	-2.24104800
C	-0.27581700	2.50666200	-2.02390200
C	0.06740500	2.17241000	-0.69903100
C	0.23500100	3.23380000	0.20349500
C	0.07727500	4.57763000	-0.19035500
C	-0.26190300	4.88217300	-1.51924200
C	-0.43638500	3.83861200	-2.43056500
H	-0.43035300	1.71374500	-2.76373600
H	0.49680600	3.04860400	1.24814000
H	-0.38869600	5.92155500	-1.82824500
H	-0.70366300	4.06164000	-3.46904400
C	0.27868300	5.63780600	0.83792000
O	0.09052000	6.87952200	0.35355400
O	0.58152200	5.43097400	1.99674400
C	0.26241800	7.96180800	1.26842300
H	-0.44861900	7.88143300	2.10775800
H	1.28939300	7.97505400	1.67055000
H	0.06835600	8.87865400	0.69350000
C	3.24979200	1.50868200	-1.82835800
C	3.34958900	2.89745200	-1.62996200
C	3.50868600	0.99188100	-3.10989700
C	3.71433300	3.74365800	-2.68174400
H	3.14300500	3.32887600	-0.64804600
C	3.86827300	1.84056500	-4.16299500
H	3.43944600	-0.08206100	-3.29838600
C	3.97497100	3.21895200	-3.95240200
H	3.79236900	4.82075600	-2.50450400
H	4.07007600	1.41710000	-5.15176200
H	4.26024500	3.88197200	-4.77495300

C	3.46647900	1.13688700	1.04674700
C	4.78901600	1.61846300	1.04596300
C	2.71709700	1.21871400	2.23249700
C	5.34934300	2.15538100	2.20861800
H	5.38734800	1.58327200	0.13150700
C	3.27837800	1.75599500	3.39698600
H	1.68119900	0.86470900	2.24196000
C	4.59598100	2.22336700	3.38719800
H	6.37913800	2.52502900	2.19276600
H	2.67999500	1.81348500	4.31104100
H	5.03560900	2.64679700	4.29541300
C	-0.43432600	-3.15705900	-1.10400000
C	-0.87412200	-4.49166600	-1.02631100
C	-0.37975100	-2.53266700	-2.36122500
C	-1.23156600	-5.18896100	-2.18395000
H	-0.94813500	-4.99150600	-0.05656100
C	-0.73738500	-3.23134500	-3.52036600
H	-0.06776900	-1.48581900	-2.43094200
C	-1.16080000	-4.56109800	-3.43377900
H	-1.57046200	-6.22672200	-2.10869900
H	-0.69140800	-2.73004900	-4.49174300
H	-1.44406200	-5.10757600	-4.33858800
C	-1.22368300	-2.65979800	1.64119100
C	-2.57539300	-2.74635500	1.26025100
C	-0.89015800	-2.85795300	2.99223000
C	-3.56404600	-3.03635100	2.20538600
H	-2.86234100	-2.58858100	0.21812900
C	-1.88216000	-3.14280000	3.93770600
H	0.15080400	-2.79992100	3.31915400
C	-3.22186100	-3.23475000	3.54780500
H	-4.60919500	-3.10595300	1.88820700
H	-1.60121900	-3.29815700	4.98399300
H	-3.99683400	-3.46138000	4.28645400

TS-3



E(RB3LYP) = -4569.26261718
Zero-point correction= 0.882502 (Hartree/Particle)
Thermal correction to Energy= 0.941508
Thermal correction to Enthalpy= 0.942453
Thermal correction to Gibbs Free Energy= 0.781888
Sum of electronic and zero-point Energies= -4568.380115
Sum of electronic and thermal Energies= -4568.321109
Sum of electronic and thermal Enthalpies= -4568.320165
Sum of electronic and thermal Free Energies= -4568.480730

C	3.88858600	-2.34145300	-0.37845000
C	4.81966400	-3.06861300	0.42194000
C	5.26209300	-2.21104000	1.47453100
C	4.61515000	-0.94770700	1.31887800
C	3.76027500	-1.01468900	0.16662900
H	3.36618300	-2.72520500	-1.25441500
H	5.11573900	-4.10725400	0.27101000
H	5.95728000	-2.47713300	2.27147600
H	4.73834900	-0.08386100	1.97049500
F	3.19425800	-2.44937900	1.56274400
C	2.49399100	-2.58338800	3.52612000
C	2.65023200	-3.89011000	2.97039500
C	1.57585700	-1.86342800	2.70638600
H	3.00844000	-2.19337600	4.40485500
C	1.82503300	-3.98359900	1.81003900
H	3.30956800	-4.67274700	3.34747600
C	1.14874100	-2.72591800	1.63370100
H	1.25322100	-0.83226300	2.85315900
H	1.74845200	-4.84912600	1.15357500
P	-0.02499500	-2.18261000	0.34185100

P	2.68034600	0.30428900	-0.53543900
P	0.21239300	0.16819000	-0.26900500
C	-3.78810000	0.87707500	0.90084000
C	-2.40835200	1.03346300	1.16765800
C	-1.96629300	1.25158300	2.48189400
C	-2.91070300	1.33569400	3.50352500
C	-4.28473400	1.19723100	3.21917100
C	-4.74667800	0.96220200	1.92375600
C	-1.73014700	0.87778400	-0.12039300
H	-0.89893000	1.33970400	2.70134900
H	-2.58655400	1.50633400	4.53435000
H	-5.01101500	1.26760400	4.03504000
H	-5.80847500	0.84467100	1.71801200
N	-2.63095100	0.63642400	-1.06019300
N	-3.88266700	0.63701200	-0.47316500
C	-4.99309900	0.40088500	-1.29372900
O	-6.11521200	0.44152700	-0.57203500
O	-4.90105700	0.19028700	-2.48129600
C	-7.44895100	0.23416400	-1.17205600
C	-8.38792900	0.37404000	0.02819900
H	-8.29007500	1.37316800	0.48647600
H	-9.43423300	0.24024900	-0.29504200
H	-8.15987300	-0.38733800	0.79383600
C	-7.72588100	1.32801700	-2.20824200
H	-7.04662600	1.24567500	-3.06984800
H	-8.76510700	1.23673300	-2.56934000
H	-7.60705900	2.32739100	-1.75401900
C	-7.53629800	-1.17423300	-1.76847000
H	-7.28008800	-1.93124100	-1.00625800
H	-8.56913200	-1.36581500	-2.10779900
H	-6.85757700	-1.28944700	-2.62660000
C	-0.55176200	2.55433700	-2.01854400
C	-0.43718900	2.16250600	-0.66151500
C	-0.14282200	3.17517900	0.27137800
C	0.06233800	4.50918000	-0.12394200
C	-0.02209600	4.86191000	-1.47965000
C	-0.33133500	3.87139300	-2.42051000
H	-0.84649300	1.81063400	-2.76440500
H	-0.06961800	2.95255100	1.33614300
H	0.13600900	5.89638000	-1.78913300
H	-0.41281600	4.13426100	-3.48017600
C	0.36200400	5.51182000	0.93961100
O	0.58271600	6.74332600	0.44789100

O	0.40746200	5.26521000	2.12858600
C	0.87716300	7.77264500	1.39318300
H	0.03955700	7.90712200	2.09794600
H	1.78919300	7.52890400	1.96321300
H	1.02966000	8.68906900	0.80543000
C	0.19814000	-3.39447700	-1.04056400
C	-0.12056200	-4.75845400	-0.90169500
C	0.67394900	-2.93425500	-2.27948400
C	0.05676800	-5.64203700	-1.97042800
H	-0.52114700	-5.13551500	0.04359700
C	0.84905600	-3.81825700	-3.35140700
H	0.90340600	-1.87206400	-2.40865500
C	0.54479700	-5.17423200	-3.19726200
H	-0.19249000	-6.70044100	-1.84634800
H	1.21904600	-3.44180700	-4.30989200
H	0.67875100	-5.86648700	-4.03422600
C	-1.66477100	-2.70929200	1.02505700
C	-1.85459600	-3.02324100	2.38094600
C	-2.77691000	-2.73702600	0.16221800
C	-3.12468100	-3.36587400	2.86182700
H	-1.00798700	-3.00783300	3.07211300
C	-4.04206400	-3.08592600	0.64198100
H	-2.65633300	-2.48857100	-0.89639700
C	-4.22104100	-3.40062500	1.99502600
H	-3.25299000	-3.61143400	3.92076400
H	-4.89404900	-3.10990700	-0.04489300
H	-5.21230000	-3.67255600	2.37067700
C	3.33275100	0.40496800	-2.26558800
C	4.68239800	0.16113700	-2.58302200
C	2.44092600	0.72177900	-3.30392600
C	5.12688600	0.24159600	-3.90608800
H	5.39373100	-0.09639700	-1.79348500
C	2.88601300	0.80381700	-4.62880300
H	1.38791400	0.90263200	-3.07352000
C	4.22977200	0.56396000	-4.93222200
H	6.17927100	0.04953600	-4.13722300
H	2.17717100	1.05074000	-5.42502000
H	4.57890400	0.62315900	-5.96774700
C	3.36039500	1.81206000	0.30047500
C	4.24791800	2.71215200	-0.31192700
C	2.93257400	2.07530300	1.61538500
C	4.70998600	3.83763700	0.38138600
H	4.58634100	2.54195900	-1.33662500

C	3.40573800	3.19066400	2.31248900
H	2.21644200	1.40378000	2.09911800
C	4.29711200	4.07658200	1.69601500
H	5.39983600	4.52945600	-0.11206700
H	3.06358400	3.37671000	3.33481300
H	4.66203600	4.95515400	2.23691700