Electronic Supplementary Material (ESI) for ChemComm.

Supplementary information

Negishi Coupling Reactions with [^{11}C]CH_3I: A Versatile Method for Efficient ^{11}C-C Bond Formation

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1 Experimental Procedures and Results

1.1 General Considerations

All commercially available reagents (analytical grade) and solvents (analytical grade) were obtained from Sigma Aldrich and used without further purification. Hihg performance liquid chromatography (HPLC) studies were performed with an Agilent 1200 Series HPLC system equipped with a radiometric detector (Gabi, Raytest) and a variable wavelength detector (wavelength for the analysis was set to 254 nm) connected in series. Unless stated otherwise, a RP-C18 column (Mediterranea Sea18, 4.6x150 mm, 5 µm particle size; Teknokroma, Spain) was used as the stationary phase and water/acetonitrile mixtures as the mobile phase at a flow rate of 1.5 mL/min. Identical conditions were used both for analysis of the reaction mixtures and to isolate products during identification of de-halogenated compounds.

The identity of all new compounds was determined by ^{1}H and ^{13}C NMR experiments, performed on 500-MHz Avance III Bruker spectrometer and UPLC/ESI-MS analyses, performed using an AQUITY UPLC separation module coupled to a LCT TOF premier XE mass spectrometer (Waters, Manchester, UK). The detection was carried out in positive mode, monitoring the most abundant isotope peaks from the mass spectra ($M\text{-}H^{+}$). GCMS analyses were performed on a 7820A GC system (Agilent Technologies), coupled to a 5975C inert XL MSD with Triple-Axis Detector (Agilent Technologies).

1.2 Synthesis of triflates

To a solution of aryl alcohol (1 mmol) and pyridine (3 mmol) in dichloromethane (1.5 mL) at -15°C, a solution of trifluoromethanesulfonyl anhydride (2 mmol) in dichloromethane (1.5 mL) was slowly added. The solution was stirred at -15°C for 1 hour. The reaction was quenched by the addition of water and the product was extracted with dichloromethane. The organic phase was dried over anhydrous magnesium sulphate, filtered, and the filtrate evaporated under vacuum. The crude product was purified by column chromatography over silica gel using ethyl acetate/petroleum ether = 1:9 mixture as the mobile phase. Pure aryl triflates were obtained in quantitative yield. The products identity was confirmed by ^{1}H and ^{13}C NMR and HRMS analysis.

4-methoxyphenyl trifluoromethanesulfonate: Colourless oil (263 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.14–7.08 (m, 2H), 6.86–6.81 (m, 2H), 3.74 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 159.09, 143.03 , 122.33, 118.77 (q, $^{1}J_{C,F}$ = 320.8 Hz), 115.03, 55.68. UPLC/ESI-MS (ESI+) m/z calcd for $C_8H_8F_3O_4S^{+}$+Na 280.196 $[M\text{-}H+Na]^{+}$, found 280.253.

4-acetophenyl trifluoromethanesulfonate: Colourless oil (281 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.02–7.96 (m, 2H), 7.34–7.27 (m, 2H), 2.55 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 196.09, 152.45, 136.86, 130.58, 121.63, 118.69 (q, $^{1}J_{C,F}$ = 320.8 Hz), 26.66. UPLC/ESI-MS (ESI+) *m/z* calculated for $C_9H_8F_3O_4S^{+}$ 269.0090 $[M\text{-}H]^{+}$, found 268.9977.

1.3 Production of $[^{11}C]CH_3I$

The synthesis of $[^{11}C]CH_3I$ was carried out using a TRACERlab $FX_{C\ Pro}$ synthesis module (GE Healthcare). $[^{11}C]CH_4$ was directly generated in an IBA Cyclone 18/9 cyclotron by irradiation (target current=22 µA) of a $N_2/5\%H_2$ gas mixture with 18 MeV protons. The radioactive gas was trapped in Carbosphere 60/80 (Alltech Associates, Inc.) at T=-140ºC, desorbed by heating (80ºC) and allowed to react with iodine at 720ºC to form $[^{11}C]CH_3I$ in a gas circulating process. $[^{11}C]CH_3I$ was selectively retained in a trap containing Porapak™ Q (50-80 mesh, Waters Corporation) at room

temperature, while unreacted [^{11}C]CH_4 was recirculated. At the end of the process (8-9 cycles), the Porapak™ Q trap was heated at 190ºC and [^{11}C]CH_3I was distilled under continuous helium flow (20 mL/min). The gas stream was passed through a trap containing phosphorous pentoxide and Ascarite II® (20-30 mesh) before being introduced in the reaction cartridge.

1.4 Formation of [^{11}C]MeZnI in zinc cartridge

A plastic solid phase extraction cartridge (reversible SPE tube, non-fluorous polypropylene, 2 mL; obtained from Sigma Aldrich, stock No. 57608) was filled with 3 g of zinc powder (<100 µm particles) and end-capped with 20 µm porosity glass frits. The cartridge was preloaded with iodine (100 µmol) in DMA (300 µL). [^{11}C]CH_3I (ca. 370 MBq) was distilled into the cartridge and the reaction was kept at 65 °C for 1 min. The cartridge was washed with dry THF (3 mL), the amount of radioactivity was measured in a dose calibrator (PETDOSE HC, Comecer) and an aliquot was submitted to HPLC analysis.

1.5 One-pot Negishi coupling reaction via *in situ* formation of [^{11}C]MeZnI

A plastic solid phase extraction cartridge (reversible SPE tube, non-fluorous polypropylene, 2 mL; obtained from Sigma Aldrich, stock No. 57608) was filled with 3 g of zinc powder (<100 µm particles) and end-capped with 20 µm porosity glass frits. During optimization in model reaction, four different scenarios were assayed (Figure S1). Finally, scenario shown in Fig. S1c was selected as optimal and applied to all other reactions.

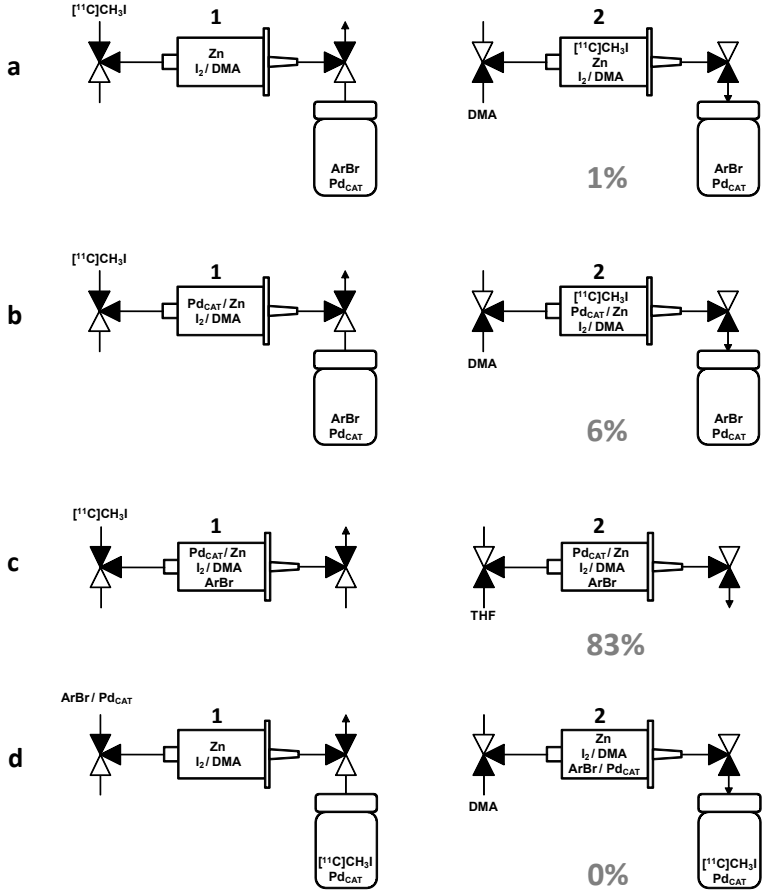


Figure S1. Experimental scenarios assayed to conduct the Negishi cross-coupling reaction. Flows associated with the generation of Zn(II)-containing nucleophiles and with ^{11}C-C Negishi

couplings are gathered on the left and on the right of each entry a-d, respectively. Filled and hollow triangles denote open and closed valves, respectively. Numbers in gray correspond to chromatographic yields of 4-[^{11}C]methylacetophenone (Ar=4-Ac-C_6H_4).

In scenario shown in Fig. S1c, the cartridge was preloaded with the corresponding aryl halide or triflate (50 µmol), tetrakistriphenylphosphine palladium (10 µmol), and iodine (100 µmol) in DMA (300 µL). [^{11}C]CH_3I (370 MBq) was distilled into the cartridge and the reaction was kept at 65 °C for 1, 3, 5 or 10 min. The cartridge was washed with dry THF (3 mL), the amount of radioactivity was measured in a dose calibrator (PETDOSE HC, Comecer) and an aliquot was submitted to HPLC analysis. Specific conditions are detailed below (entries correspond to Table 1 in the main document):

[^{11}C]4-Methylacetophenone

a) **Entry 1:** 4-Bromoacetophenone reacted for 5 minutes, resulting in 83% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (40/60); rt_{prod} = 6.02 min (radioactive detector), rt_{stand} = 6.09 min (UV detector).
b) **Entry 14:** 4-Acetophenyl trifluoromethanesulfonate reacted for 5 minutes, resulting in 73% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (40/60); rt_{prod} = 6.02 min (radioactive detector), rt_{stand} = 6.09 min (UV detector).

For this compound, a kinetic study to determine the percentage of radioactivity present as [^{11}C]4-methylacetophenone, [^{11}C]CH_3I and [^{11}C]CH_4 (the latter formed by hydrolysis of [^{11}C]MeZnI) was carried out (Figure S1).

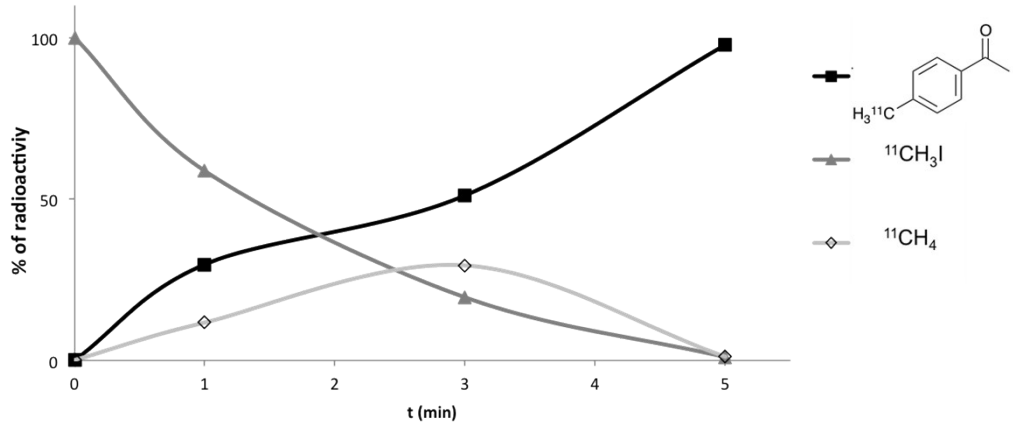


Figure S2. Kinetic study of the formation of [^{11}C]4-methylacetophenone: HPLC chromatographs of reaction mixture after 1, 3, and 5 minutes of reaction (top) and a graphical representation of the contents of $^{11}CH_3I$, $^{11}CH_4$, and final [^{11}C]4-methylacetophenone in the reaction mixture at different times (bottom).

[^{11}C]3-Methylacetophenone

a) **Entry 2:** 3-Bromoacetophenone reacted for 10 minutes, resulting in 35% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (40:60); rt_{prod} = 6.17 min (radioactive detector), rt_{stand} = 6.25 min (UV detector).

[^{11}C]2-Methylacetophenone

a) **Entry 3:** 2-Bromoacetophenone reacted for 10 minutes, resulting in 53% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (40/60); rt_{prod} = 6.27 min (radioactive detector), rt_{stand} = 6.35 min (UV detector).

b) **Entry 10:** 2-Iodoacetophenone reacted for 5 minutes, resulting in 23% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (40/60); rt_{prod} = 6.27 min (radioactive detector), rt_{stand} = 6.35 min (UV detector).

[^{11}C]Ethyl-4-methylbenzoate

a) **Entry 4:** Ethyl-4-bromobenzoate reacted for 5 minutes, resulting in 69% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60:40); rt_{prod} = 4.58 min (radioactive detector), rt_{stand} = 4.65 min (UV detector).

[^{11}C]1-Methylnaphthalene.

a) **Entry 5:** 1-Bromonaphthalene reacted for 10 minutes, resulting in 21% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60/40); rt_{prod} = 6.87 min (radioactive detector), rt_{stand} = 6.98 min (UV detector).
b) **Entry 11:** 1-Iodonaphthalene reacted for 10 minutes, resulting in 26% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60:40); rt_{prod} = 6.87 min (radioactive detector), rt_{stand} = 6.98 min (UV detector).

[^{11}C]4-Methylaniline

a) **Entry 6:** 4-Bromoaniline reacted for 10 minutes, resulting in 19% conversion into the product. HPLC analysis: ACN/0.1M NaOAc in ultrapure water (25/75); rt_{prod} = 6.85 min (radioactive detector), rt_{stand} = 6.85 min (UV detector).

[^{11}C]2-Methylaniline

a) **Entry 7:** 2-Bromoaniline reacted for 10 minutes, resulting in 2% conversion into the product. HPLC analysis: ACN/0.1M NaOAc in ultrapure water (25/75); rt_{prod} = 5.50 min (radioactive detector), rt_{stand} = 5.63 min (UV detector).
b) **Entry 12:** 2-Iodonaniline reacted for 10 minutes, resulting in 12% conversion into the product. HPLC analysis: ACN/0.1M NaOAc in ultrapure water (25/75); rt_{prod} = 5.50 min (radioactive detector), rt_{stand} = 5.63 min (UV detector).

[^{11}C]4-Methylanisole.

a) **Entry 8:** 4-Bromoanisole reacted for 10 minutes, resulting in 8% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60/40); rt_{prod} = 3.70 min (radioactive detector), rt_{stand} = 3.77 min (UV detector).
b) **Entry 13:** 4-Iodoanisole reacted for 10 minutes, resulting in 33% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60/40); rt_{prod} = 3.70 min (radioactive detector), rt_{stand} = 3.77 min (UV detector).
c) **Entry 15:** 4-Methoxyphenyl trifluoromethanesulfonate reacted for 10 minutes, resulting no product.

[^{11}C]2,4-Dichlorotoluene

a) **Entry 9:** 2,4-Dichloroiodobenzene reacted for 10 minutes, resulting in 60% conversion into the product. HPLC analysis: ACN/0.1% TFA in ultrapure water (60/40); rt_{prod} = 9.10 min (radioactive detector), rt_{stand} = 9.17 min (UV detector).

[^{11}C]Thymidine.

A zinc-filled (3 g of zinc powder) cartridge was preloaded with a solution of Idoxuridine (50 µmol), tetrakistriphenylphosphine palladium (10 µmol), and iodine

(100 µmol) in DMA (300 µL). [^{11}C]CH_3I (1.5 GBq) was distilled into the cartridge and the reaction was kept at 65 °C for 5 min. The crude was eluted from the cartridge with 20% MeOH solution in 10 mM NaH_2PO_4 in ultrapure water (pH 5.4; 1.5 mL). The eluted fraction was filtered through cotton and purified by HPLC. A Mediteranea Sea 18 column (5 µm, 25x1 cm; Teknokroma, Spain) was used as the stationary phase and 20% MeOH solution in 10 mM NaH_2PO_4 in ultrapure water (pH 5.4) was used as the mobile phase (flow = 5 mL/min). The product (Rt = 11-13 min) was collected and reformulated by trapping in a C-18 cartridge and subsequent elution with ethanol (1 mL). Chemical and radiochemical purity were determined by HPLC using an Agilent Zorbax XDB-C18 column (5 µm, 4.6 x 50mm) as stationary phase.

1.6 De-halogenation of aryl iodides

A plastic solid phase extraction cartridge (reversible SPE tube, non-fluorous polypropylene, 2 mL; obtained from Sigma Aldrich, stock No. 57608) was filled with 3 g of zinc powder (<100 µm particles) and end-capped with 20 µm porosity glass frits. The cartridge was preloaded with the corresponding aryl halide (0.5 mmol), tetrakistriphenylphosphine palladium (0) (10 µmol), and iodine (100 µmol) in anhydrous DMA (300 µL). The cartridge was kept at 65 °C for 10 min. The cartridge was washed with THF (1 mL) and an aliquot was submitted to HPLC analysis. A small sample of the reaction mixture was injected in the HPLC, the different products were isolated and analysed by GCMS. See Figure S2 for example of analysis of the dehalogenation product resulting from entry 9 in Table 1.

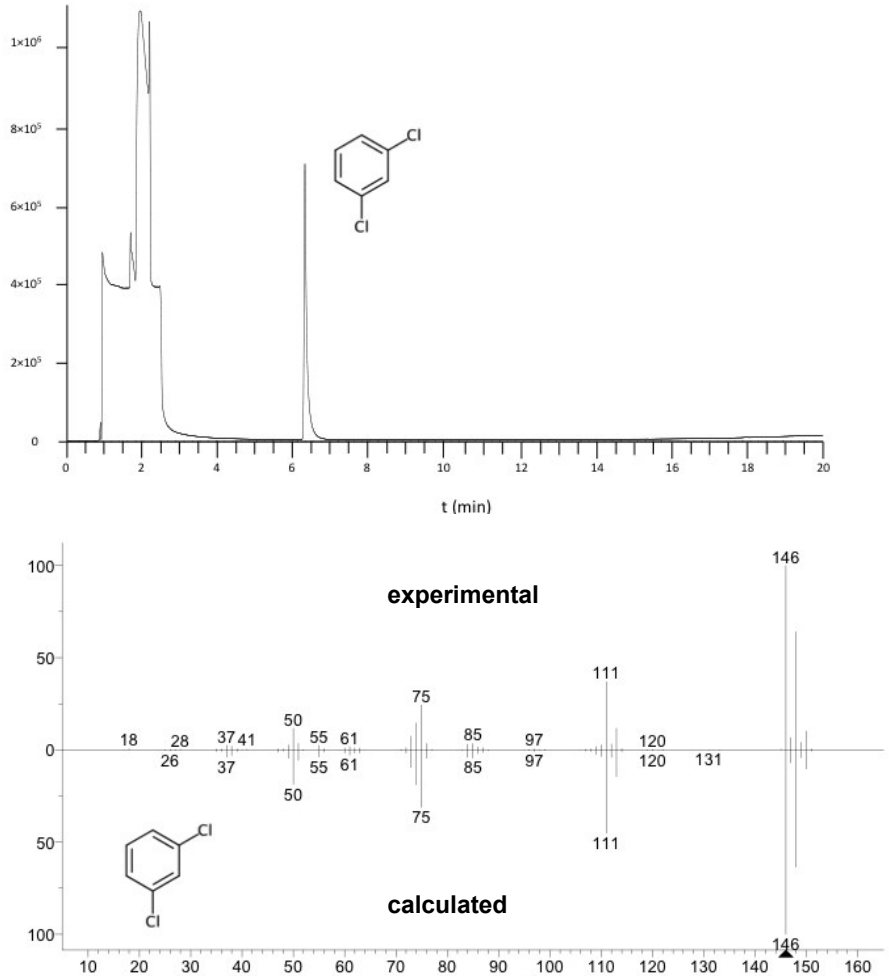


Figure S3. Gas chromatography chromatogram (top) and experimental mass spectrum of the peak observed at rt = 6.4 min (bottom). The calculated spectrum for 1,3-dichlorobenzene is also included to show exact matching.

2 Computational methods

2.1 Standard 1M free energies in solution

All the reaction energies in solution were calculated at the 1M standard state. Since the harmonic analyses and the thermodynamic calculations were performed at P = 1 atm, the conversion between both states was performed by means of the following expression:[1,2]

$$\Delta G_{rxn}^{1M} = \Delta G_{rxn}^{1atm} - RT\Delta n[ln(24.45)] \quad (1)$$

where Δn is a stoichiometric term given by

$$\Delta n = \sum_{i}^{products} n_i - \sum_{j}^{reactants} n_j \quad (2)$$

At T=333.15 K eq. (1) becomes

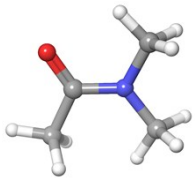
$$\Delta G_{rxn}^{1M}(333.15) = \Delta G_{rxn}^{1atm}(333.15) - 2.1\Delta \text{(kcal/mol)}. \quad (3)$$

Since activation energies shown in Figure 3 correspond to intramolecular processes via **TSa-c**, Δn=0 and therefore in this particular case $\Delta G_{a}^{1M} = \Delta G_{a}^{1atm}$.

2.2 Energies, imaginary frequencies and geometries of the stationary points discussed in Figures 2 and 3

All energies are given in atomic units (hartree/particle) and have been calculated at the B3LYP-D3 (PCM, solvent=*N,N*-dimethylacetamide)/6-31G* (C,H,O,N,P) & LANL2DZ (Zn,Pd,I) level of theory. Harmonic analyses were computed at 333.15 K and 1atm. When necessary ^{11}C isotopes were considered.

DMA (NIMAG=0)



E= -287.8471998

Zero-point correction=	0.130965
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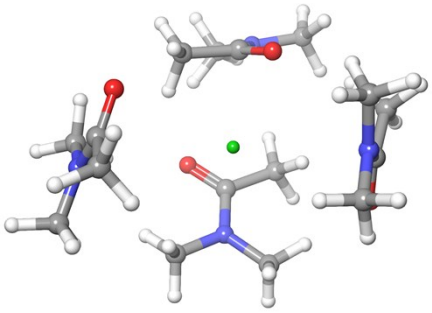
Thermal correction to Enthalpy=	0.141254
Thermal correction to Gibbs Free Energy=	0.093543
Sum of electronic and zero-point Energies=	-287.716235
Sum of electronic and thermal Energies=	-287.707001
Sum of electronic and thermal Enthalpies=	-287.705946
Sum of electronic and thermal Free Energies=	-287.753657

[1] C. P. Kelly, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2006**, *110*, 16066-16081.

[2] C. P. Kelly, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2007**, *111*, 408-422.

$Zn(DMA)_4$ (NIMAG=0)



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Sum of electronic and thermal Energies= -1216.459997
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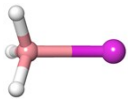
$[^{11}C]CH_3I$ (NIMAG=0)



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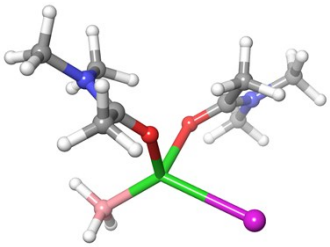
1 (NIMAG=0)



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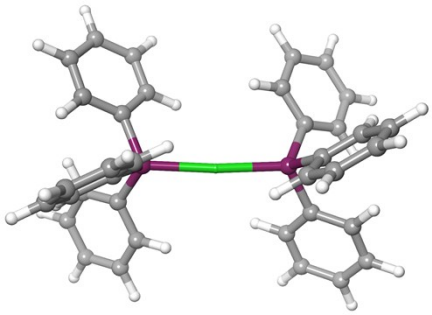
Sum of electronic and zero-point Energies= -692.403980
Sum of electronic and thermal Energies= -692.375717

Sum of electronic and thermal Enthalpies= -692.374662
Sum of electronic and thermal Free Energies= -692.473560

$Pd(PPh_3)_2$ (NIMAG=0)



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Sum of electronic and thermal Energies= -2198.888501
Sum of electronic and thermal Enthalpies= -2198.887446
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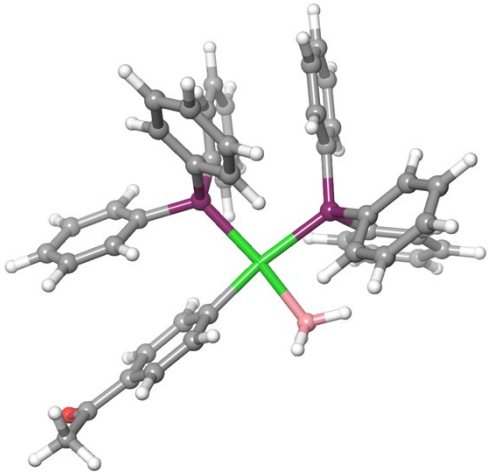
cis-5a (NIMAG=0)



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[^{11}C]-cis-5a
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Thermal correction to Gibbs Free Energy= 0.617582
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Sum of electronic and thermal Energies= -2622.914457
Sum of electronic and thermal Enthalpies= -2622.913402
Sum of electronic and thermal Free Energies= -2623.071036
[^{12}C]-cis-5a
Zero-point correction= 0.717209
Thermal correction to Energy= 0.773968

Thermal correction to Enthalpy= 0.775023
Thermal correction to Gibbs Free Energy= 0.617305
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Sum of electronic and thermal Energies= -2622.914650
Sum of electronic and thermal Enthalpies= -2622.913594
Sum of electronic and thermal Free Energies= -2623.071312

[^{13}C]-cis-5a

Zero-point correction= 0.716826
Thermal correction to Energy= 0.773660
Thermal correction to Enthalpy= 0.774715
Thermal correction to Gibbs Free Energy= 0.616583
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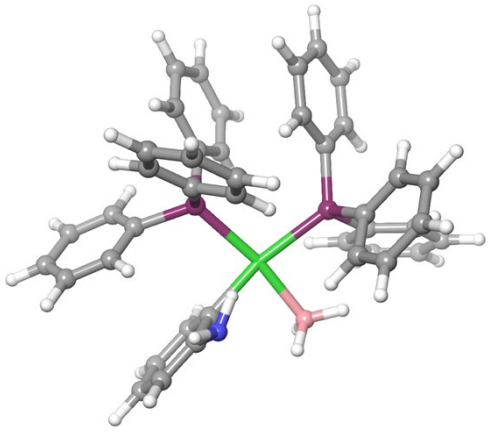
cis-5b (NIMAG=0)



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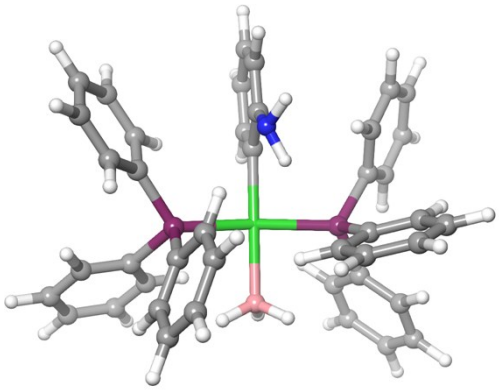
Thermal correction to Gibbs Free Energy= 0.602161
Sum of electronic and zero-point Energies= -2525.693762
Sum of electronic and thermal Energies= -2525.639765
Sum of electronic and thermal Enthalpies= -2525.638710
Sum of electronic and thermal Free Energies= -2525.788588

trans-5b (NIMAG=0)



E=-2526.3847093
Zero-point correction= 0.697213
Thermal correction to Energy= 0.751005
Thermal correction to Enthalpy= 0.752060
Thermal correction to Gibbs Free Energy= 0.602397
Sum of electronic and zero-point Energies= -2525.687497
Sum of electronic and thermal Energies= -2525.633704
Sum of electronic and thermal Enthalpies= -2525.632649
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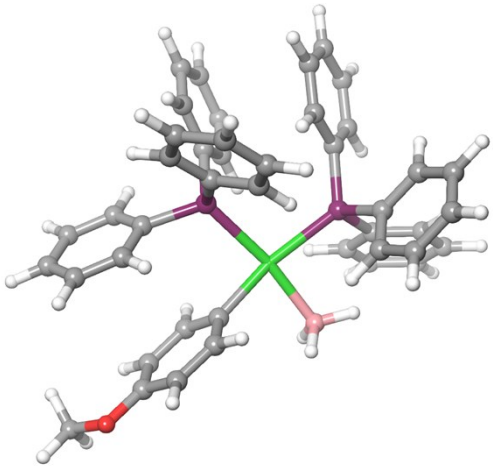
cis-5c (NIMAG=0)



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Zero-point correction= 0.712369
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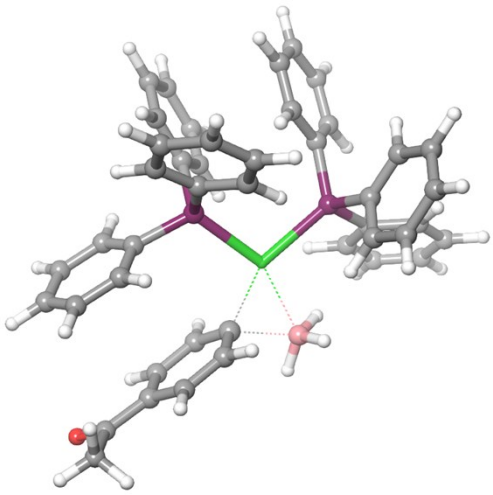
Thermal correction to Enthalpy= 0.769127
Thermal correction to Gibbs Free Energy= 0.613287
Sum of electronic and zero-point Energies= -2584.841445
Sum of electronic and thermal Energies= -2584.785741
Sum of electronic and thermal Enthalpies= -2584.784686
Sum of electronic and thermal Free Energies= -2584.940526

TSa (NIMAG=1, -424.4882 cm^{-1})



E= -2623.6600402

[^{11}C]-TSa

Zero-point correction= 0.715761
Thermal correction to Energy= 0.772347
Thermal correction to Enthalpy= 0.773402
Thermal correction to Gibbs Free Energy= 0.614178
Sum of electronic and zero-point Energies= -2622.944279
Sum of electronic and thermal Energies= -2622.887693
Sum of electronic and thermal Enthalpies= -2622.886638
Sum of electronic and thermal Free Energies= -2623.045862

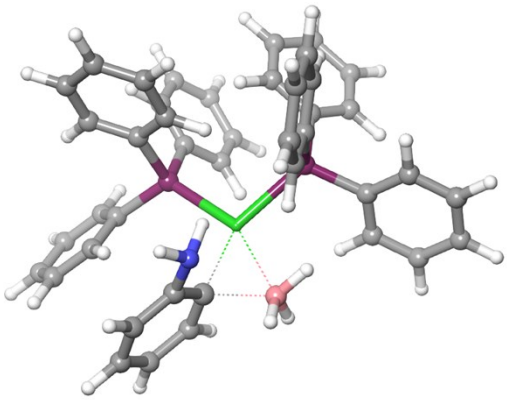
[^{12}C]-TSa

Zero-point correction= 0.715590
Thermal correction to Energy= 0.772206
Thermal correction to Enthalpy= 0.773261
Thermal correction to Gibbs Free Energy= 0.613958
Sum of electronic and zero-point Energies= -2622.944450
Sum of electronic and thermal Energies= -2622.887834
Sum of electronic and thermal Enthalpies= -2622.886779
Sum of electronic and thermal Free Energies= -2623.046083

[^{13}C]-TSa

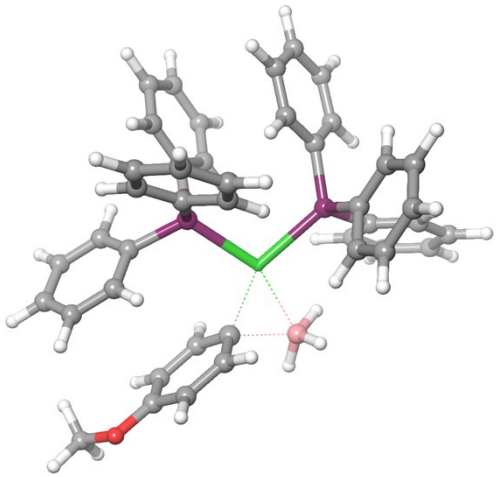
Zero-point correction= 0.715441
Thermal correction to Energy= 0.772085
Thermal correction to Enthalpy= 0.773140
Thermal correction to Gibbs Free Energy= 0.613761
Sum of electronic and zero-point Energies= -2622.944599
Sum of electronic and thermal Energies= -2622.887956
Sum of electronic and thermal Enthalpies= -2622.886901
Sum of electronic and thermal Free Energies= -2623.046279

TSb (NIMAG=1, -453.6319 cm^{-1})



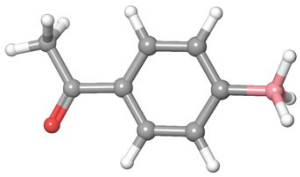
E= -2526.3581933
Zero-point correction= 0.695720
Thermal correction to Energy= 0.749618
Thermal correction to Enthalpy= 0.750673
Thermal correction to Gibbs Free Energy= 0.597731
Sum of electronic and zero-point Energies= -2525.662473
Sum of electronic and thermal Energies= -2525.608575
Sum of electronic and thermal Enthalpies= -2525.607520
Sum of electronic and thermal Free Energies= -2525.760463

TSc (NIMAG=1, -445.2012 cm^{-1})



E= -2585.5231036
Zero-point correction= 0.711137
Thermal correction to Energy= 0.766543
Thermal correction to Enthalpy= 0.767598
Thermal correction to Gibbs Free Energy= 0.612027
Sum of electronic and zero-point Energies= -2584.811967
Sum of electronic and thermal Energies= -2584.756560
Sum of electronic and thermal Enthalpies= -2584.755505
Sum of electronic and thermal Free Energies= -2584.911077

6a (NIMAG=0)



E= -424.2351882

[^{11}C]-6a

Zero-point correction= 0.166264
Thermal correction to Energy= 0.177949
Thermal correction to Enthalpy= 0.179004
Thermal correction to Gibbs Free Energy= 0.125011
Sum of electronic and zero-point Energies= -424.068925
Sum of electronic and thermal Energies= -424.057239
Sum of electronic and thermal Enthalpies= -424.056184
Sum of electronic and thermal Free Energies= -424.110178

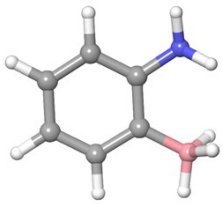
[^{12}C]-6a

Zero-point correction= 0.166044
Thermal correction to Energy= 0.177753
Thermal correction to Enthalpy= 0.178808
Thermal correction to Gibbs Free Energy= 0.124733
Sum of electronic and zero-point Energies= -424.069144
Sum of electronic and thermal Energies= -424.057435
Sum of electronic and thermal Enthalpies= -424.056380
Sum of electronic and thermal Free Energies= -424.110456

[^{13}C]-6a

Zero-point correction= 0.165854
Thermal correction to Energy= 0.177584
Thermal correction to Enthalpy= 0.178639
Thermal correction to Gibbs Free Energy= 0.124485
Sum of electronic and zero-point Energies= -424.069335
Sum of electronic and thermal Energies= -424.057604
Sum of electronic and thermal Enthalpies= -424.056549
Sum of electronic and thermal Free Energies= -424.110703

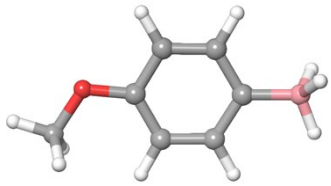
6b (NIMAG=0)



E= -326.9366451

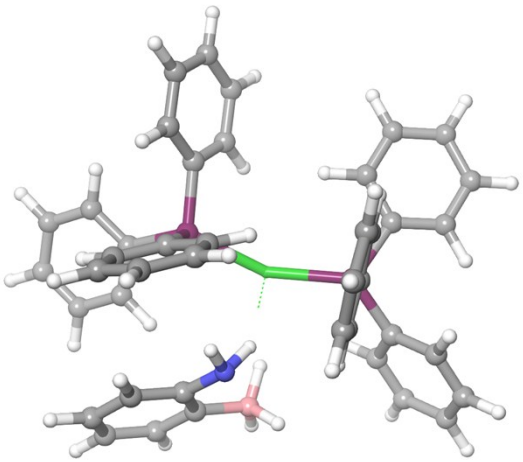
Zero-point correction= 0.145796
Thermal correction to Energy= 0.154657
Thermal correction to Enthalpy= 0.155712
Thermal correction to Gibbs Free Energy= 0.110317
Sum of electronic and zero-point Energies= -326.790849
Sum of electronic and thermal Energies= -326.781988
Sum of electronic and thermal Enthalpies= -326.780933
Sum of electronic and thermal Free Energies= -326.826328

6c (NIMAG=0)



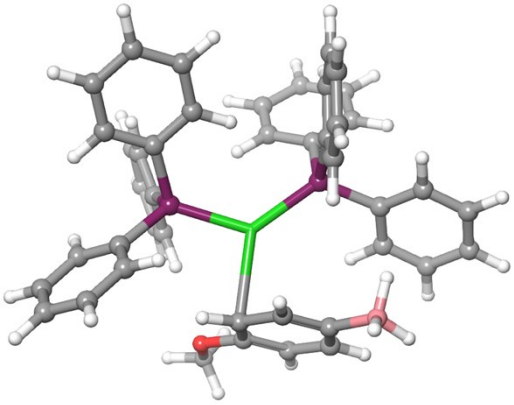
E= -386.1051017
Zero-point correction= 0.161239
Thermal correction to Energy= 0.171892
Thermal correction to Enthalpy= 0.172947
Thermal correction to Gibbs Free Energy= 0.120528
Sum of electronic and zero-point Energies= -385.943863
Sum of electronic and thermal Energies= -385.933210
Sum of electronic and thermal Enthalpies= -385.932155
Sum of electronic and thermal Free Energies= -385.984574

6b' (NIMAG=0)



E= -2526.4407084
Zero-point correction= 0.699222
Thermal correction to Energy= 0.753441
Thermal correction to Enthalpy= 0.754496
Thermal correction to Gibbs Free Energy= 0.599504
Sum of electronic and zero-point Energies= -2525.741486
Sum of electronic and thermal Energies= -2525.687268
Sum of electronic and thermal Enthalpies= -2525.686213
Sum of electronic and thermal Free Energies= -2525.841204

6c' (NIMAG=0)



E= -2585.6050521
Zero-point correction= 0.714129
Thermal correction to Energy= 0.770251
Thermal correction to Enthalpy= 0.771306
Thermal correction to Gibbs Free Energy= 0.611978
Sum of electronic and zero-point Energies= -2584.890923
Sum of electronic and thermal Energies= -2584.834801
Sum of electronic and thermal Enthalpies= -2584.833746
Sum of electronic and thermal Free Energies= -2584.993074

2.3 Complete reference 13h

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian, Inc.*, Wallingford CT, 2013.

2.4 Cartesian coordinates of the stationary points discussed in Figures 2 and 3

DMA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.073646	-1.462324	0.007811
2	6	0	0.731631	-0.291229	-0.004640
3	6	0	1.758663	0.819856	0.002006
4	7	0	-0.591802	0.079970	-0.032636
5	6	0	-1.085823	1.434322	0.009305
6	6	0	-1.609862	-0.945863	0.004446
7	1	0	2.743430	0.349412	0.047641
8	1	0	1.704973	1.434953	-0.905202
9	1	0	1.643949	1.486469	0.865780
10	1	0	-1.823269	1.592363	-0.791586

11	1	0	1.585192	1.646805	0.968320
12	1	0	-0.282495	2.161272	-0.127512
13	1	0	-1.118950	-1.920529	-0.030315
14	1	0	-2.289783	-0.844425	-0.853819
15	1	0	-2.206860	-0.870033	0.925965

$Zn(DMA)_4$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.702125	1.354628	-1.804283
2	8	0	-1.427142	1.853302	-1.738470
3	30	0	0.743682	-1.209563	-0.800005
4	8	0	0.547901	1.058370	2.529038
5	8	0	-3.913663	-1.796613	0.749349
6	6	0	-0.272709	0.146882	2.324589
7	6	0	3.936121	0.221753	-1.362997
8	6	0	-0.797730	2.509962	-0.892143
9	6	0	-3.624442	-1.302589	-0.351243
10	6	0	4.151369	-0.954919	-2.303386
11	6	0	-4.178971	0.051217	-0.763863
12	7	0	0.001265	-1.150275	2.638947
13	6	0	-0.812619	-2.297439	2.251714
14	6	0	1.314401	-1.497553	3.168326
15	7	0	4.021882	-0.045858	-0.027104
16	6	0	4.192361	-1.400768	0.489335
17	6	0	3.722348	0.999273	0.947937
18	6	0	-1.612844	0.462505	1.689937
19	6	0	0.698619	2.347599	-0.721341
20	7	0	-1.411128	3.398996	-0.061263
21	6	0	-0.702780	4.059679	1.038152
22	6	0	-2.845305	3.635949	-0.179445
23	7	0	-2.798267	-1.933198	-1.235276
24	6	0	-2.455772	-1.405391	-2.552320
25	6	0	-2.357849	-3.299292	-0.979000
26	1	0	4.051533	-0.593125	-3.327730
27	1	0	5.142518	-1.405239	-2.177537
28	1	0	3.398207	-1.730587	-2.120774
29	1	0	-4.815245	0.412645	0.045433
30	1	0	-3.380606	0.776636	-0.950738
31	1	0	-4.774048	-0.028734	-1.681041
32	1	0	-0.298008	-2.862887	1.462700
33	1	0	-0.957309	-2.954445	3.117734
34	1	0	-1.787478	-2.003583	1.867756
35	1	0	1.201405	-2.223362	3.981046
36	1	0	1.935145	-1.946352	2.381828
37	1	0	1.804789	-0.599921	3.540760
38	1	0	4.391509	-1.342617	1.561281
39	1	0	3.283912	-2.000402	0.336486
40	1	0	5.037049	-1.909232	0.016610
41	1	0	4.523672	1.053108	1.694231
42	1	0	3.649757	1.950980	0.423970
43	1	0	2.773462	0.800585	1.460599
44	1	0	-1.792627	1.531400	1.795778
45	1	0	-1.554590	0.227655	0.621331
46	1	0	-2.453367	-0.094268	2.106331
47	1	0	0.908481	1.822208	0.216701
48	1	0	1.094691	1.748083	-1.539466
49	1	0	1.221689	3.308997	-0.688721
50	1	0	-1.442573	4.517065	1.698351
51	1	0	-0.126678	3.337431	1.624026
52	1	0	-0.034617	4.849821	0.674378
53	1	0	-3.051462	4.706807	-0.084134
54	1	0	-3.184238	3.287277	-1.154225
55	1	0	-3.402398	3.100418	0.600689
56	1	0	-3.144117	-1.776061	-3.324754

57	1	0	-2.450809	-0.316352	-2.551842
58	1	0	-1.440008	-1.733158	-2.796891
59	1	0	-2.729074	-3.969437	-1.765175
60	1	0	-1.261415	-3.338314	-0.969020
61	1	0	-2.742829	-3.622519	-0.013526

$[^{11}C]CH_3I$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.040653	-2.184246
2	6(11)	0	0.000000	0.000000	-1.867573
3	1	0	0.901232	-0.520327	-2.184246
4	1	0	-0.901232	-0.520327	-2.184246
5	53	0	0.000000	0.000000	0.335060

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	-1.865764	-1.902882	-0.376878
2	30	0	0.342563	-0.459675	1.019859
3	8	0	1.749270	-0.456019	-0.572159
4	8	0	-0.477660	1.442458	0.679821
5	6	0	2.985501	-0.299077	-0.746800
6	6	0	-1.146293	1.877000	-0.299310
7	6	0	-0.673935	1.622705	-1.713171
8	7	0	3.637448	0.785036	-0.297354
9	6	0	5.079373	0.993163	-0.431353
10	6(11)	0	2.924835	1.867129	0.384039
11	6	0	1.125162	-0.900503	2.866004
12	7	0	-2.269181	2.580061	-0.091951
13	6	0	-3.102950	3.140455	-1.153606
14	6	0	-2.780060	2.793258	1.262630
15	6	0	3.749265	-1.365405	-1.504411
16	1	0	0.219869	1.001737	-1.664996
17	1	0	-1.437232	1.099504	-2.295876
18	1	0	-0.431223	2.562285	-2.221343
19	1	0	5.281224	1.783936	-1.162998
20	1	0	5.483820	1.302301	0.537640
21	1	0	5.589169	0.083159	-0.739472
22	1	0	1.857560	1.804371	0.181734
23	1	0	3.089076	1.807382	1.466133
24	1	0	3.308419	2.825100	0.020807
25	1	0	0.375169	-0.821932	3.663984
26	1	0	1.535914	-1.918400	2.895172
27	1	0	1.942164	-0.206491	3.108767
28	1	0	-2.618855	3.067059	-2.124387
29	1	0	-4.061728	2.610898	-1.192188
30	1	0	-3.295736	4.196689	-0.939393
31	1	0	-2.779714	3.863798	1.495026
32	1	0	-3.807712	2.419742	1.324632
33	1	0	-2.152497	2.262899	1.975045
34	1	0	4.307467	-0.948418	-2.348101
35	1	0	3.027225	-2.093571	-1.874331
36	1	0	4.460082	-1.878609	-0.847360

$Pd(PPh_3)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.002096	-0.027371	-0.183415

2	15	0	-2.311193	-0.009887	-0.060318
3	15	0	2.315483	-0.010634	-0.063193
4	6	0	3.862886	0.094122	4.325869
5	6	0	2.666976	-0.550043	3.995011
6	6	0	2.219474	-0.556169	2.673231
7	6	0	2.967721	0.071321	1.662390
8	6	0	4.165545	0.718091	2.004184
9	6	0	4.608651	0.729045	3.329429
10	1	0	4.208167	0.106986	5.355979
11	1	0	2.078313	-1.039081	4.766379
12	1	0	1.279085	-1.040453	2.419544
13	1	0	4.753268	1.216259	1.239137
14	1	0	5.536274	1.235424	3.582029
15	6	0	-4.213704	4.141635	-0.959224
16	6	0	-4.826928	3.304688	-0.023611
17	6	0	-4.274135	2.055864	0.271613
18	6	0	-3.097881	1.632008	-0.366018
19	6	0	-2.482162	2.485406	-1.297139
20	6	0	-3.039716	3.729223	-1.596801
21	1	0	-4.644498	5.112983	-1.185885
22	1	0	-5.736636	3.622544	0.478528
23	1	0	-4.759881	1.414577	1.000668
24	1	0	-1.558838	2.172410	-1.779687
25	1	0	-2.553783	4.378782	-2.319700
26	6	0	4.369630	-3.721699	-1.976972
27	6	0	4.962197	-3.119983	-0.863837
28	6	0	4.365232	-2.007769	-0.264715
29	6	0	3.164707	-1.487429	-0.772848
30	6	0	2.570629	-2.105998	-1.885689
31	6	0	3.172453	-3.211766	-2.488146
32	1	0	4.834664	-4.587673	-2.439889
33	1	0	5.889826	-3.515769	-0.459375
34	1	0	4.834631	-1.548920	0.600212
35	1	0	4.963981	0.393637	-1.472985
36	1	0	2.702676	-3.680378	-3.348572
37	6	0	-4.451893	-2.954985	-2.959383
38	6	0	-3.189029	-3.244853	-2.434331
39	6	0	-2.562579	-2.336577	-1.579551
40	6	0	-3.196495	-1.133181	-1.227547
41	6	0	-4.462797	-0.848783	-1.762496
42	6	0	-5.085116	-1.755289	-2.624488
43	1	0	-4.937103	-3.657703	-3.631134
44	1	0	-2.688268	-4.172705	-2.696982
45	1	0	-1.572888	-2.554281	-1.184063
46	1	0	-4.964393	0.080789	-1.510182
47	1	0	-6.064446	-1.522904	-3.033944
48	6	0	3.142326	1.410518	-0.901781
49	6	0	2.449771	2.632412	-0.939673
50	6	0	4.416413	1.331417	-1.485264
51	6	0	3.025832	3.756445	-1.533168
52	1	0	1.452996	2.694430	-0.508205
53	6	0	4.988439	2.455640	-2.086476
54	1	0	1.629189	-1.720840	-2.271519
55	6	0	4.296773	3.669520	-2.109275
56	1	0	2.479577	4.695511	-1.554295
57	1	0	5.974507	2.381423	-2.536939
58	1	0	4.742975	4.541680	-2.579075
59	6	0	-2.971707	-0.499695	1.593062
60	6	0	-2.196596	-0.187937	2.723224
61	6	0	-4.202191	-1.150935	1.770575
62	6	0	-2.650498	-0.504345	4.004406
63	1	0	-1.230635	0.294517	2.592017
64	6	0	-4.652195	-1.472774	3.053777
65	1	0	-4.810945	-1.410059	0.909758
66	6	0	-3.880108	-1.148318	4.172052
67	1	0	-2.040860	-0.257069	4.869211
68	1	0	-5.606119	-1.978081	3.177931
69	1	0	-4.231170	-1.402126	5.168455

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.242340	-1.105626	-0.070681
2	15	0	-0.753705	1.252027	0.041498
3	15	0	2.168988	-0.891405	-0.009207
4	6	0	-5.058501	-1.967277	-0.128914
5	6	0	-4.304979	-2.176886	1.039572
6	6	0	-2.922707	-1.990338	1.035572
7	6	0	-2.236566	-1.565133	-0.117918
8	6	0	-3.001034	-1.385000	-1.289234
9	6	0	-4.377218	-1.582868	-1.298667
10	1	0	-4.794233	-2.479025	1.961527
11	1	0	-4.955957	-1.420688	-2.203624
12	6	0	3.871758	-3.374239	-3.555063
13	6	0	2.764300	-2.536274	-3.716446
14	6	0	2.271288	-1.814478	-2.629196
15	6	0	2.892511	-1.901765	-1.371394
16	6	0	4.000977	-2.745406	-1.217720
17	6	0	4.483972	-3.480085	-2.304379
18	1	0	4.250566	-3.945542	-4.397908
19	1	0	2.277988	-2.452402	-4.684373
20	1	0	1.397336	-1.181505	-2.755226
21	1	0	4.486302	-2.843813	-0.252502
22	1	0	5.339569	-4.136180	-2.169899
23	6	0	0.259441	3.149620	4.158596
24	6	0	-0.398736	3.917705	3.192065
25	6	0	-0.717228	3.361340	1.953031
26	6	0	-0.360394	2.034325	1.656754
27	6	0	0.275846	1.265265	2.642296
28	6	0	0.587424	1.819941	3.885923
29	1	0	0.503788	3.584330	5.123741
30	1	0	-0.670323	4.947495	3.406342
31	1	0	-1.252287	3.956342	1.218405
32	1	0	0.527710	0.229248	2.436074
33	1	0	1.084362	1.211828	4.636634
34	6	0	4.297431	3.236750	-0.397279
35	6	0	4.159908	2.417834	-1.519208
36	6	0	3.538814	1.172351	-1.412704
37	6	0	3.050091	0.724900	-0.176606
38	6	0	3.187528	1.558434	0.946270
39	6	0	3.805367	2.804026	0.836231
40	1	0	4.779496	4.206508	-0.484349
41	1	0	4.529642	2.749048	-2.485267
42	1	0	3.438677	0.553512	-2.297600
43	1	0	4.891894	-0.842827	1.218397
44	1	0	3.904247	3.432245	1.717328
45	6	0	1.338781	3.505172	-3.436801
46	6	0	0.756301	2.248146	-3.620976
47	6	0	0.160489	1.593312	-2.543367
48	6	0	0.125974	2.192352	-1.271246
49	6	0	0.722218	3.446511	-1.093703
50	6	0	1.326430	4.096127	-2.172238
51	1	0	1.811073	4.014751	-4.272004
52	1	0	0.771445	1.774439	-4.598588
53	1	0	-0.287578	0.613126	-2.687955
54	1	0	0.738310	3.913200	-0.115423
55	1	0	1.797789	5.062571	-2.018276
56	6	0	2.877534	-1.556958	1.555478
57	6	0	2.036623	-2.230984	2.455170
58	6	0	4.232351	-1.383774	1.890137
59	6	0	2.540357	-2.727100	3.660216
60	1	0	0.986838	-2.361442	2.210426
61	6	0	4.735066	-1.885682	3.090708

62	1	0	2.825899	1.232745	1.914699
63	6	0	3.889439	-2.558078	3.978606
64	1	0	1.876505	-3.241171	4.349650
65	1	0	5.784212	-1.746047	3.335574
66	1	0	4.280565	-2.942263	4.916564
67	6	0	-2.515391	1.744394	-0.192938
68	6	0	-3.435469	1.380366	0.804880
69	6	0	-2.982369	2.389486	-1.345795
70	6	0	-4.792765	1.651718	0.649646
71	1	0	-3.092772	0.864341	1.696046
72	6	0	-4.345450	2.662406	-1.498661
73	1	0	-2.290361	2.679919	-2.129279
74	6	0	-5.253197	2.293423	-0.505031
75	1	0	-5.492969	1.352619	1.424649
76	1	0	-4.693652	3.164649	-2.397265
77	1	0	-6.312655	2.500455	-0.628470
78	1	0	-2.373058	-2.160876	1.959127
79	1	0	-2.515988	-1.048388	-2.203350
80	6(11)	0	-0.007878	-3.207129	-0.201571
81	1	0	-0.621681	-3.691414	0.565988
82	1	0	-0.360640	-3.528997	-1.188627
83	1	0	1.033344	-3.524735	-0.081645
84	6	0	-6.535487	-2.110884	-0.170634
85	8	0	-7.167718	-1.940736	-1.213135
86	6	0	-7.272728	-2.463422	1.111925
87	1	0	-6.935350	-3.429065	1.506204
88	1	0	-7.084923	-1.712538	1.888270
89	1	0	-8.343697	-2.511979	0.905682

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.211470	-1.227245	-0.319779
2	15	0	-1.469390	0.827957	-0.040022
3	15	0	2.074609	-0.426392	-0.070055
4	6	0	-4.430240	-3.670827	-0.762250
5	6	0	-3.885413	-3.443691	0.502754
6	6	0	-2.674660	-2.745005	0.648334
7	6	0	-1.989000	-2.266562	-0.490286
8	6	0	-2.551866	-2.518878	-1.746000
9	6	0	-3.763809	-3.208415	-1.898074
10	1	0	-4.404141	-3.803309	1.390830
11	1	0	-4.178581	-3.376716	-2.889630
12	6	0	4.876975	-2.579785	-3.085166
13	6	0	3.586218	-2.185219	-3.450541
14	6	0	2.755728	-1.564979	-2.516565
15	6	0	3.211495	-1.317959	-1.211743
16	6	0	4.506855	-1.714839	-0.852855
17	6	0	5.333176	-2.347329	-1.785360
18	1	0	5.521859	-3.070128	-3.809098
19	1	0	3.223546	-2.368555	-4.458188
20	1	0	1.743728	-1.281082	-2.794080
21	1	0	4.874006	-1.535211	0.152796
22	1	0	6.333484	-2.656621	-1.494966
23	6	0	-1.664935	2.055446	4.449895
24	6	0	-2.626396	2.549997	3.562954
25	6	0	-2.592695	2.189006	2.214940
26	6	0	-1.589499	1.331495	1.731150
27	6	0	-0.640335	0.828337	2.635660
28	6	0	-0.672909	1.190265	3.984022
29	1	0	-1.696328	2.336511	5.498752
30	1	0	-3.407615	3.214405	3.921444
31	1	0	-3.360786	2.560324	1.543535
32	1	0	0.126518	0.143620	2.290115
33	1	0	0.072542	0.787715	4.664214

34	6	0	3.289708	4.035807	-0.612523
35	6	0	3.833294	3.070249	-1.459989
36	6	0	3.493353	1.723625	-1.303885
37	6	0	2.602255	1.328320	-0.296200
38	6	0	2.061100	2.308668	0.552296
39	6	0	2.402722	3.649775	0.396743
40	1	0	3.550058	5.083047	-0.738465
41	1	0	4.524114	3.360557	-2.246977
42	1	0	3.925535	0.985964	-1.971087
43	1	0	4.312091	0.637411	1.612243
44	1	0	1.965976	4.394819	1.055364
45	6	0	0.083797	4.472510	-2.463135
46	6	0	0.380202	3.165318	-2.853644
47	6	0	-0.079926	2.089164	-2.093489
48	6	0	-0.846026	2.308746	-0.939587
49	6	0	-1.142782	3.624944	-0.556286
50	6	0	-0.677231	4.700180	-1.313030
51	1	0	0.451195	5.311579	-3.047439
52	1	0	0.982364	2.981843	-3.738733
53	1	0	0.168568	1.072404	-2.385887
54	1	0	-1.724300	3.817256	0.339213
55	1	0	-0.904944	5.716165	-1.002172
56	6	0	2.693897	-0.797378	1.629335
57	6	0	2.027240	-1.765257	2.399777
58	6	0	3.793260	-0.123303	2.187328
59	6	0	2.450286	-2.050493	3.699647
60	1	0	1.168312	-2.282288	1.983163
61	6	0	4.216915	-0.413546	3.485496
62	1	0	1.364450	2.028071	1.335967
63	6	0	3.545227	-1.375538	4.245159
64	1	0	1.919968	-2.795491	4.286285
65	1	0	5.067466	0.116630	3.904857
66	1	0	3.871012	-1.593965	5.258328
67	6	0	-3.232493	0.772052	-0.573119
68	6	0	-4.182687	0.119344	0.228740
69	6	0	-3.629228	1.281649	-1.818028
70	6	0	-5.501729	-0.012864	-0.202527
71	1	0	-3.891611	-0.290653	1.189786
72	6	0	-4.950955	1.143989	-2.250348
73	1	0	-2.910658	1.788815	-2.454347
74	6	0	-5.890453	0.497727	-1.444416
75	1	0	-6.223194	-0.523964	0.428708
76	1	0	-5.244130	1.546481	-3.216275
77	1	0	-6.918156	0.391579	-1.780942
78	7	0	-2.135732	-2.559209	1.942896
79	1	0	-2.044058	-2.156895	-2.639045
80	6(11)	0	0.567885	-3.189573	-0.501914
81	1	0	0.005327	-3.876249	0.137735
82	1	0	0.435138	-3.487825	-1.548531
83	1	0	1.631658	-3.255134	-0.251633
84	1	0	-5.372775	-4.205946	-0.854066
85	1	0	-1.494980	-1.772553	1.981276
86	1	0	-2.841154	-2.469405	2.668064

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.007205	-0.209784	-0.462263
2	15	0	-2.311943	-0.307376	-0.137515
3	15	0	2.318633	-0.336118	-0.131902
4	6	0	0.032266	4.734407	-0.554722
5	6	0	0.166418	3.986851	-1.726355
6	6	0	0.183397	2.586278	-1.642944
7	6	0	0.061771	1.898836	-0.428275
8	6	0	-0.047208	2.679033	0.743705

9	6	0	-0.067645	4.081913	0.676216
10	1	0	0.257795	4.482618	-2.690616
11	1	0	-0.155922	4.663492	1.593523
12	6	0	3.006598	-1.375940	4.350862
13	6	0	1.764411	-1.599772	3.752626
14	6	0	1.570670	-1.293357	2.404387
15	6	0	2.617821	-0.753436	1.638190
16	6	0	3.862542	-0.526558	2.250050
17	6	0	4.055029	-0.840042	3.596619
18	1	0	3.157209	-1.611185	5.400747
19	1	0	0.938731	-2.005736	4.330478
20	1	0	0.600377	-1.464371	1.948411
21	1	0	4.677746	-0.092266	1.679200
22	1	0	5.021957	-0.659367	4.057670
23	6	0	-4.770185	-2.310146	-3.531271
24	6	0	-5.415168	-1.886294	-2.364189
25	6	0	-4.682375	-1.289345	-1.338882
26	6	0	-3.292790	-1.120274	-1.465016
27	6	0	-2.654564	-1.543302	-2.639111
28	6	0	-3.391686	-2.134871	-3.668574
29	1	0	-5.342859	-2.771516	-4.331050
30	1	0	-6.488277	-2.016601	-2.255556
31	1	0	-5.190913	-0.950782	-0.440341
32	1	0	-1.581846	-1.412340	-2.740819
33	1	0	-2.887597	-2.458301	-4.575078
34	6	0	4.432351	-3.523086	-2.763923
35	6	0	4.774055	-3.430405	-1.412799
36	6	0	4.153771	-2.484043	-0.592534
37	6	0	3.177255	-1.627338	-1.118367
38	6	0	2.827386	-1.736898	-2.474550
39	6	0	3.458688	-2.671680	-3.295268
40	1	0	4.917418	-4.258807	-3.399294
41	1	0	5.525188	-4.094098	-0.993536
42	1	0	4.430774	-2.422170	0.454958
43	1	0	4.339930	0.479527	-2.189065
44	1	0	3.182804	-2.743273	-4.343597
45	6	0	-2.661762	-2.915942	3.691081
46	6	0	-2.143682	-1.617545	3.747359
47	6	0	-2.088498	-0.833353	2.595173
48	6	0	-2.562585	-1.334979	1.369169
49	6	0	-3.087024	-2.633864	1.321511
50	6	0	-3.133764	-3.419141	2.477617
51	1	0	-2.697793	-3.528575	4.587551
52	1	0	-1.778117	-1.215321	4.688386
53	1	0	-1.679468	0.172191	2.642927
54	1	0	-3.457051	-3.039683	0.385884
55	1	0	-3.540274	-4.425421	2.425275
56	6	0	3.355285	1.164496	-0.389107
57	6	0	3.216933	2.241165	0.503624
58	6	0	4.213125	1.299332	-1.489612
59	6	0	3.923416	3.424647	0.298845
60	1	0	2.553616	2.157153	1.357598
61	6	0	4.916766	2.490041	-1.695470
62	1	0	2.051879	-1.093058	-2.881751
63	6	0	4.773824	3.554385	-0.804021
64	1	0	3.802975	4.248652	0.996603
65	1	0	5.579241	2.579539	-2.552086
66	1	0	5.321042	4.479101	-0.965167
67	6	0	-3.309623	1.209517	0.172370
68	6	0	-3.169390	2.279832	-0.725515
69	6	0	-4.236006	1.315074	1.220734
70	6	0	-3.938791	3.433458	-0.575512
71	1	0	-2.441857	2.221277	-1.526957
72	6	0	-5.000940	2.474908	1.372196
73	1	0	-4.362957	0.498380	1.923685
74	6	0	-4.854130	3.536031	0.476161
75	1	0	-3.812487	4.256716	-1.273278
76	1	0	-5.712283	2.545350	2.190652

77	1	0	-5.447961	4.437970	0.597061
78	1	0	0.286615	2.015539	-2.567123
79	6(11)	0	-0.006700	-2.366927	-0.673426
80	1	0	0.314839	-2.597194	-1.697209
81	1	0	0.700863	-2.851231	0.011736
82	1	0	-0.988717	-2.823114	-0.510630
83	1	0	0.017001	5.821432	-0.591079
84	7	0	-0.167170	2.043650	2.003472
85	1	0	0.284382	1.134303	2.019481
86	1	0	0.166842	2.608091	2.779151

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.211905	-1.139886	-0.081086
2	15	0	-1.051471	1.146948	-0.012091
3	15	0	2.194510	-0.754648	-0.052700
4	6	0	-4.910513	-2.501474	0.110709
5	6	0	-4.124439	-2.499734	1.270041
6	6	0	-2.772551	-2.159082	1.200042
7	6	0	-2.159351	-1.794025	-0.012724
8	6	0	-2.962533	-1.834246	-1.160484
9	6	0	-4.319127	-2.185699	-1.116773
10	1	0	-4.593051	-2.755554	2.217431
11	1	0	-4.899614	-2.181349	-2.033184
12	6	0	4.322933	-3.731299	-2.917197
13	6	0	3.104238	-3.139334	-3.262462
14	6	0	2.474486	-2.268810	-2.372275
15	6	0	3.063700	-1.966794	-1.133985
16	6	0	4.286462	-2.562432	-0.795544
17	6	0	4.909622	-3.444520	-1.682181
18	1	0	4.810044	-4.416250	-3.605658
19	1	0	2.639927	-3.362629	-4.219034
20	1	0	1.514032	-1.830483	-2.630951
21	1	0	4.754074	-2.343793	0.159277
22	1	0	5.853951	-3.906024	-1.406740
23	6	0	-0.658146	2.912394	4.278351
24	6	0	-1.561900	3.490383	3.381213
25	6	0	-1.707002	2.968087	2.095044
26	6	0	-0.941487	1.863418	1.683346
27	6	0	-0.055166	1.277283	2.601112
28	6	0	0.091481	1.800807	3.887618
29	1	0	-0.548667	3.320637	5.279161
30	1	0	-2.158485	4.346365	3.684101
31	1	0	-2.430897	3.410101	1.417494
32	1	0	0.515389	0.400343	2.314980
33	1	0	0.784937	1.332381	4.580632
34	6	0	4.143974	3.312621	-1.204013
35	6	0	4.433300	2.177102	-1.960895
36	6	0	3.868958	0.943525	-1.624640
37	6	0	3.006482	0.833571	-0.524969
38	6	0	2.721928	1.982913	0.231160
39	6	0	3.286425	3.211074	-0.104560
40	1	0	4.578403	4.272318	-1.469789
41	1	0	5.099147	2.246100	-2.816919
42	1	0	4.105403	0.070343	-2.222878
43	1	0	4.719374	0.048723	1.345697
44	1	0	3.047214	4.091109	0.485412
45	6	0	0.959647	4.108185	-2.972702
46	6	0	0.967905	2.731775	-3.205926
47	6	0	0.376900	1.865111	-2.285306
48	6	0	-0.233650	2.364699	-1.125753
49	6	0	-0.239874	3.749313	-0.900797
50	6	0	0.355661	4.614667	-1.818513
51	1	0	1.428817	4.783610	-3.682742

52	1	0	1.447222	2.329956	-4.093920
53	1	0	0.400873	0.792296	-2.457826
54	1	0	-0.695058	4.157516	-0.004670
55	1	0	0.352432	5.684770	-1.629760
56	6	0	2.872605	-1.038757	1.641825
57	6	0	2.107922	-1.767013	2.568841
58	6	0	4.118679	-0.527333	2.042748
59	6	0	2.578149	-1.976568	3.867034
60	1	0	1.138308	-2.156528	2.273856
61	6	0	4.588344	-0.741297	3.339826
62	1	0	2.053999	1.922136	1.084900
63	6	0	3.818476	-1.464097	4.255408
64	1	0	1.971797	-2.534796	4.574945
65	1	0	5.552892	-0.338242	3.635808
66	1	0	4.181732	-1.622761	5.266954
67	6	0	-2.831272	1.381376	-0.437341
68	6	0	-3.819830	0.998031	0.483625
69	6	0	-3.225152	1.840074	-1.702630
70	6	0	-5.169761	1.071486	0.146159
71	1	0	-3.534949	0.621004	1.459638
72	6	0	-4.579899	1.914608	-2.038857
73	1	0	-2.478736	2.142351	-2.430499
74	6	0	-5.555495	1.530350	-1.117037
75	1	0	-5.920456	0.759705	0.866939
76	1	0	-4.869157	2.275342	-3.022378
77	1	0	-6.608416	1.585392	-1.380111
78	1	0	-2.192996	-2.165429	2.121588
79	1	0	-2.546636	-1.550557	-2.125720
80	6(11)	0	0.183436	-3.220481	-0.030216
81	1	0	-0.423292	-3.691398	0.750323
82	1	0	-0.104210	-3.641370	-1.001158
83	1	0	1.238899	-3.451206	0.147425
84	8	0	-6.237417	-2.820124	0.282826
85	6	0	-7.094602	-2.703326	-0.844847
86	1	0	-8.099788	-2.937378	-0.488059
87	1	0	-7.081384	-1.684147	-1.254517
88	1	0	-6.821476	-3.410535	-1.639686

TSa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.110436	-1.018282	-0.098350
2	15	0	-0.940694	1.228273	-0.039787
3	15	0	2.334296	-0.785721	-0.000708
4	6	0	-4.765349	-2.198110	-0.097465
5	6	0	-4.020170	-2.261217	1.096770
6	6	0	-2.633308	-2.193099	1.084023
7	6	0	-1.910299	-2.037690	-0.126971
8	6	0	-2.670201	-2.013238	-1.330363
9	6	0	-4.049952	-2.076434	-1.309540
10	1	0	-4.527503	-2.350453	2.053438
11	1	0	-4.616541	-2.016648	-2.234235
12	6	0	4.400364	-4.261606	-2.298161
13	6	0	3.282444	-3.608400	-2.824794
14	6	0	2.674942	-2.576638	-2.106912
15	6	0	3.188111	-2.172294	-0.861860
16	6	0	4.311392	-2.832660	-0.342836
17	6	0	4.910147	-3.874055	-1.056104
18	1	0	4.868998	-5.070920	-2.851070
19	1	0	2.878203	-3.906461	-3.788202
20	1	0	1.797042	-2.079532	-2.513789
21	1	0	4.721953	-2.534744	0.616934
22	1	0	5.778018	-4.379948	-0.641823
23	6	0	-0.356037	3.323338	4.079615
24	6	0	-1.314009	3.821630	3.190663

25	6	0	-1.517919	3.201965	1.956621
26	6	0	-0.759905	2.076437	1.589391
27	6	0	0.182420	1.572721	2.499867
28	6	0	0.389093	2.194040	3.733697
29	1	0	-0.200717	3.807509	5.039739
30	1	0	-1.906234	4.691952	3.459668
31	1	0	-2.280876	3.584390	1.285478
32	1	0	0.750223	0.683652	2.249320
33	1	0	1.125142	1.787016	4.421682
34	6	0	4.342243	3.062809	-1.677213
35	6	0	4.618112	1.833583	-2.276689
36	6	0	4.050732	0.659703	-1.772175
37	6	0	3.193474	0.705000	-0.664009
38	6	0	2.918862	1.949142	-0.069696
39	6	0	3.492681	3.116188	-0.567989
40	1	0	4.780937	3.974817	-2.072496
41	1	0	5.278908	1.782043	-3.137974
42	1	0	4.280417	-0.288674	-2.246673
43	1	0	4.765044	0.266418	1.439644
44	1	0	3.262767	4.069229	-0.100711
45	6	0	1.047832	3.969082	-3.229593
46	6	0	1.019216	2.581465	-3.381532
47	6	0	0.424284	1.784691	-2.402427
48	6	0	-0.158963	2.365077	-1.265462
49	6	0	-0.128603	3.760498	-1.123537
50	6	0	0.473856	4.556364	-2.098676
51	1	0	1.522873	4.590206	-3.984007
52	1	0	1.475201	2.116966	-4.251184
53	1	0	0.427999	0.702887	-2.507684
54	1	0	-0.559480	4.231675	-0.246386
55	1	0	0.498780	5.635473	-1.972701
56	6	0	-6.236579	-2.205112	-0.130632
57	8	0	-6.865735	-2.151498	-1.192868
58	6	0	-6.998589	-2.264804	1.187244
59	1	0	-8.070408	-2.258595	0.978565
60	1	0	-6.746115	-3.169572	1.752481
61	1	0	-6.749508	-1.406004	1.821835
62	6	0	2.956600	-0.880059	1.733282
63	6	0	2.179964	-1.576724	2.674925
64	6	0	4.154747	-0.279868	2.152077
65	6	0	2.590545	-1.669617	4.005930
66	1	0	1.242003	-2.031390	2.365772
67	6	0	4.562617	-0.370023	3.484693
68	1	0	2.251808	2.008609	0.785102
69	6	0	3.781611	-1.062678	4.414034
70	1	0	1.976608	-2.206466	4.723710
71	1	0	5.489676	0.102946	3.796782
72	1	0	4.098030	-1.126282	5.451398
73	6	0	-2.736351	1.408974	-0.399628
74	6	0	-3.677241	1.119776	0.602332
75	6	0	-3.194263	1.707836	-1.692238
76	6	0	-5.042293	1.144957	0.320739
77	1	0	-3.344289	0.871726	1.604957
78	6	0	-4.562108	1.726769	-1.972721
79	1	0	-2.482760	1.929533	-2.482301
80	6	0	-5.490560	1.446216	-0.967438
81	1	0	-5.756634	0.918585	1.107562
82	1	0	-4.900860	1.963403	-2.977973
83	1	0	-6.554570	1.455003	-1.186833
84	1	0	-2.089111	-2.250363	2.023648
85	1	0	-2.153634	-1.924341	-2.283421
86	6(11)	0	-0.353718	-3.308256	-0.152802
87	1	0	-1.087067	-4.026992	-0.511574
88	1	0	0.510801	-3.359288	-0.822239
89	1	0	-0.072451	-3.566744	0.871378

TSb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.158055	-1.072073	-0.553040
2	15	0	-1.590086	0.806849	-0.093204
3	15	0	2.131803	-0.247505	-0.139083
4	6	0	-4.090055	-3.908862	-0.616067
5	6	0	-3.304237	-3.804000	0.538809
6	6	0	-2.038650	-3.208359	0.501482
7	6	0	-1.528356	-2.689392	-0.725204
8	6	0	-2.339820	-2.810795	-1.867641
9	6	0	-3.606743	-3.403167	-1.822401
10	1	0	-3.677814	-4.189707	1.486505
11	1	0	-4.207654	-3.463608	-2.726735
12	6	0	5.330416	-2.596564	-2.559901
13	6	0	4.076191	-2.315800	-3.107656
14	6	0	3.125449	-1.623204	-2.354477
15	6	0	3.423695	-1.192018	-1.052123
16	6	0	4.686438	-1.479425	-0.509929
17	6	0	5.632945	-2.179799	-1.259475
18	1	0	6.068635	-3.141885	-3.141464
19	1	0	3.834335	-2.642401	-4.115298
20	1	0	2.142334	-1.420702	-2.772653
21	1	0	4.929067	-1.153574	0.497439
22	1	0	6.607084	-2.398282	-0.830411
23	6	0	-1.923356	1.685401	4.471585
24	6	0	-2.953831	2.096704	3.620390
25	6	0	-2.879752	1.839141	2.249585
26	6	0	-1.770245	1.166560	1.710535
27	6	0	-0.749214	0.744768	2.577684
28	6	0	-0.820080	1.007288	3.947297
29	1	0	-1.985325	1.885960	5.537634
30	1	0	-3.817914	2.617585	4.023999
31	1	0	-3.689603	2.155489	1.598566
32	1	0	0.100230	0.198359	2.183035
33	1	0	-0.016862	0.672835	4.598371
34	6	0	3.327455	4.215400	-0.690452
35	6	0	3.987271	3.234196	-1.431805
36	6	0	3.666752	1.884306	-1.258779
37	6	0	2.672132	1.501170	-0.346854
38	6	0	2.004907	2.499633	0.385410
39	6	0	2.336321	3.842584	0.222633
40	1	0	3.577788	5.263984	-0.825799
41	1	0	4.759089	3.514465	-2.143806
42	1	0	4.196402	1.132840	-1.835431
43	1	0	3.540152	1.234218	2.116974
44	1	0	1.805332	4.598278	0.793178
45	6	0	-0.177666	4.759689	-2.093404
46	6	0	0.085148	3.516716	-2.674076
47	6	0	-0.334392	2.347575	-2.038754
48	6	0	-1.034357	2.405889	-0.823430
49	6	0	-1.297506	3.658675	-0.250051
50	6	0	-0.867871	4.827931	-0.880306
51	1	0	0.161179	5.670650	-2.579024
52	1	0	0.632005	3.455979	-3.610929
53	1	0	-0.105421	1.378890	-2.476827
54	1	0	-1.831024	3.725557	0.692965
55	1	0	-1.070300	5.792326	-0.422014
56	1	0	-5.069943	-4.376007	-0.561946
57	6	0	2.534386	-0.616635	1.632061
58	6	0	2.100073	-1.851153	2.151351
59	6	0	3.190509	0.277837	2.490288
60	6	0	2.304479	-2.173736	3.492556
61	1	0	1.587716	-2.561150	1.509244
62	6	0	3.388311	-0.043491	3.836809
63	1	0	1.222396	2.227745	1.087392
64	6	0	2.943302	-1.265911	4.343431

65	1	0	1.955852	-3.129507	3.874137
66	1	0	3.891943	0.665866	4.487900
67	1	0	3.092877	-1.510887	5.391192
68	6	0	-3.347473	0.720017	-0.647136
69	6	0	-4.115604	-0.372253	-0.210816
70	6	0	-3.934566	1.659013	-1.510129
71	6	0	-5.443504	-0.511552	-0.611943
72	1	0	-3.672138	-1.127996	0.428295
73	6	0	-5.264325	1.513638	-1.916065
74	1	0	-3.360260	2.508965	-1.863654
75	6	0	-6.023731	0.431166	-1.465773
76	1	0	-6.015022	-1.370047	-0.270853
77	1	0	-5.705520	2.251090	-2.581647
78	1	0	-7.057100	0.319415	-1.783104
79	7	0	-1.222832	-3.183120	1.652308
80	1	0	-1.958336	-2.443681	-2.818187
81	6(11)	0	0.296664	-3.270235	-1.128051
82	1	0	0.296150	-3.303572	-2.219144
83	1	0	1.311984	-3.059064	-0.779868
84	1	0	0.030846	-4.246952	-0.725520
85	1	0	-0.660008	-2.338468	1.703889
86	1	0	-1.743629	-3.299636	2.516372

TSc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.151689	-1.063555	-0.220100
2	15	0	-1.134320	1.137862	-0.042753
3	15	0	2.266241	-0.687030	-0.055028
4	6	0	-4.685648	-2.611871	0.117163
5	6	0	-3.825458	-2.720961	1.215684
6	6	0	-2.449081	-2.563053	1.055227
7	6	0	-1.879592	-2.267228	-0.203601
8	6	0	-2.765259	-2.204185	-1.300090
9	6	0	-4.143301	-2.367871	-1.151421
10	1	0	-4.253254	-2.917653	2.195651
11	1	0	-4.781925	-2.277519	-2.023251
12	6	0	4.615635	-3.828570	-2.556059
13	6	0	3.483949	-3.188993	-3.069892
14	6	0	2.794238	-2.258798	-2.290156
15	6	0	3.237692	-1.940035	-0.994307
16	6	0	4.375162	-2.586681	-0.488692
17	6	0	5.056356	-3.528104	-1.264287
18	1	0	5.148421	-4.559885	-3.157495
19	1	0	3.133065	-3.419781	-4.071984
20	1	0	1.905977	-1.772424	-2.687570
21	1	0	4.732733	-2.354288	0.509628
22	1	0	5.934842	-4.023673	-0.859800
23	6	0	-0.844152	2.890543	4.269117
24	6	0	-1.812777	3.391617	3.393467
25	6	0	-1.927620	2.875050	2.101532
26	6	0	-1.069383	1.852586	1.661260
27	6	0	-0.116331	1.343093	2.557915
28	6	0	0.001641	1.861236	3.849783
29	1	0	-0.758139	3.293601	5.274440
30	1	0	-2.482391	4.183688	3.717618
31	1	0	-2.697719	3.258681	1.439065
32	1	0	0.528944	0.527485	2.249831
33	1	0	0.747585	1.451196	4.525424
34	6	0	4.093931	3.402987	-1.326738
35	6	0	4.464738	2.248069	-2.016232
36	6	0	3.953991	1.003669	-1.634563
37	6	0	3.057836	0.901749	-0.561313
38	6	0	2.687703	2.072678	0.123488
39	6	0	3.205377	3.310036	-0.251169

40	1	0	4.489148	4.369759	-1.626250
41	1	0	5.156861	2.309554	-2.852004
42	1	0	4.258695	0.114874	-2.177538
43	1	0	4.613156	0.363196	1.526327
44	1	0	2.901787	4.203924	0.285980
45	6	0	0.791095	4.280223	-2.883221
46	6	0	0.879355	2.911614	-3.144964
47	6	0	0.300128	1.995321	-2.266136
48	6	0	-0.383177	2.433756	-1.121398
49	6	0	-0.470434	3.811306	-0.869964
50	6	0	0.116302	4.727802	-1.743853
51	1	0	1.253037	4.995411	-3.558412
52	1	0	1.415183	2.555576	-4.020263
53	1	0	0.395669	0.928590	-2.452464
54	1	0	-0.985297	4.174255	0.013669
55	1	0	0.048910	5.791923	-1.533324
56	8	0	-6.029455	-2.739996	0.384329
57	6	0	2.853099	-0.881363	1.686016
58	6	0	2.087606	-1.676800	2.555642
59	6	0	4.011386	-0.260097	2.180527
60	6	0	2.469187	-1.846292	3.887930
61	1	0	1.178866	-2.148189	2.189160
62	6	0	4.390779	-0.426976	3.514127
63	1	0	1.990508	2.018774	0.954102
64	6	0	3.620440	-1.218165	4.370985
65	1	0	1.862910	-2.459693	4.548751
66	1	0	5.287103	0.063537	3.883897
67	1	0	3.913896	-1.341515	5.409762
68	6	0	-2.927961	1.273465	-0.445116
69	6	0	-3.860377	0.707502	0.439922
70	6	0	-3.388077	1.818799	-1.653697
71	6	0	-5.219916	0.704086	0.133967
72	1	0	-3.521389	0.248671	1.363055
73	6	0	-4.751230	1.808733	-1.962580
74	1	0	-2.684166	2.257597	-2.354482
75	6	0	-5.671621	1.256007	-1.068598
76	1	0	-5.923749	0.246076	0.823124
77	1	0	-5.092435	2.239732	-2.900278
78	1	0	-6.731644	1.250776	-1.308142
79	1	0	-1.804657	-2.666944	1.925274
80	1	0	-2.370602	-2.017299	-2.296390
81	6(11)	0	-0.228423	-3.350194	-0.483188
82	1	0	0.638156	-3.234523	-1.144139
83	1	0	0.088975	-3.717879	0.495960
84	1	0	-0.883602	-4.086911	-0.942943
85	6	0	-6.936704	-2.539035	-0.691300
86	1	0	-7.937729	-2.636809	-0.266039
87	1	0	-6.822273	-1.538364	-1.128527
88	1	0	-6.805584	-3.292415	-1.480056

6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.026005	1.168839	-0.003899
2	6	0	-1.367286	1.218028	-0.009056
3	6	0	-2.132999	0.044324	-0.009084
4	6	0	-1.458866	-1.189020	-0.008784
5	6	0	-0.071181	-1.244089	-0.003445
6	6(11)	0	-3.640819	0.094742	0.012746
7	1	0	-4.016015	1.076650	-0.291422
8	1	0	-4.021002	-0.107482	1.022659
9	1	0	-4.073865	-0.661808	-0.650822
10	1	0	-2.034946	-2.111311	-0.014271
11	6	0	0.694699	-0.065119	-0.000616
12	1	0	0.445720	-2.198325	-0.004411

13	1	0	0.584305	2.099462	-0.005492
14	1	0	-1.868223	2.182759	-0.014337
15	6	0	2.183782	-0.176420	0.002677
16	6	0	3.012325	1.094908	0.004188
17	1	0	2.793346	1.704441	-0.880161
18	1	0	4.071121	0.830093	0.008337
19	1	0	2.786909	1.706902	0.885203
20	8	0	2.732336	-1.274818	0.004544

6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895807	-0.820501	0.008760
2	6	0	-0.633247	-1.419840	0.009873
3	6	0	0.544393	-0.666551	0.000588
4	6	0	0.445465	0.745672	-0.004375
5	6	0	-0.824398	1.348180	-0.004971
6	6(11)	0	1.899491	-1.330980	-0.012312
7	1	0	1.805720	-2.418905	-0.077844
8	1	0	2.476357	-1.105967	0.896718
9	1	0	2.505028	-0.990425	-0.862751
10	7	0	1.602197	1.534559	-0.078673
11	6	0	-1.983239	0.572881	-0.001633
12	1	0	-0.895190	2.433998	-0.008954
13	1	0	-2.793191	-1.432634	0.014362
14	1	0	-0.553884	-2.505085	0.015898
15	1	0	-2.953714	1.062662	-0.001386
16	1	0	1.462544	2.495643	0.213368
17	1	0	2.414999	1.145631	0.385719

6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.098455	1.380728	-0.000048
2	6	0	-1.277100	1.185534	-0.000127
3	6	0	-1.835205	-0.104988	-0.000181
4	6	0	-0.954271	-1.188761	-0.000254
5	6	0	0.435595	-1.015094	-0.000178
6	6(11)	0	-3.334226	-0.297265	0.000323
7	1	0	-3.798199	0.169048	-0.877982
8	1	0	-3.796362	0.159422	0.884683
9	1	0	-3.601969	-1.358782	-0.005059
10	1	0	-1.352407	-2.201023	-0.000392
11	6	0	0.968201	0.278142	-0.000053
12	1	0	1.079164	-1.887126	-0.000297
13	1	0	0.524703	2.379708	-0.000053
14	1	0	-1.934673	2.052284	-0.000176
15	8	0	2.303270	0.575638	-0.000028
16	6	0	3.230867	-0.505725	0.000264
17	1	0	4.222582	-0.050250	0.000504
18	1	0	3.118310	-1.131864	0.894702
19	1	0	3.118793	-1.131947	-0.894179

6b′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.268640	-0.006906	-0.810861
2	15	0	-1.764993	1.011066	-0.327410
3	15	0	2.502099	-0.176996	-0.267338

4	6	0	-4.163494	-3.685277	0.402690
5	6	0	-3.125766	-3.077107	1.107961
6	6	0	-1.826689	-3.025770	0.575755
7	6	0	-1.570036	-3.605620	-0.691069
8	6	0	-2.629572	-4.204509	-1.380284
9	6	0	-3.922938	-4.251469	-0.850912
10	1	0	-3.318538	-2.612327	2.071720
11	1	0	-4.726556	-4.722704	-1.409780
12	6	0	5.023041	-3.876840	-1.513786
13	6	0	3.957962	-3.428821	-2.299691
14	6	0	3.213033	-2.318217	-1.897527
15	6	0	3.530587	-1.637491	-0.711845
16	6	0	4.601739	-2.096273	0.072443
17	6	0	5.342698	-3.210050	-0.326998
18	1	0	5.598349	-4.745808	-1.820943
19	1	0	3.700605	-3.948271	-3.218580
20	1	0	2.372916	-1.979470	-2.498510
21	1	0	4.850714	-1.588250	0.999505
22	1	0	6.167961	-3.557760	0.288311
23	6	0	-2.739951	0.138728	4.145329
24	6	0	-3.773305	0.111089	3.207080
25	6	0	-3.513366	0.394447	1.861824
26	6	0	-2.213326	0.704539	1.441081
27	6	0	-1.178442	0.735128	2.394560
28	6	0	-1.439897	0.458166	3.736001
29	1	0	-2.942955	-0.090095	5.187854
30	1	0	-4.784994	-0.136546	3.516956
31	1	0	-4.324397	0.359760	1.141896
32	1	0	-0.160219	0.950571	2.081158
33	1	0	-0.623692	0.474915	4.452343
34	6	0	4.978822	3.596079	-1.415805
35	6	0	5.638983	2.374491	-1.256331
36	6	0	4.922121	1.224403	-0.917148
37	6	0	3.530864	1.282071	-0.743064
38	6	0	2.874041	2.513012	-0.916084
39	6	0	3.593847	3.663829	-1.241152
40	1	0	5.540273	4.488311	-1.678947
41	1	0	6.715213	2.315181	-1.394451
42	1	0	5.449981	0.283811	-0.794679
43	1	0	3.037196	1.940663	1.785403
44	1	0	3.069497	4.607539	-1.366146
45	6	0	-1.259328	5.633639	-0.582336
46	6	0	-0.652295	4.789236	-1.517000
47	6	0	-0.822146	3.407099	-1.422614
48	6	0	-1.605884	2.849812	-0.398082
49	6	0	-2.214883	3.705787	0.532459
50	6	0	-2.040501	5.089394	0.440380
51	1	0	-1.120136	6.709139	-0.648033
52	1	0	-0.039005	5.204387	-2.312151
53	1	0	-0.330746	2.750770	-2.137071
54	1	0	-2.821496	3.293474	1.333335
55	1	0	-2.514001	5.740876	1.169881
56	1	0	-5.162776	-3.702806	0.830415
57	6	0	2.554626	-0.157296	1.581609
58	6	0	2.203769	-1.325074	2.281977
59	6	0	2.767922	1.025931	2.304306
60	6	0	2.067622	-1.307407	3.669369
61	1	0	2.022693	-2.250060	1.742726
62	6	0	2.626178	1.042311	3.694993
63	1	0	1.795426	2.566663	-0.794148
64	6	0	2.274581	-0.121734	4.382061
65	1	0	1.792573	-2.218788	4.193179
66	1	0	2.793057	1.967735	4.239611
67	1	0	2.163038	-0.106868	5.462650
68	6	0	-3.339652	0.670833	-1.223342
69	6	0	-3.551474	-0.642130	-1.674077
70	6	0	-4.333250	1.638195	-1.442244
71	6	0	-4.740777	-0.985811	-2.318626

72	1	0	-2.793063	-1.400990	-1.506771
73	6	0	-5.516968	1.294999	-2.099912
74	1	0	-4.186067	2.657528	-1.098187
75	6	0	-5.724350	-0.016972	-2.536155
76	1	0	-4.892785	-2.010739	-2.643766
77	1	0	-6.278355	2.052063	-2.267879
78	1	0	-6.647816	-0.281491	-3.044201
79	7	0	-0.773517	-2.451641	1.305245
80	1	0	-2.432084	-4.643587	-2.356093
81	6(11)	0	-0.183204	-3.549636	-1.278790
82	1	0	-0.117180	-4.125712	-2.207036
83	1	0	0.110440	-2.511017	-1.505119
84	1	0	0.569825	-3.932219	-0.577729
85	1	0	-0.159602	-1.870404	0.727718
86	1	0	-1.098383	-1.877653	2.077652

6c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.009902	-0.605784	-0.406021
2	15	0	2.126114	0.311974	-0.187675
3	15	0	-2.028594	0.436447	0.080871
4	6	0	0.547218	-3.683717	0.085878
5	6	0	0.622205	-2.973069	-1.133360
6	6	0	-0.538491	-2.798193	-1.900623
7	6	0	-1.775612	-3.349621	-1.503258
8	6	0	-1.809039	-4.074679	-0.314181
9	6	0	-0.670337	-4.230537	0.493918
10	1	0	1.596714	-2.677973	-1.505671
11	1	0	-0.749087	-4.794322	1.416311
12	6	0	-6.002604	-1.983451	0.314561
13	6	0	-4.848551	-2.404181	0.982925
14	6	0	-3.675512	-1.655059	0.892235
15	6	0	-3.641256	-0.464875	0.147228
16	6	0	-4.805224	-0.048043	-0.517456
17	6	0	-5.977155	-0.805680	-0.436484
18	1	0	-6.913757	-2.572310	0.375534
19	1	0	-4.857961	-3.323705	1.562198
20	1	0	-2.772639	-2.005074	1.385232
21	1	0	-4.797838	0.867433	-1.101127
22	1	0	-6.870542	-0.472237	-0.957983
23	6	0	2.597602	4.707787	-1.660477
24	6	0	3.739798	3.919785	-1.484606
25	6	0	3.621449	2.597504	-1.051269
26	6	0	2.356533	2.045220	-0.789231
27	6	0	1.217679	2.844768	-0.969865
28	6	0	1.335594	4.167699	-1.400483
29	1	0	2.692601	5.734909	-2.002368
30	1	0	4.723864	4.334569	-1.686338
31	1	0	4.514912	1.994257	-0.918267
32	1	0	0.235896	2.425312	-0.780434
33	1	0	0.438917	4.765477	-1.541435
34	6	0	-2.060470	2.882807	4.051052
35	6	0	-3.273574	2.578462	3.424456
36	6	0	-3.286835	1.840189	2.239242
37	6	0	-2.084325	1.396771	1.663146
38	6	0	-0.874024	1.707020	2.301368
39	6	0	-0.859831	2.445631	3.486518
40	1	0	-2.054059	3.453536	4.975814
41	1	0	-4.210747	2.914630	3.860210
42	1	0	-4.235283	1.607097	1.763618
43	1	0	-2.507799	3.432575	0.098683
44	1	0	0.090061	2.667019	3.966071
45	6	0	2.935001	0.468278	4.392326
46	6	0	2.640050	-0.736357	3.742947

47	6	0	2.436871	-0.756768	2.364124
48	6	0	2.546948	0.424498	1.606393
49	6	0	2.854434	1.624708	2.262517
50	6	0	3.040810	1.645455	3.649428
51	1	0	3.078766	0.487182	5.469095
52	1	0	2.556560	-1.657848	4.313212
53	1	0	2.188797	-1.690198	1.865297
54	1	0	2.940758	2.547990	1.698193
55	1	0	3.271838	2.584520	4.145443
56	8	0	1.727056	-3.791893	0.772224
57	6	0	-2.331652	1.723308	-1.211735
58	6	0	-2.301037	1.309413	-2.556781
59	6	0	-2.485774	3.088281	-0.930229
60	6	0	-2.431312	2.235746	-3.590309
61	1	0	-2.163562	0.256290	-2.791727
62	6	0	-2.598213	4.019371	-1.968719
63	1	0	0.058875	1.359095	1.872104
64	6	0	-2.572929	3.597473	-3.298851
65	1	0	-2.410751	1.898302	-4.623131
66	1	0	-2.708902	5.074557	-1.733108
67	1	0	-2.659782	4.321694	-4.104020
68	6	0	3.597525	-0.540638	-0.911736
69	6	0	3.489245	-0.976031	-2.244352
70	6	0	4.785688	-0.798341	-0.211912
71	6	0	4.545998	-1.641234	-2.866396
72	1	0	2.566749	-0.795658	-2.793267
73	6	0	5.840528	-1.475256	-0.831701
74	1	0	4.889976	-0.472615	0.818605
75	6	0	5.725177	-1.896244	-2.158531
76	1	0	4.446392	-1.968616	-3.897796
77	1	0	6.754320	-1.669706	-0.276311
78	1	0	6.545815	-2.423168	-2.637457
79	1	0	-0.463514	-2.290199	-2.859639
80	1	0	-2.747235	-4.511154	0.017553
81	6(11)	0	-3.018152	-3.108525	-2.323966
82	1	0	-3.816776	-3.808036	-2.057596
83	1	0	-3.402369	-2.095332	-2.150417
84	1	0	-2.818994	-3.206586	-3.397775
85	6	0	1.708202	-4.449271	2.036629
86	1	0	2.728466	-4.391659	2.419098
87	1	0	1.027868	-3.946140	2.735812
88	1	0	1.413796	-5.501466	1.936766