Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Co-SAC catalyzed utilization of methanol and ethanol in the transfer hydrogenation of azo bonds: experimental and theoretical studies

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Table of Contents

1. General Consideration

Reagent information.

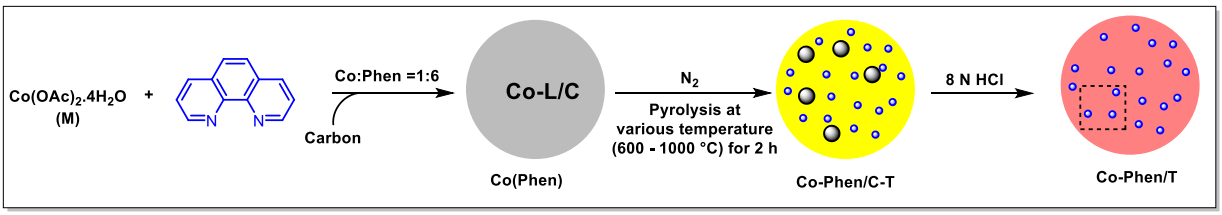
Unless otherwise stated, all the experiments were carried out under argon atmosphere using either argon filled Glove box or standard Schlenk line technique. Glass apparatus were oven dried immediately prior to use. Solvents were dried according to literature methods. All the solvents were eventually distilled over sodium under argon atmosphere and deoxygenated prior to use. All the reagents were purchased from Sigma-Aldrich, Alfa-Aesar, SD-fine chemicals, Avra, Spectrochem. Silica gel (100-200 mesh) was used for the column chromatography with a gradient elution of hexane/ethyl acetate, based on alumina TLC plate.

Analytical information.

^{1}H and ^{13}C NMR spectra were recorded on JEOL 400 MHz and 500 MHz spectrometer using $CDCl_3$ and DMSO-d_6. All ^{1}H NMR experiments were reported in parts per million (ppm) unit and were measured relative to the signals for residual chloroform (7.24 ppm) or DMSO-d_6 (2.50 ppm) in the deuterated solvent and coupling constant (J) was reported in hertz (Hz). All ^{1}H decoupled ^{13}C NMR spectra were reported in ppm relative to deuterated chloroform (77.1 ppm) or DMSO-d_6 (39.5 ppm). All the GC analysis were performed using Perkin Elmer Clarus 600 Gas Chromatograph and High-resolution mass spectra were recorded on Agilent 6230 LC/TOF mass spectrometer.

2. Procedure for synthesis of Co-Phen/T catalysts

The catalysts were synthesized following literature reports[1-3] with slight modifications. At first, $Co(OAc)_2.4H_2O$ (2 mmol) was dissolved in ethanol (30 mL) then phenanthroline (12 mmol) was added and reaction mixture was heated at 60 °C for 2h. Next, the reaction mixture was cooled to room temperature and carbon powder (carbon black, acetylene, Thermo-Fisher Chemicals; CAS: 1333-86-4) (3 g) was added. Afterwards, the resultant reaction mixture was stirred for 24 h at room temperature. Next, ethanol was removed slowly under reduced pressure and the reaction mixture was dried and the sample was grinded to fine powder. Then, it was subjected for pyrolysis at various temperature (600 °C - 1000 °C) for 2 h with the ramp of 1 °C/min under N_2 atmosphere. Afterwards, 100 mL 8 N HCl solution was added and stirred for 24 h at room temperature. Then the slurry was filtered and washed with deionized water. Afterwards, the material was centrifuged with ethanol followed by drying in air at 80 ℃ for overnight to prepare the cobalt catalysts. (Scheme S1).



Scheme S1. Preparation of the catalysts.

3. Procedure for synthesis of azo compounds

Symmetric azobenzene:

Method-I[4]

In a 100 mL RB, 1.0 g of amine was dissolved in 50 mL of toluene. To this solution, 10 equiv. of activated MnO_2 was added. Then, the mixture was refluxed for 24-48 h. Then, the reaction mixture was filtered through Celite and washed with toluene. Finally, the desired product was purified by flash column chromatography using silica (eluted with ethyl acetate/hexane).

Method-II[5]

In a 100 mL RB, 1.0 g of amine was dissolved in 10 mL of methanol and kept in ice bath. To this solution, NaOCl (20 equiv.) was added dropwise. Then, the mixture was stirred for overnight. Next, the reaction mixture was extracted with EtOAc and dried over anh. Na_2SO_4. Finally, the desired product was purified by flash column chromatography using silica (eluted with ethyl acetate/hexane).

Unsymmetric azobenzene:[4]

To a solution of nitrosobenzene (5 mmol) in glacial acetic acid (12 mL) and EtOH (3 mL), the amine (1.0 equiv.) was added. The reaction mixture was stirred at room temperature for 12 h. Then, the mixture was poured into ice water and filtered. Finally, the desired product was purified by flash column chromatography using silica (eluted with ethyl acetate/hexane).

4. General synthetic procedures

Transfer hydrogenation of azo compounds using ethanol

To an oven dried 9 mL screw cap tube, a magnetic stir-bar, azobenzene (0.5 mmol), Cs_2CO_3 (0.125 mmol), Co-Phen/800 (2.2 mol % Co) and ethanol (5 mL) were added under argon atmosphere. Then, the tube was sealed and placed in a preheated oil bath at 130 °C for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, 25 µL reaction mixture was syringed out and filtered through a small plug of silica and subjected for GC analysis using mesitylene as internal standard to determine conversion of the azo

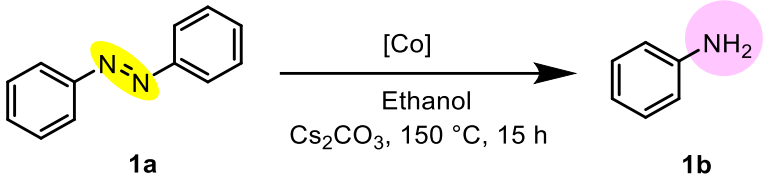
compounds. The remaining solvent was evaporated under reduced pressure and the final product was purified by basic alumina column chromatography using ethyl acetate/hexane as eluent.

Transfer hydrogenation of azo compounds using methanol

To an oven dried 9 mL screw cap tube, a magnetic stir-bar, azobenzene (0.5 mmol), Cs_2CO_3 (0.375 mmol), Co-Phen/800 (8 mol % Co) and methanol (5 mL) were added under argon atmosphere. Then, the tube was sealed and placed in a preheated oil bath at 130 °C for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, a 25 µL reaction mixture was syringed out and filtered through a small plug of silica and subjected for GC analysis using mesitylene as internal standard to determine conversion of the azo compounds. The remaining solvent was evaporated under reduced pressure and the final product was purified by basic alumina column chromatography using ethyl acetate/hexane as eluent.

5. Optimization details for the transfer hydrogenation azobenzene

Table S1. Catalyst screening [a]

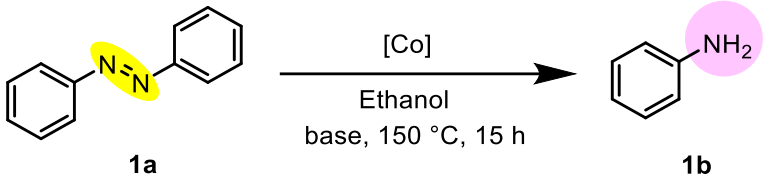


1a **1b**

Entry	Catalyst (mol%)	Conversion of 1a (%)	Yield of 1b (%)
1	**Co-Phen/800 (1.3)**	**>99**	**>99**
2	Co-Phen/600 (1.3)	15	15
3	Co-Phen/700 (1.3)	44	44
4	Co-Phen/900 (1.3)	61	61
5	Co-Phen/1000 (1.3)	40	40

[a]Reaction conditions: Azobenzene (0.15 mmol), Co-cat. (1.3 mol%) and Cs_2CO_3 (0.075 mmol) at 150 °C for 15 h; conversions and yields were determined by GC using mesitylene as an internal standard.

Table S2. Base screening [a]

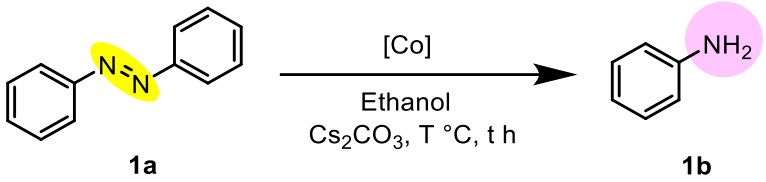


1a 1b

Entry	Base	Conversion of 1a (%)	Yield of 1b (%)
1	**Cs_2CO_3 (0.75)**	**>99 (22)[a]**	**>99 (22)[a]**
2	Na_2CO_3 (0.75)	40	40
3	K_2CO_3 (0.75)	75	75
4	NaOH (0.75)	>99 (12) [b]	>99 (12) [b]
5	KOH (0.75)	70	70
6	$CsOH.H_2O$ (0.75)	>99 (9) [b]	>99 (9) [b]
7	^{t}BuOK (0.75)	88	88
8	NaOMe	70	70

[a] Reaction conditions: Azobenzene (0.15 mmol), Co-cat. (1.3 mol%) and bases (0.075 mmol) at 150 °C for 15 h; [b] 3 h; conversions and yields were determined by GC using mesitylene as an internal standard.

Table S3. Optimization of the catalyst, base and temperature (using ethanol) [a]



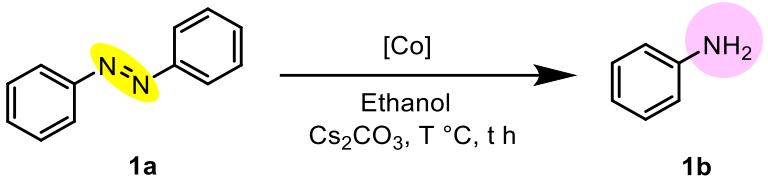
1a 1b

Entry	Cat (mol%)	Base (equiv.)	Time (h)	Temp. (℃)	Conv. of 1a (%)	Yield of 1b (%)
1	1.3	0.75	15	150	>99	>99
2	1.3	0.75	15	140	87	87
3	1.3	0.75	15	130	66	66
4	1.3	0.75	15	120	45	45
5	1.3	0.75	15	110	24	24
6	1.3	0.75	24	130	73	73
7	1.3	0.75	24	130	>99	>99
8	2.2	0.5	24	130	>99	98
9	**2.2**	**0.25**	**24**	**130**	**90**	**90**

10	2.2	0.1	24	130	24	24
11	-	0.25	24	130	N.D.	N.D.
12	2.2	-	24	130	N.D.	N.D.

[a] Reaction conditions: Azobenzene (0.15 mmol), Co-cat. (2.2 mol%) and bases (x mmol) at 150 °C for 24 h; conversions and yields were determined by GC using mesitylene as an internal standard.

Table S4. Optimization of the catalyst, base and temperature (using methanol) [a]



1a **1b**

Entry	Cat (mol%; Co)	Cs_2CO_3 (equiv.)	Conv. of 1a (%)	Yield of 1b (%)
1	2.2	0.25	26	26
2	3	0.25	32	32
3	6	0.25	44	44
4	7.5	0.25	50	50
5	8	0.25	62	62
6	8	0.5	75	75
7	**8**	**0.75**	**88**	**88**
8	-	0.75	N.D.	N.D.
9	8	-	N.D.	N.D.
10 [b]	2.2	0.75	87	87

[a] Reaction conditions: Azobenzene (0.15 mmol), Co-cat. (x mol%) and bases (x mmol) at 130 °C for 24 h; [b]150 ℃ for 24 h; conversions and yields were determined by GC using mesitylene as an internal standard.

6. Procedure for catalyst recyclization

The recyclization of the catalyst was carried out for the transfer hydrogenation of azobenzene using the procedure as follows: azobenzene (2.5 mmol), Co-Phen/800 (2.2/ 8 mol%), Cs_2CO_3 (1.25/ 3.75 mmol), ethanol/ methanol (35 mL) were taken in a 100 mL pressure tube. Afterwards, the tube was placed in a preheated oil bath at 130 °C (oil bath temperature) for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature and yields were determined by GC using mesitylene as the internal standard. In each run, after reaction, the catalyst was separated by centrifugation, washed thoroughly with methanol, and

dried at 90 ℃. Then, the dried catalyst was further used, without any purification or reactivation (Fig. **S1**).

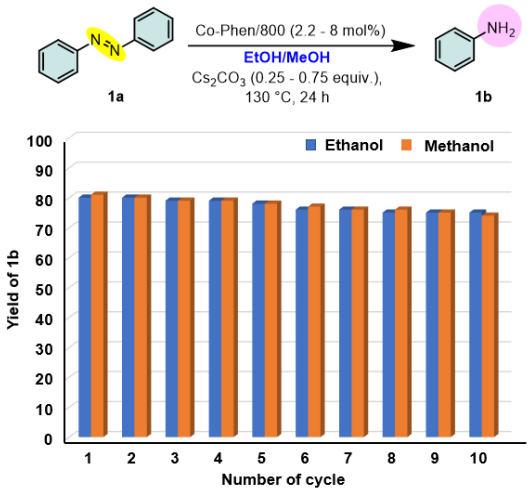


Fig. S1 Recyclability test of Co-Phen/800 catalyst.

7. The time-dependent experiment

Several experiments for the transfer hydrogenation of azobenzene using ethanol were conducted following the outlined procedure with varying time (0.5 h, 1 h, 3 h, 6 h, 9 h, 12 h and 15 h); An oven dried pressure tube was charged with azobenzene (0.15 mmol), Co-Phen/800 (2.2 mol % Co), Cs_2CO_3 (0.0375 mmol) followed by the addition of ethanol (1.5 mL). All the tubes were placed in a preheated oil-baths at 130 °C with stirring and the progress of the reaction was analysed by GC using mesitylene as the internal standard. All the reactions were repeated twice, and the average data was plotted as concentration (mmol) vs time (h) (Fig. **S2**).

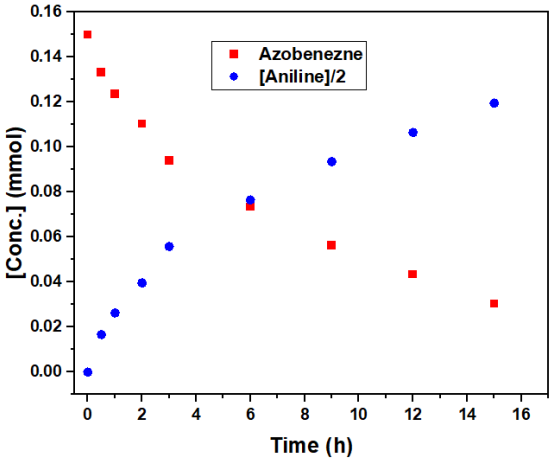
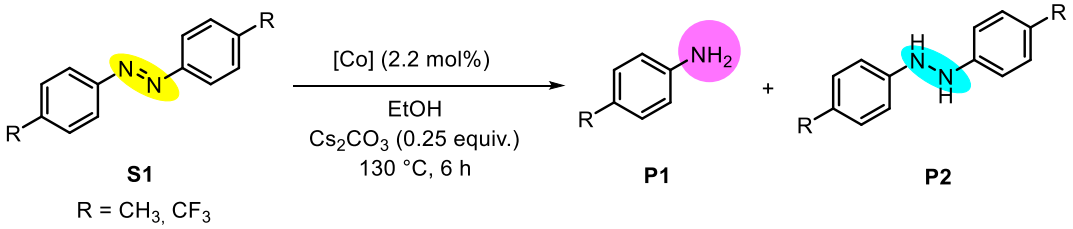


Fig. S2 Time dependent product distribution experiment for the transfer hydrogenation of azobenzene.

8. Kinetic and control experiments

8.1. Study of electronic effect for *p*-substituted symmetric azobenzene

In two different 4 mL pressure tube, (4,4'-CH_3)-azobenzene (0.15 mmol) and (4,4'-CF_3)-azobenzene (0.15 mmol) were taken along with Cs_2CO_3 (0.0375 mmol), Co-Phen/800 (2.2 mol%) and ethanol (1.5 mL) under argon atmosphere. Then, the tubes were sealed and placed in a preheated oil bath at 130 °C for 6 h. After completion of the reaction, the tube was allowed to cool at room temperature. The conversions and yields of the reaction were determined by GC analysis using mesitylene as internal standard.



S1
R = CH_3, CF_3

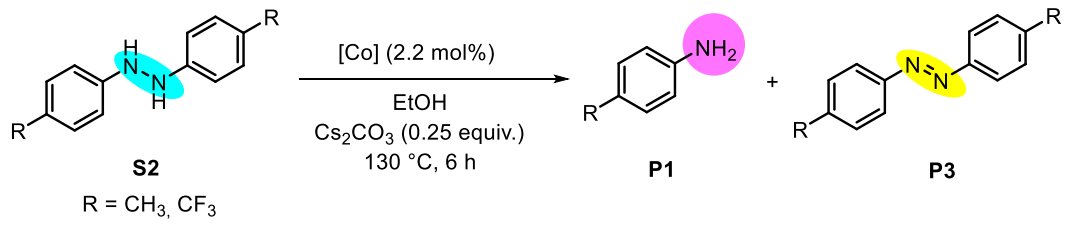
P1 + **P2**

R =	Conv. of **S1**	Yield of **P1**	Yield of **P2**
CH_3	68%	68%	N.D.
CF_3	8%	Trace	6%

Scheme S2. Controls experiments for electronic studies of *p*-substituted symmetric azobenzenes.

8.2. Study of electronic effect for *p*-substituted symmetric hydrazobenezene

In two different 4 mL pressure tube, (4-CH_3)-hydrazobenezene (0.15 mmol) and (4-CF_3)-hydrazobenezene (0.15 mmol) were taken, along with Cs_2CO_3 (0.0375 mmol), Co-Phen/800 (2.2 mol%) and ethanol (1.5 mL) under argon atmosphere. Then, the tubes were sealed and placed in a preheated oil bath at 130 °C for 6 h. After completion of the reaction, the tube was allowed to cool at room temperature. The conversions and yields were calculated by GC analysis using mesitylene as internal standard.



S2
R = CH_3, CF_3

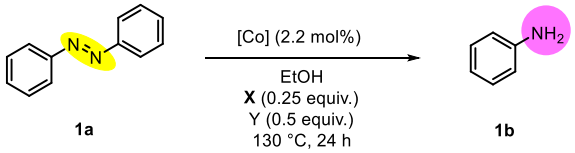
P1 + **P3**

R =	Conv. of **S2**	Yield of **P1**	Yield of **P3**
CH_3	100%	62%	38%
CF_3	15%	5%	10%

Scheme S3. Controls experiments for electronic studies of *p*-substituted symmetric hydrazobenzenes.

8.3. Study on the effect of counter-cation in the transfer hydrogenation azobenezene

In two different 4 mL pressure tube, azobenzene (0.15 mmol) along with Co-Phen/800 (2.2 mol%) and ethanol (1.5 mL) were taken under argon atmosphere. In one pressure tube K_2CO_3 (0.0375 mmol) and 18-crown-ether (0.075 mmol) and in another tube Cs_2CO_3 (0.0375 mmol) and dibenzo-21-crown-7 (0.075 mmol) were added. Then, the tubes were sealed and placed in a preheated oil bath at 130 °C for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. The conversions and yields of the reaction were determined by GC analysis using mesitylene as internal standard.

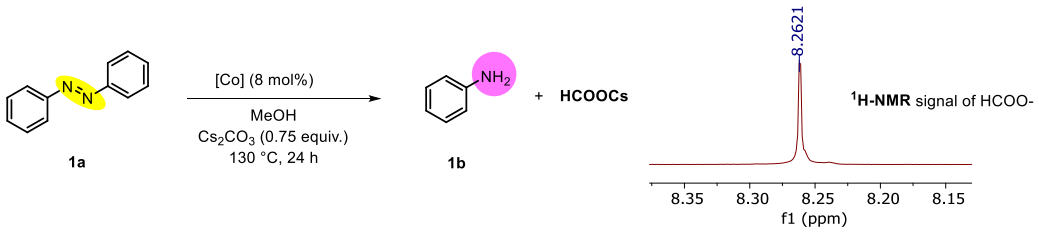


X =	crown-ether (Y)	Yield of **1b** (without crown-ether)	Yield of **1b** (with crown-ether)
K_2CO_3	18-crown-6	75%	45%
Cs_2CO_3	dibenzo-21-crown-7	99%	57%

Scheme S4. Controls experiments on the study of counter-cation.

8.4. Study of the detection of formate in the reaction medium

In a 4 mL pressure tube, azobenzene (0.15 mmol), Co-Phen/800 (8 mol%), and Cs_2CO_3 (0.1125 mmol) were taken in 1.5 mL methanol under argon atmosphere. Then, the tubes were sealed and placed in a preheated oil bath at 130 °C for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then the crude reaction mixture was analyzed though **^{1}H-NMR** in DMSO-d_6.



Scheme S5. Controls experiments for the detection of formate.

8.5. Study on the transfer hydrogenation of *p*-$COCH_3$ substituted azobenzene at various time interval

In a 4 mL pressure tube, azoarene **15a** (0.15 mmol), Co-Phen/800 (2.2 mol%), and Cs2CO3 (0.0375 mmol), were taken in 1.5 mL ethanol. Then, the tube was sealed and placed in a

preheated oil bath at 130 °C (oil bath temperature) for 3-12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected for ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as internal standard to determine conversion and yield of the product (Fig. S3).

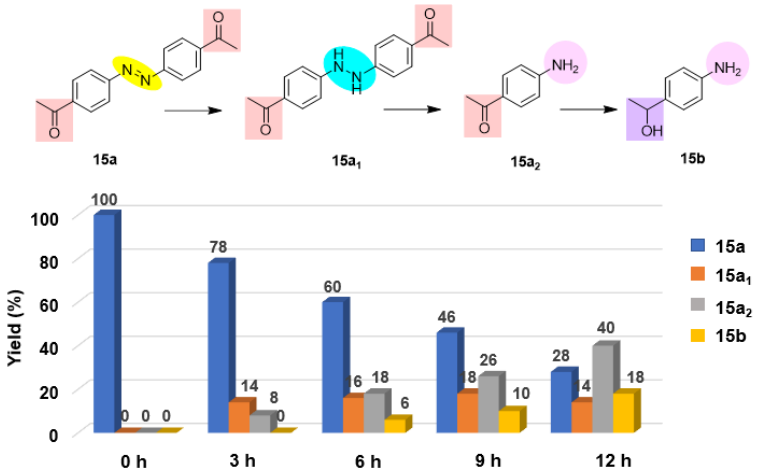


Fig. S3 Time dependent product distribution experiment for the transfer hydrogenation of *p*-$COCH_3$ substituted azobenzene.

8.6. Study on the transfer hydrogenation of *p*-$COCH_3$/NO_2 substituted unsymmetric azobenzene at various time interval

In a 4 mL pressure tube, azoarene **34a** (0.15 mmol), Co-Phen/800 (2.2 mol%), and Cs2CO3 (0.0375 mmol), were taken in 1.5 mL ethanol. Then, the tube was sealed and placed in a preheated oil bath at 130 °C (oil bath temperature) for 3-12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected for ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as internal standard to determine conversion and yield of the product (Fig. S4).

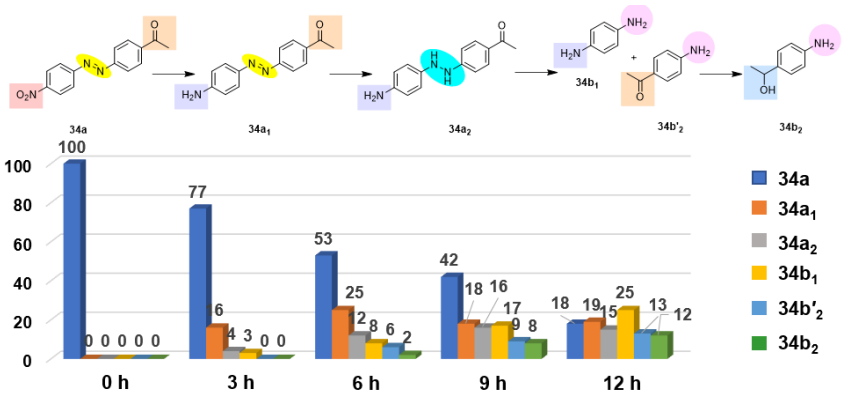
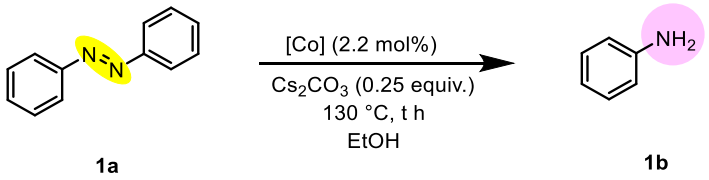


Fig. S4 Time dependent product distribution experiment for the transfer hydrogenation of *p*-$COCH_3$/NO_2 substituted azobenzene.

8.7. Determination of reaction order



1a 1b

No.	1a (mmol)	Cat. (mol%)	Cs_2CO_3 (mmol)	Ethanol (mL)
Run 1:	0.15	2.2	0.0375	1.5
Run 2:	0.3	2.2	0.0375	1.5

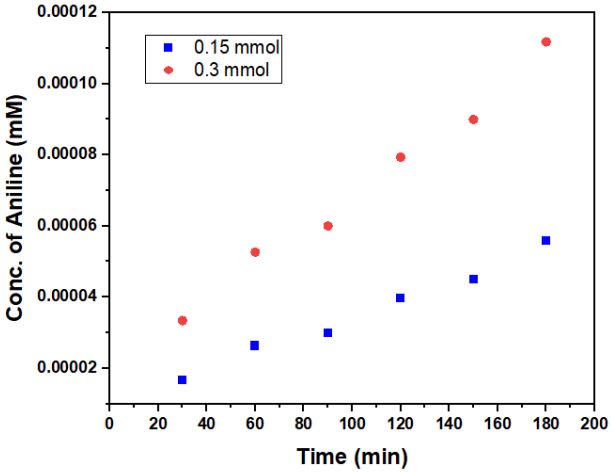


Fig. S5 Determination of initial slopes for the transfer hydrogenation of azobenzene using ethanol; yields were calculated through GC analysis using mesitylene as internal standard.

Considering steady state approximation for ethanol

Initial slope for run 1 at 40 min (r_1) = 4.75 x 10^{-7}(mM)/min = k [**1a** (0.15 mmol)]^x

Initial slope for run 2 at 40 min (r_2) = 9.71 x 10^{-7} (mM)/min = k [**1a** (0.30 mmol)]^x

Comparing the initial slopes,

$$r_1/r_2 = 4.75 \times 10^{-7}/9.71 \times 10^{-7} = (0.15/0.30)^x$$

$$\text{or, } 0.49 = (0.5)^x$$

$$\text{or, } \log(0.49) = \log(0.50)^x$$

$$\text{or, } x = \log(0.49)/\log(0.50)$$

$$\text{or, } x = 1.03 \approx 1$$

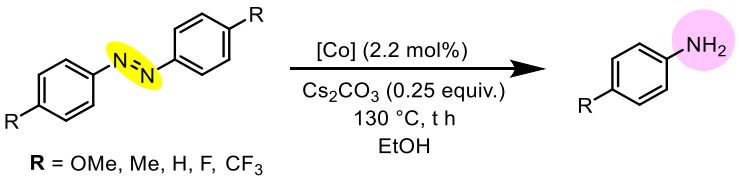
$$\text{So, rate} = k[\mathbf{1a}]^1$$

This experiment stated that the transfer hydrogenation of azobenzene follow a first order kinetics with respect to the azobenzene concentration.

8.8. Hammett studies

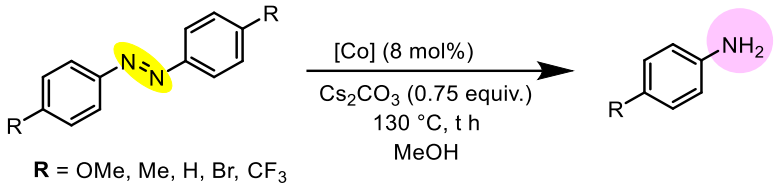
An oven dried screw cap tube was charged with *para*-substituted azobenzene derivative (0.15 mmol), Co-Phen/800 (2.2 mol % for Ethanol; 8 mol% for Methanol)), Cs_2CO_3 (0.0375 mmol), followed by the addition of Ethanol or Methanol (1.5 mL). All the tubes were placed in a preheated oil baths at 130 °C with stirring. The progress of the reaction was analysed by GC using mesitylene as internal standard. (Figure 1b and 1c (see manuscript); Table S5; Figure S4 and S5).

Table S5. Hammett Analysis with the *para*-Substitution Constant (σ_P)



R = OMe, Me, H, F, CF_3

Substrate	-(k x10^{-4} (min))	k_x/k_H	$\log(k_x/k_H)$	σ_p	ρ
4-4'-MeO-azobenezene	75.83	3.07	0.48803	-0.27	-1.74
4-4'-Me-azobenezene	51.87	2.10	0.3255	-0.17	
azobenezene	24.70	1	0	0	
4-4'-F-azobenezene	14.65	0.5932	-0.22675	0.06541	
4-4'-CF_3-azobenezene	3.03	0.1227	-0.91098	0.54	



R = OMe, Me, H, Br, CF_3

Substrate	- (k ×10^{-4} (min))	k_x/k_H	$\log(k_x/k_H)$	σ_p	ρ
4-4'-MeO-azobenezene	61.10	2.74	0.43866	-0.27	-1.72
4-4'-Me-azobenezene	39.92	1.79	0.25525	-0.17	
azobenezene	22.3	1	0	0	
4-4'-Br-azobenezene	6.58	0.295	-0.52935	0.232	
4-4'-CF_3-azobenezene	2.65	0.119	-0.92301	0.54	

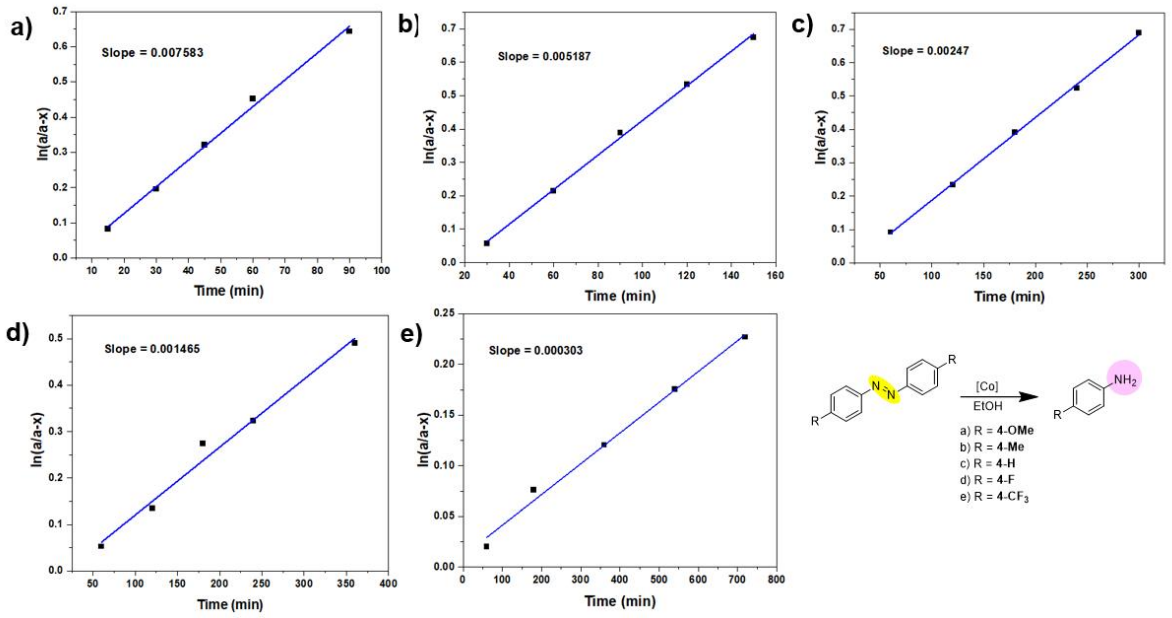


Fig. S6 Determination of rate constant for the *para*-substituted azobenzene substrates during transfer hydrogenation using ethanol.

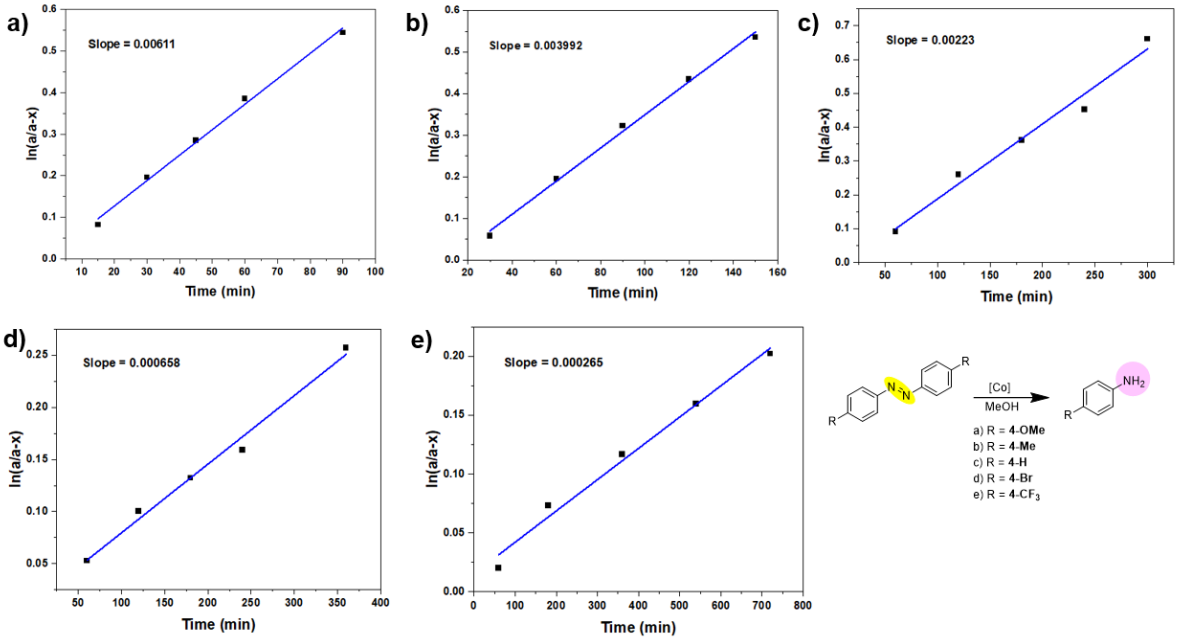


Fig. S7 Determination of rate constant for the *para*-substituted azobenzene substrates during transfer hydrogenation using methanol.

8.9. Kinetic isotope effect (KIE) studies:

Parallel reactions for the transfer hydrogenation azobenzene were carried out using CH_3OH and CD_3OD under identical conditions following the outlined procedure. All the tubes were placed in a preheated oil-baths at 130 °C with stirring and the progress of the reaction was analysed by GC using mesitylene as internal standard.

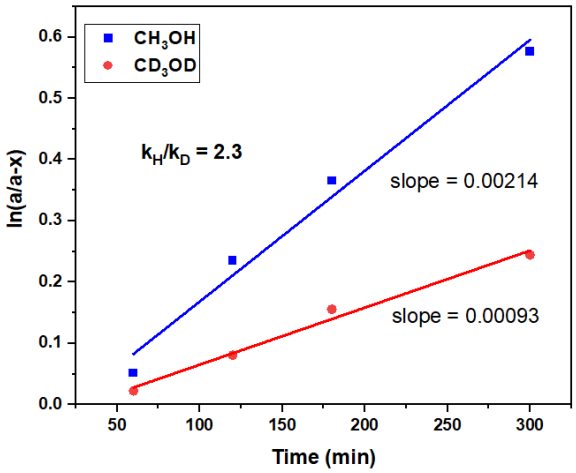


Fig. S8 Kinetic isotopic effect analysis during the transfer hydrogenation azobenzene.

9. Material characterization

Powder X-ray diffraction (XRD) technique was used to investigate the effect of doped heteroatom on carbon structure. The analysis was performed by using Panalytical XPert diffractometer in presence of Cu-Kα as X-ray source (1.54 Å). The ICPMS data was acquired using Agilent ICPMS 7900. X-Ray Photoelectron Spectroscopy (XPS) data was obtained by using PHI5000 Versa Probe II (FEI Inc.). Scanning transmission electron microscopy experiment was performed on a Thermo-Fisher probe-corrected Titan Themis at an operating voltage of 300 kV. High angle annular dark imaging was performed at a camera length of 195 mm. The microscope is equipped with Bruker SuperX detector for energy dispersive X-ray spectroscopy (EDX). Here, samples were deposited without any pretreatment on a holey carbon supported Cu-grid (mesh 300) and transferred to the microscope. Co K-edge XANES measurement was carried out in the fluorescence mode, using RIGAKU R-XAS laboratory spectrometer, equipped with a 3 kW X-ray source and Ge(220) monochromator. The incident and transmitted intensities were measured using a gas-filled ionization chamber and scintillation detector, respectively. The edge energy was calibrated using a Co metal foil in which Co is in Co(0) state. CoO (Sigma-Aldrich, 99.99\% purity), Co_3O_4 (Sigma-Aldrich, 99.99\% purity) and Cobalt(II) Phthalocyanine (TCI Chemicals, >98% purity), where Co is in 2+ state. Textural and surface properties of heteroatom doped catalysts were characterized by N_2-adsorption-desorption isotherms, measured at 77 K using Quantachrome Autosorb® iQ-MP / iQ-XR. Surface area and pore size of the catalyst were determined using the Brunauer–Emmett–Teller (BET) equation.

Table S6 Comparative study between the Co-Phen/T catalysts

Catalysts	C[a] (at %)	O[a] (at %)	N[a] (at %)	Co[a] wt% (at %)	Co[b] wt%	$BET_{Surface\ area}$ (m^2/g)	Average pore size radius (nm)[c]
Co-Phen/ 600	88.0	7.8	3.9	1.41 (0.3)	1.35	43.36	0.10
Co-Phen/700	94.0	2.3	3.4	0.96 (0.2)	0.92	36.11	0.31
Co-Phen/800	89.5	4.8	5.6	0.48 (0.1)	0.52	50.78	0.16
Co-Phen/900	88.5	5.8	5.6	0.47 (0.1)	0.41	36.24	0.29
Co-Phen/1000	81.9	9.5	8.2	1.85 (0.4)	1.70	49.82	0.38

[a] From XPS analysis; [b] ICPMS; [c] BET analysis (BJH method)

9.1. PXRD pattern of the Co-Phen/T catalysts

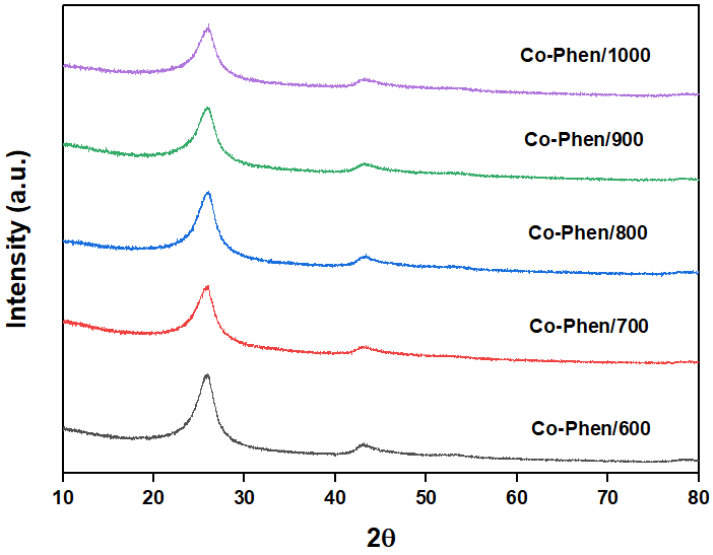


Fig. S9 PXRD pattern of the Co-Phen/T catalysts.

9.2. XPS analysis of the Co-Phen/T catalysts

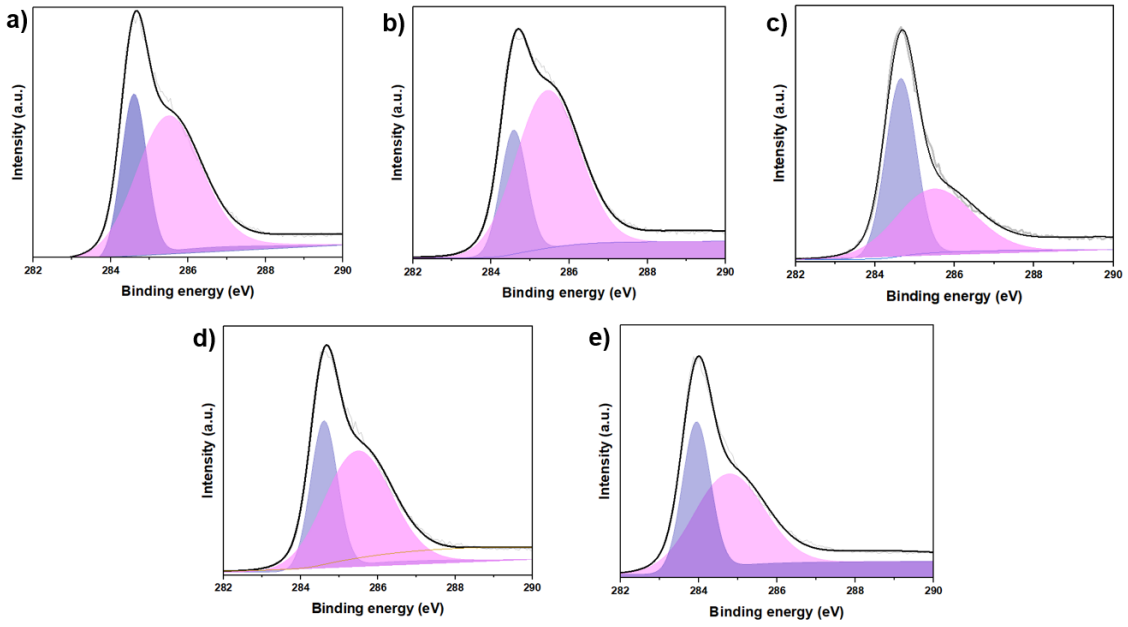


Fig. S10 C_{1s} XPS spectra of a) Co-Phen/600; b) Co-Phen/700; c) Co-Phen/800; d) Co-Phen/900; e) Co-Phen/1000

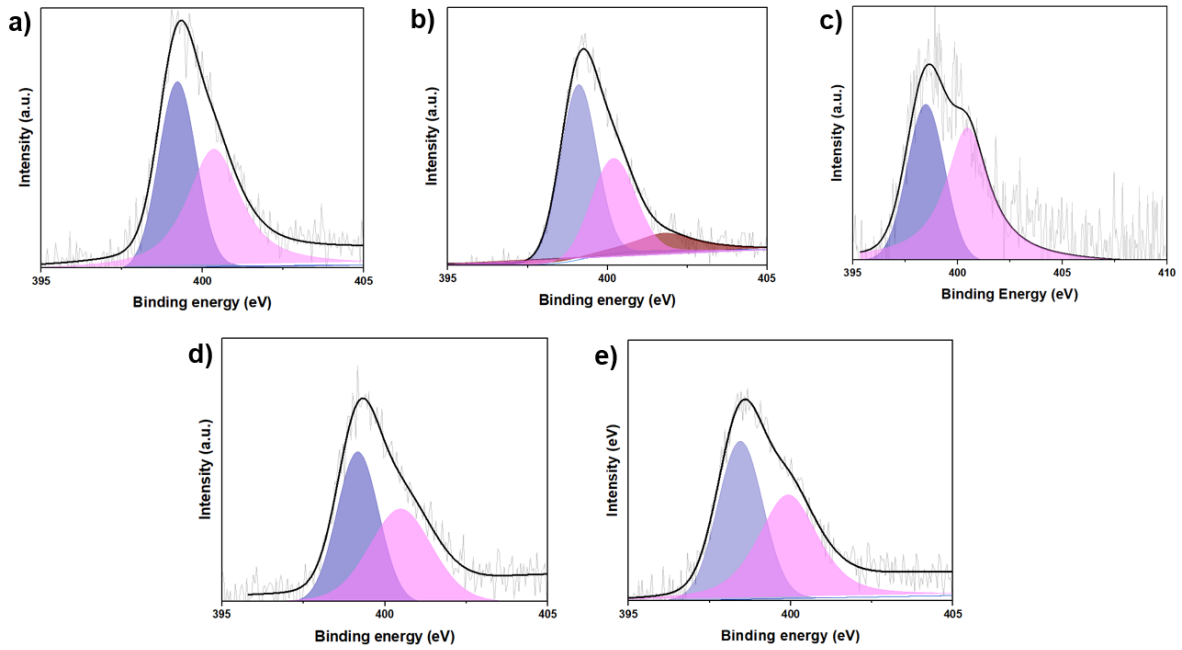


Figure S11. N_{1s} XPS spectra of a) Co-Phen/600; b) Co-Phen/700; c) Co-Phen/800; d) Co-Phen/900; e) Co-Phen/1000.

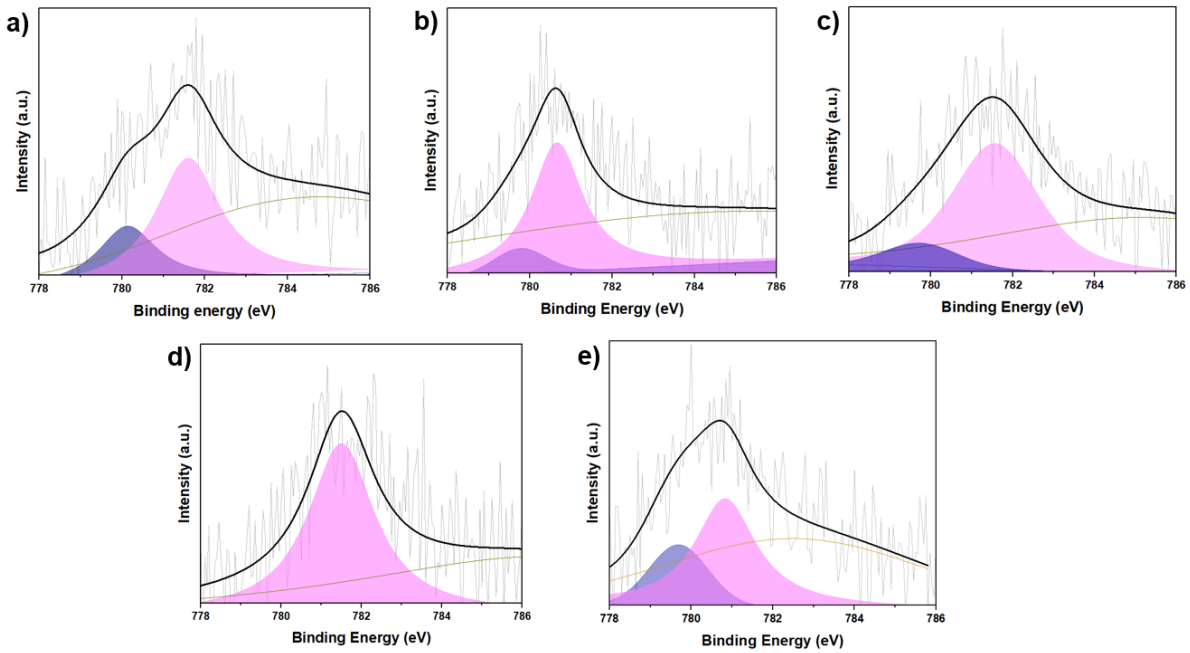


Fig. S12 Co_{2p} high resolution XPS spectra of a) Co-Phen/600; b) Co-Phen/700; c) Co-Phen/800; d) Co-Phen/900; e) Co-Phen/1000.

9.3. XAS analysis of Co-Phen/800

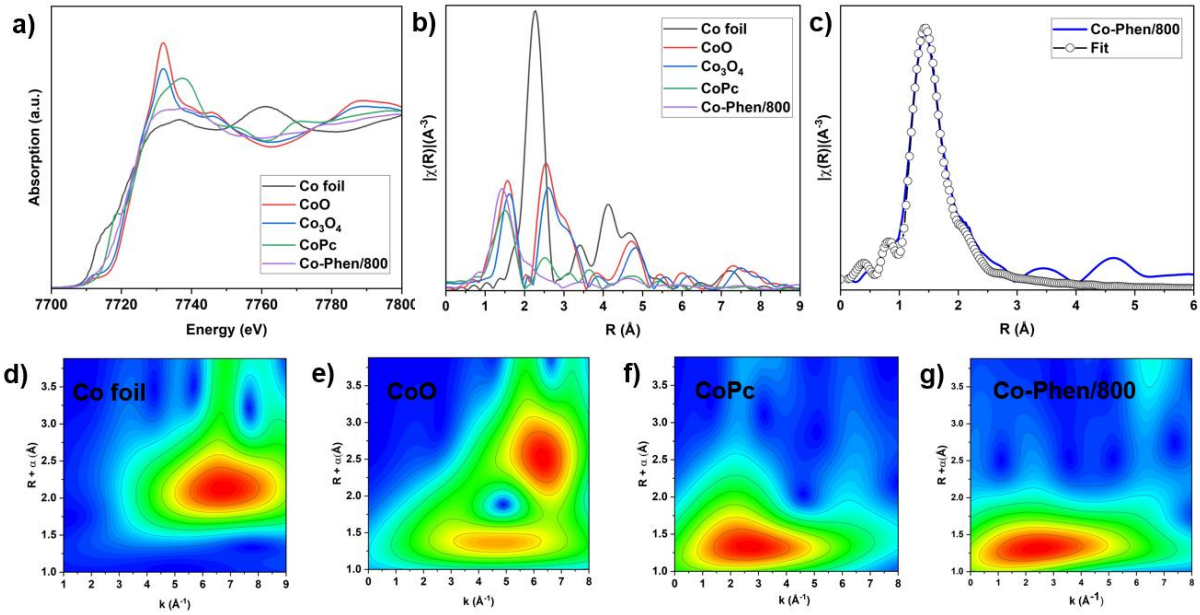


Fig. S13 a) Comparative XANES b) FT-EXAFS spectra of Co(0), CoO, Co_3O_4, Co-phthalocyanine (CoPc) and Co-Phen/800, c) FT-EXAFS fitting result of Co-Phen/800 d-g) WT-EXAFS signals of Co-foil, CoO, CoPc and Co-Phen/800 respectively.

Table S7. EXAFS data fitting results of Co-Phen/800 catalyst.

Sample	Path	N[a]	R (Å)[b]
Co-Phen/800	Co-N	3.6	1.89

[a] N is the coordination number. [b] R is the interatomic distance.

9.4. BET analysis of the Co-Phen/T catalyst

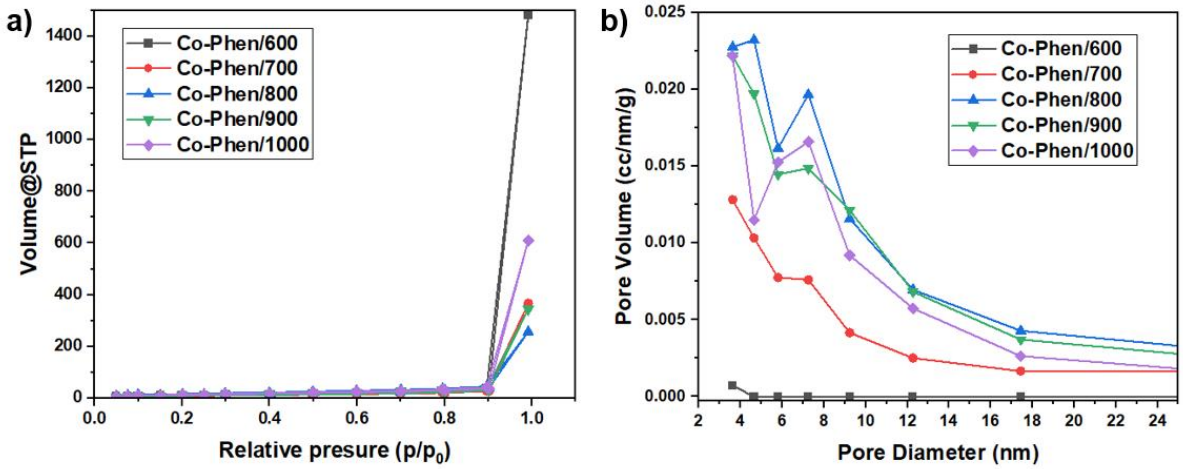


Fig. S14 a) N_2 adsorption-desorption isotherm and b) pore-size distribution plot (BJH method) of Co-Phen/T catalysts.

9.5. BET analysis of the Co-Phen/800 catalyst

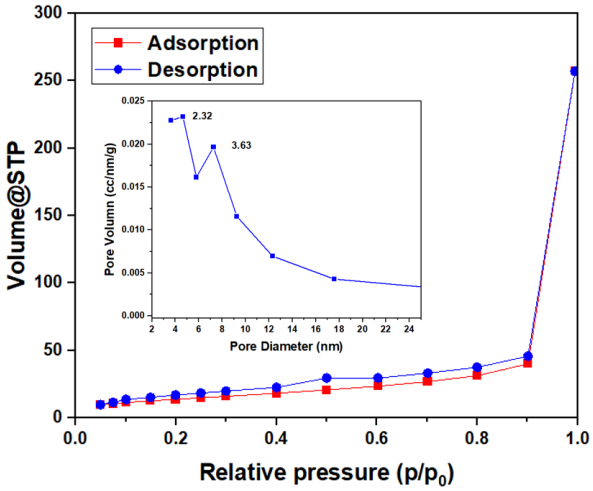


Fig. S15 N_2 adsorption-desorption isotherm and pore-size distribution plot (BJH method) of Co-Phen/800 catalyst.

9.6. Characterization of Co-Phen/800 catalyst

The PXRD pattern of Co-Phen/800 did not show any peaks assignable to cobalt metal or its compounds, only the peaks corresponded to (002) and (100) graphitic planes were observed, which indicated the Co species in the sample were either highly dispersed or amorphous (Fig. S16a). Later, HRTEM was employed to examine the dispersed Co-species. However, no cobalt-containing nanoparticles were observed, only graphitic layers were revealed which was in accordance with the PXRD pattern (Fig. S16b). This implied that the cobalt species must be highly dispersed as tiny clusters or single atoms that are undetectable or invisible by PXRD, TEM techniques.

Later, in order to get information at atomic scale, sub-Ångström-resolution HAADF-STEM technique was used to examine the Co-Phen/800. Interestingly, a large number of uniformly dispersed Co single atoms were observed (Fig. S16c,d). Additionally, the EDX analysis also demonstrated homogeneous distribution of the Co-SACs on the carbon support (Fig. S16e-i).

Next, XPS analysis was performed to gain the information about the electronic states of the elements present in the surface. The high resolution deconvoluted $Co2p_{3/2}$ spectra revealed Co(II)-CoNx (781.6 eV) was present as the major Co-species (Fig. S16j). Later the oxidation state of cobalt as Co(II) was further confirmed by XANES analysis where the adsorption K-edges of Co-Phen/800 were more-or-less overlayed the cobalt phthalocyanine (CoPc) and the CoO edge (Fig. S13). This indicated the Co(II) oxidation state of Co-Phen/800. In the N_{1s} XPS spectra, two peaks were observed at 399.02 eV and 400.7 eV, the lower energy peak

corresponded to pyridinic nitrogen whereas the higher energy peak represented the overlap of CoNx and pyrrolic nitrogen (Fig. S16k).

The FT-EXAFS spectra for Co-Phen/800 (Fig. S13b) presented only one prominent peak at 1.43 Å, which could be ascribed to the Co–Nx coordination of Co at the first shell. Note that the Co–O coordination was located at slightly higher R values in the CoO (1.55 Å) and Co_3O_4 (1.6 Å) samples. Besides, it was also be found, the FT-EXAFS curve of Co-Phen/800 indicated similar characteristic peaks to those of CoPc but different peak-distributions to those of Co foil, CoO, and Co_3O_4. This result suggested that the coordination environment of Co-Phen/800 was closer to that of CoPc, where the Co atoms are coordinated with nitrogen to form Co–Nx bonds. Meanwhile, no obvious Co–Co peak, typically at 2.1 Å, was found in Co-Phen/800, which ruled out the possibility of aggregated Co nanoparticles, consistent with the HAADF-STEM observation. Moreover, the EXAFS fitting was performed to extract the quantitative structural parameters of Co sites in Co-Phen/800. The EXAFS R-space fitting curve of Co-Phen/800 (Fig. S13c) and the fitted parameters summarized in Table S7 clearly suggested that the atomically dispersed cobalt sites existed in the Co–N_4 configuration with a bond distance of 1.89 Å. The WT-EXAFS of Co-Phen/800 in Fig. S13g exhibited a maximum peak at around 2.3 $Å^{-1}$, which was similar to that of CoPc (Fig. S13f) and could be assigned to the Co–N coordination. No intensity maximum corresponding to Co–Co coordination was observed, in sharp contrast with those of Co foil, CoO, and Co_3O_4, demonstrating Co aggregation were not present in Co-Phen/800.

The textural properties of Co-Phen/800 catalysts were investigated through N_2-adsorption desorption studies. The Co-Phen/800 presented a type-II isotherm. BET surface area and pore volume of the catalyst were found to be 64.96 m^2/g, 0.398 cc/g, respectively. Further, the pore size distribution was derived using BJH method, and two peaks were observed at 2.32 nm and 3.63 nm, which signified the meso-porous nature of the catalyst (Fig. S15).

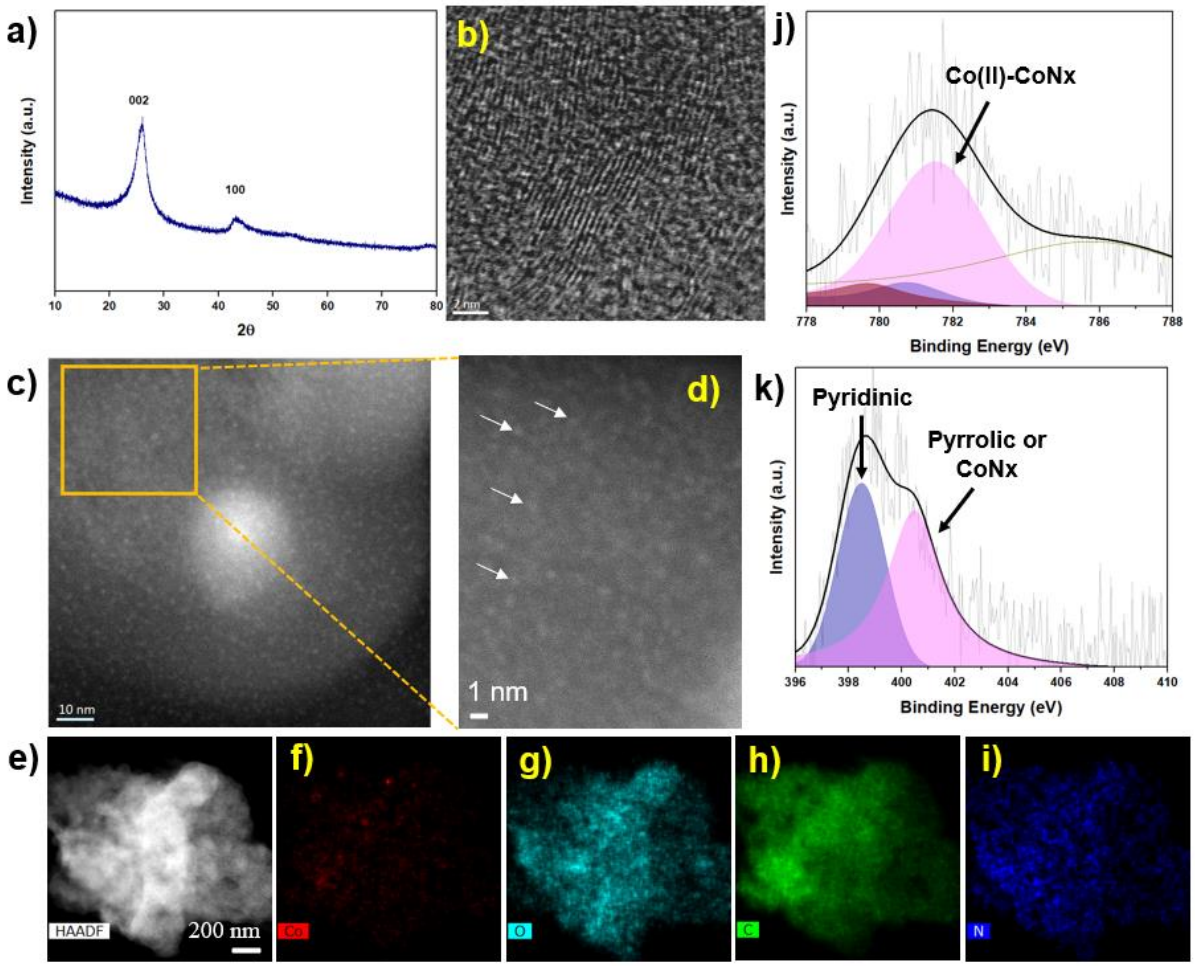
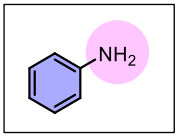


Fig. S16 a) PXRD pattern; b) HRTEM; c) and d) AC-HAADF image; e-i) EDX analysis; j) High-resolution deconvoluted $Co2p_{3/2}$, k) N_{1s} XPS spectra of Co-Phen/800.

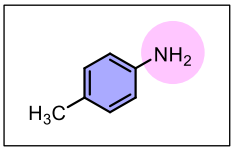
10. Spectral data for the amines

Aniline (1b):[6]



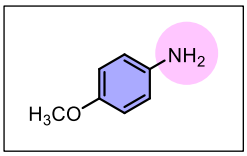
From **1a**, 75.5 mg (81%) (EtOH), 76.4 mg (82%) (MeOH); From **25a**, 41.9 mg (90%) (EtOH), 38.6 mg (83%) (MeOH); From **26a**, 42.4 mg (91%) (EtOH), 38.2 mg (82%) (MeOH); From **27a**, 43.7 mg (94%) (EtOH), 42.8 mg (92%) (MeOH); From **28a**, 7.9 mg (17%); 22.3 mg (48%) (EtOH), 7.0 mg (15%); 24.7 mg (53%) (MeOH); From **29a**, 8.4 mg (18%); 24.2 mg (52%) (EtOH), 10.24 mg (22%); 20.9 mg (45%) (MeOH); From **30a**, 76.4 mg (82%) (EtOH), 70.8 mg (76%) (MeOH); From **31a**, 26.5 mg (57%); 36.3 mg (78%) (EtOH), 24.2 mg (52%) (MeOH); 33.5 mg (72%); From **36a**, 12.6 mg (27%); 26.5 mg (57%) (EtOH), 11.2 mg (24%); 20.5 mg (44%) (MeOH); isolated yield; yellowish liquid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.15 (t, $J_{H,H}$ = 7.8 Hz, 2H), 6.76 (t, $J_{H,H}$ = 7.4 Hz, 1H), 6.68 (d, $J_{H,H}$ = 8.0 Hz, 2H), 3.51 (s, 2H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 146.4, 129.3, 118.5, 115.1.

***p*-toluidine (2b):[6]**



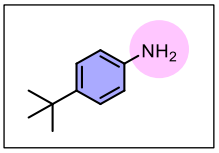
From **2a**, 99.6 mg (93%) (EtOH), 94.3 mg (88%) (MeOH); From **25a**, 48.2 mg (90%) (EtOH), 44.4 mg (83%) (MeOH); From **27a**, 50.3 mg (94%) (EtOH), 49.3 mg (92%) (MeOH); From **33a**, 11.25 mg (21%); 27.8 mg (52%) (EtOH), 14.5 mg (27%); 26.8 mg (50%) (MeOH); isolated yield; yellow orange solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.97 (d, $J_{H,H}$ = 7.9 Hz, 2H), 6.61 (d, $J_{H,H}$ = 8.0 Hz, 2H), 3.46 (s, 2H), 2.25 (s, 3H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 143.9, 129.8, 127.8, 115.3, 20.5.

4-methoxyaniline (3b):[7]



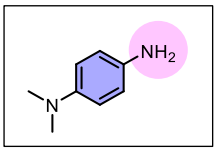
From **3a**, 115.7 mg (94%) (EtOH), 107.2 mg (87%) (MeOH); From **26a**, 56 .0 mg (91%) (EtOH), 50.5 mg (82%) (MeOH); From **27a**, 57.86 mg (94%) (EtOH), 56.6 mg (92%) (MeOH); From **35a**, 48.0 mg (78%) (EtOH), 50.5 mg (82%) (MeOH); isolated yield; yellowish solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.73 (d, $J_{H,H}$ = 9.0 Hz, 2H), 6.63 (d, $J_{H,H}$ = 9.1 Hz, 2H), 3.73 (s, 3H), 3.38 (s, 2H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 152.9, 140.0, 116.5, 114.9, 55.8.

4-(*tert*-butyl)aniline (4b):[8]



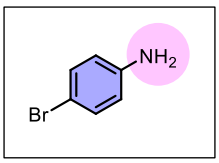
From **4a**, 129.8 mg (87%) (EtOH), 134.3 mg (90%) (MeOH); From **32a**, 28.4 mg (38%); 51.5 mg (69%) (EtOH), 23.9 mg (32%); 50 mg (67%) (MeOH); isolated yield; yellowish oil. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.19 (d, $J_{H,H}$ = 8.6 Hz, 2H), 6.65 (d, $J_{H,H}$ = 8.6 Hz, 2H), 3.50 (s, 2H), 1.29 (s, 9H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 143.8, 141.5, 126.1, 115.0, 34.0, 31.6.

N,N-dimethylbenzene-1,4-diamine (5b):[9]



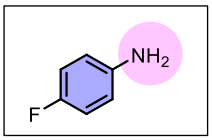
From **5a**, 128.0 mg (93%) (EtOH), 123.9 mg (91%) (MeOH); isolated yield; reddish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.70 - 6.62 (m, 4H), 3.33 (s, 2H), 2.81 (s, 6H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 145.0, 137.9, 116.7, 115.7, 42.2.

4-bromoaniline (6b):[10]



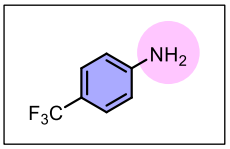
From **6a**, 77.4 mg (45%); 130 mg (76%) (EtOH), 60.2 mg (35%); 127.3 mg (74%) (MeOH); From **28a**, 14.6 mg (17%); 41.3 mg (48%) (EtOH), 12.9 mg (15%); 45.6 mg (53%) (MeOH); From **33a**, 18.1 mg (21%); 44.8 mg (52%) (EtOH), 20.7 mg (27%); 42.8 mg (50%) (MeOH); isolated yield; yellowish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.22 (d, $J_{H,H}$ = 8.9 Hz, 2H), 6.55 (d, $J_{H,H}$ = 8.6 Hz, 2H), 3.63 (s, 2H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 145.5, 132.1, 116.8, 110.3.

4-fluoroaniline (7b):[6]



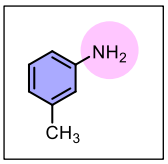
From **7a**, 42.2 mg (38%); 74.4 mg (67%) (EtOH), 36.7 mg (33%); 63.33 mg (57%) (MeOH); isolated yield; yellowish oil.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.86 (t, $J_{H,H}$ = 8.6 Hz, 2H), 6.63 - 6.54 (m, 2H), 3.53 (s, 2H). **^{13}C {^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 157.63, 155.29, 142.76, 116.19 ($J_{C\text{-}F}$ = 8.0 Hz), 115.76 ($J_{C\text{-}F}$ = 22 Hz).

4-(trifluoromethyl)aniline (8b):[6]



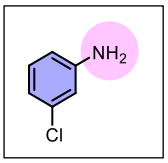
From **8a**, 29.0 mg (18%); 62.8 mg (39%) (EtOH), 22.5 mg (14%); 54.8 mg (34%) (MeOH); From **32a**, 30.6 mg (38%); 55.6 mg (69%) (EtOH), 25.6 mg (32%); 54.0 mg (67%) (MeOH); From **36a**, 21.7 mg (27%); 46.9 mg (57%) (EtOH), 19.5 mg (24%); 35.4 mg (44%) (MeOH); isolated yield; yellow oil. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.38 (d, $J_{H,H}$ = 8.3 Hz, 2H), 6.67 (d, $J_{H,H}$ = 8.3 Hz, 2H), 3.92 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 149.4, 126.8 (d, $J_{C\text{-}F}$ = 3 Hz), 126.2, 124.0, 120.2 (q, $J_{C\text{-}F}$ = 33 Hz), 114.24.

m-toluidine (9b):[11]



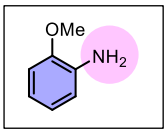
From **9a**, 93.2 mg (87%) (EtOH), 98.6 mg (92%) (MeOH); isolated yield; yellowish oil.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.07 (t, $J_{H,H}$ = 7.4 Hz, 1H), 6.62 (d, $J_{H,H}$ = 7.5 Hz, 1H), 6.52 (d, $J_{H,H}$ = 8.8 Hz, 2H), 3.57 (s, 2H), 2.30 (s, 3H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 146.5, 139.2, 129.3, 119.6, 116.1, 112.4, 21.5.

3-chloroaniline (10b):[7]



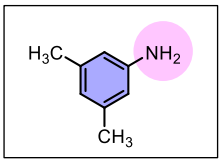
From **10a**, 84.2 mg (66%) (EtOH), 82.9 mg (65%) (MeOH); isolated yield; yellowish solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.06 (t, $J_{H,H}$ = 8.0 Hz, 1H), 6.74 (d, $J_{H,H}$ = 7.9 Hz, 1H), 6.65 (d, $J_{H,H}$ = 3.0 Hz, 1H), 6.52 (dd, $J_{H,H}$ = 8.0, 2.3 Hz, 1H), 3.72 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 147.69, 147.66, 134.64, 130.30, 130.27, 130.23, 118.25, 114.80, 113.20, 113.17, 113.12.

2-methoxyaniline (11b):[11]



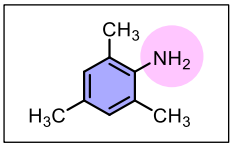
From **11a**, 64.1 mg (52%); 92.4 mg (75%) (EtOH), 55.4 mg (45%); 82.5 mg (67%) (MeOH); isolated yield; colourless liquid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.83 - 6.78 (m, 2H), 6.77 - 6.71 (m, 2H), 3.85 (s, 3H), 3.71 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 147.37, 136.11, 121.09, 118.53, 115.09, 110.47, 55.43.

3,5-dimethylaniline (12b):[11]



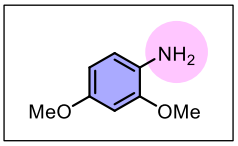
From **12a**, 109 mg (90%) (EtOH), 106.7 mg (88%) (MeOH); isolated yield; yellowish oil.**^{1}H NMR** ($CDCl_3$, 500 MHz) δ = 6.44 (s, 1H), 6.34 (s, 2H), 3.55 (s, 2H), 2.25 (s, 6H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 125 MHz) δ = 146.38, 120.50, 113.11, 21.32.

2,4,6-trimethylaniline (13b):[12]



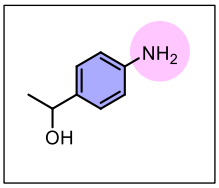
From **13a**, 60.9 mg (45%); 81 mg (60%) (EtOH), 69.1 mg (51%), 87.9 mg (65%) (MeOH); isolated yield; yellow liquid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.80 (s, 2H), 3.46 (s, 2H), 2.24 (s, 3H), 2.19 (s, 6H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 140.2, 128.9, 127.1, 121.9, 20.4, 17.6.

2,4-dimethoxyaniline (14b):[12]



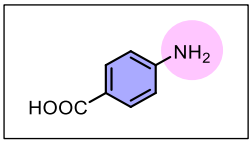
From **14a**, 79.65 mg (52%); 119.4 mg (78%) (EtOH), 72.1 mg (47%); 105.7 mg (69%) (MeOH); isolated yield; yellow liquid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 6.63 (d, $J_{H,H}$ = 8.1 Hz, 1H), 6.44 (d, $J_{H,H}$ = 2.6 Hz, 1H), 6.33 (dd, $J_{H,H}$ = 8.3, 2.7 Hz, 1H), 3.81 (s, 3H), 3.73 (s, 3H), 3.50 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 153.17, 148.39, 129.77, 115.26, 104.19, 99.39, 55.80, 55.51.

1-(4-aminophenyl)ethan-1-ol (15b):[13]



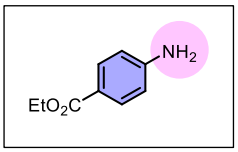
From **15a**, 56.24 mg (41%); 93.28 mg (68%) (EtOH), 59.0 mg (43%); 89.2 mg (65%) (MeOH); From **34a**, 20.5 mg (30%); 44.6 mg (65%) (EtOH), 18.5 mg (27%); 42.5 mg (62%) (MeOH); yellowish liquid .**^{1}H NMR** (DMSO-d_6, 400 MHz) δ = 6.95 (d, $J_{H,H}$ = 7.8 Hz, 2H), 6.47 (d, $J_{H,H}$ = 8.3 Hz, 2H), 4.81 (s, 2H), 4.54 - 4.48 (m, 1H), 1.22 (d, $J_{H,H}$ = 6.7 Hz, 3H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 147.31, 134.74, 126.22, 113.68, 68.16, 25.93.

4-aminobenzoic acid (16b):[6]



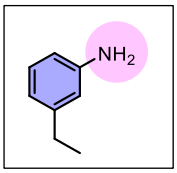
From **16a**, 115.2 mg (84%) (EtOH), 97.4 mg (71%) (MeOH); isolated yield; white solid.**^{1}H NMR** (DMSO-d_6, 400 MHz) δ = 7.55 (d, $J_{H,H}$ = 8.4 Hz, 2H), 6.49 (d, $J_{H,H}$ = 8.4 Hz, 2H), 5.79 (s, 2H). **^{13}C{^{1}H} NMR** (DMSO-d_6, 100 MHz) δ = 167.7, 153.2, 131.3, 117.0, 112.7.

ethyl 4-aminobenzoate (17b):[11]



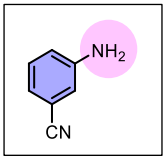
From **17a**, 130.5 mg (79%) (EtOH); isolated yield; yellowish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.84 (d, $J_{H,H}$ = 8.2 Hz, 1H), 6.62 (d, $J_{H,H}$ = 8.6 Hz, 1H), 4.30 (q, $J_{H,H}$ = 6.9 Hz, 1H), 4.01 (s, 1H), 1.34 (t, $J_{H,H}$ = 7.0 Hz, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 166.8, 150.8, 131.6, 120.3, 113.9, 60.4, 14.5.

3-ethylaniline (18b):[12]



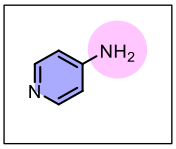
From **18a**, 101.8 mg (84%) (EtOH), 100.6 mg (83%) (MeOH); isolated yield; yellow liquid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.09 (t, $J_{H,H}$ = 7.7 Hz, 1H), 6.63 (d, $J_{H,H}$ = 7.3 Hz, 1H), 6.59 - 6.50 (m, 2H), 3.60 (s, 2H), 2.58 (q, $J_{H,H}$ = 7.5 Hz, 2H), 1.23 (t, $J_{H,H}$ = 7.44 Hz, 3H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 146.52, 145.68, 129.34, 118.38, 114.86, 112.65, 28.96, 15.62.

3-aminobenzonitrile (19b):[6]



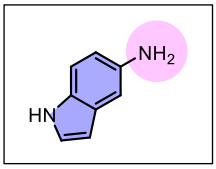
From **19a**, 63.8 mg (54%); 85 mg (72%) (EtOH), 47.2 mg (40%); 82.7 mg (71%) (MeOH); isolated yield; yellow-orange solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.17 (t, $J_{H,H}$ = 7.9 Hz, 1H), 6.96 (d, $J_{H,H}$ = 7.9 Hz, 1H), 6.87 - 6.82 (m, 2H), 3.92 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 147.2, 130.2, 121.9, 119.4, 119.3, 117.5, 112.8.

pyridin-4-amine (20b):[14]



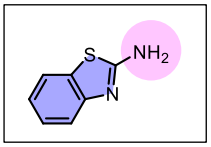
From **20a**, 75.3 mg (80%) (EtOH), 67.8 mg (72%) (MeOH); isolated yield; yellowish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 8.16 (d, $J_{H,H}$ = 5.4 Hz, 2H), 6.48 (d, $J_{H,H}$ = 5.5 Hz, 2H), 4.23 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 152.8, 150.2, 109.7.

1H-indol-5-amine (21b): [15]



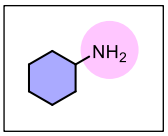
From **21a**, 103 mg (78%) (EtOH), 92.5 mg (70%) (MeOH); isolated yield; yellowish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.94 (s, 1H), 7.18 (d, $J_{H,H}$ = 8.5 Hz, 1H), 7.11 (t, $J_{H,H}$ = 2.8 Hz, 1H), 6.93 (d, $J_{H,H}$ = 2.3 Hz, 1H), 6.65 (dd, $J_{H,H}$ = 8.3, 2.1 Hz, 1H), 6.36 (t, $J_{H,H}$ = 2.5 Hz, 1H), 3.47 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 139.64, 130.76, 128.89, 124.78, 113.06, 111.59, 105.64, 101.68.

benzo[d]thiazol-2-amine (22b):[16]



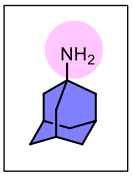
From **22a**, 37.5 mg (25%); 87.1 mg (58%) (EtOH), 27 mg (18%); 76.6 mg (51%) (MeOH); isolated yield; yellowish solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.57 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.52 (d, $J_{H,H}$ = 8.0 Hz, 1H), 7.29 (t, $J_{H,H}$ = 7.7 Hz, 1H), 7.11 (t, $J_{H,H}$ = 7.6 Hz, 1H), 5.58 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 166.52, 151.99, 131.43, 125.99, 122.23, 120.95, 118.99.

Cyclohexanamine (23b):[17]



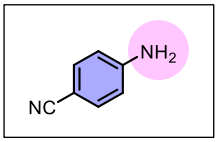
From **23a**, 54.6 mg (55%); 78.4 mg (79%) (EtOH), 40.6 mg (41 %); 67.4 mg (68%) (MeOH); From **35a**, 38.6 mg (78%) (EtOH), 40.6 mg (82%) (MeOH); isolated yield; yellowish liquid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 2.55 (tt, $J_{H,H}$ = 10.8, 3.9 Hz, 1H), 1.74 (dt, $J_{H,H}$ = 12.4, 3.8 Hz, 2H), 1.64 (dq, $J_{H,H}$ = 11.5, 3.8 Hz, 2H), 1.58 - 1.47 (m, 1H), 1.29 - 1.12 (m, 4H), 1.12 - 1.04 (m, 1H), 1.04 - 0.89 (m, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 50.5, 36.9, 25.7, 25.2.

Adamantan-1-amine (24b):[18]



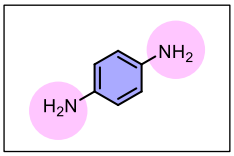
From **24a**, 90.8 mg (60%); 124 mg (82%) (EtOH), 76.6 mg (52%); 113.4 mg (75%) (MeOH); isolated yield; white solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 2.03 (s, 2H), 1.78 - 1.41 (m, 15H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 47.5, 46.2, 36.3, 29.9.

4-aminobenzonitrile (29b2):[6]



From **29a**, 10.6 mg (18%); 30.7 mg (52%) (EtOH), 13.0 mg (22%); 26.6 mg (45%) (MeOH); isolated yield; yellow solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 7.39 (d, $J_{H,H}$ = 8.5 Hz, 2H), 6.62 (d, $J_{H,H}$ = 8.6 Hz, 2H), 4.12 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 150.4, 133.9, 120.2, 114.5, 100.4.

benzene-1,4-diamine (30b2):[8]



From **30a**, 44.3 mg (82%) (EtOH), 41.1 mg (76%) (MeOH); From **31a**, 30.8 mg (57%); 42.2 mg (78%) (EtOH), 28.2 mg (52%); 39.0 mg (72%); (MeOH); From **34a**, 22.6 mg (42%); 41.6 mg (77%) (EtOH), 20.5 mg (38%); 42.7 mg (79%) (MeOH); isolated yield; white solid.**^{1}H NMR** ($CDCl_3$, 400 MHz) δ = 8.16 (d, $J_{H,H}$ = 5.4 Hz, 2H), 6.48 (d, $J_{H,H}$ = 5.5 Hz, 2H), 4.23 (s, 2H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ = 152.8, 150.2, 149.9, 109.7.

11. Computational details:

Possible geometries on the designed reaction pathways were optimized using Gaussian 09 software[19] and structure were presented using CYLview20.[20] Construction of trial geometries, monitoring the progress of calculations and visualization of the final output were done by several graphical user interface softwares like Gauss View, Molden etc. We have chosen hybrid density functional M06-2X as a method for performing optimization of structures. 6-31G (d, p)[21] basis set was employed for all non-metal atoms and the LANL2DZ basis set[22] was employed for cobalt. The optimized geometries are further refined with single-point energy calculations at the M06-2X/6-311+G(2df, p)[23] level of theory. To find out the geometries of several transition structures on the potential energy surface (PES) of the reaction pathway, relaxed scan method was used. Each structure was characterized as corresponding to a minimum or a saddle point on the energy hyper surface by means of frequency analysis. A transition structure (TS) possesses only a single imaginary frequency while the structure at minimum contains no imaginary frequency at all. Further confirmation of the TS was done by following the intrinsic reaction coordinate (IRC) pathway. All the relative energies on the reaction path were calculated with respect to the energy sum of the free reactant and catalyst. Solvent effect was approximated by introducing a polarizable continuum model (PCM).[24] We used the standard parameters for the solvent Ethanol at 403.15 K temperature.

11.1. The reason for considering A as the active site:

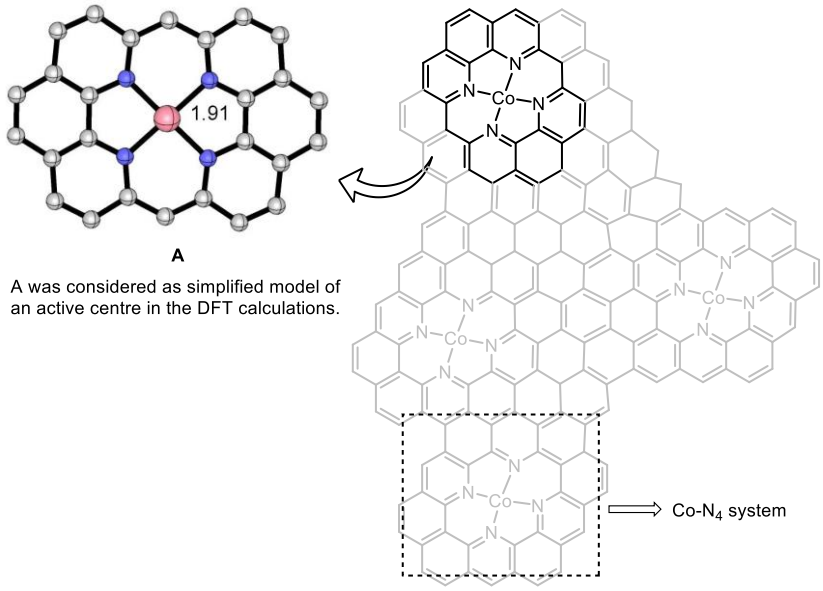


Fig. S17 The reason for considering **A** as the active site.

Table S8. Comparison of FT-EXAFS fitting data and theoretical model

	CN	**R (Å)**
FT-EXAFS fitting	3.6	1.89
Theoretical model	4	1.91

The FT-EXAFS and WT-EXAFS clearly suggested in this catalyst only the Co-N bond is present in the active site. Further, the fitting study demonstrated, CN= ~4 (3.6) and R = 1.89 Å, which suggested the existence of **Co-N_4** unit. On the other hand, in the theoretical model, cobalt is bound with 4 nitrogens with the length of 1.91 Å. Based on these structural information **A** is considered as the model active site.

11.2. Kinetic Isotope Study:

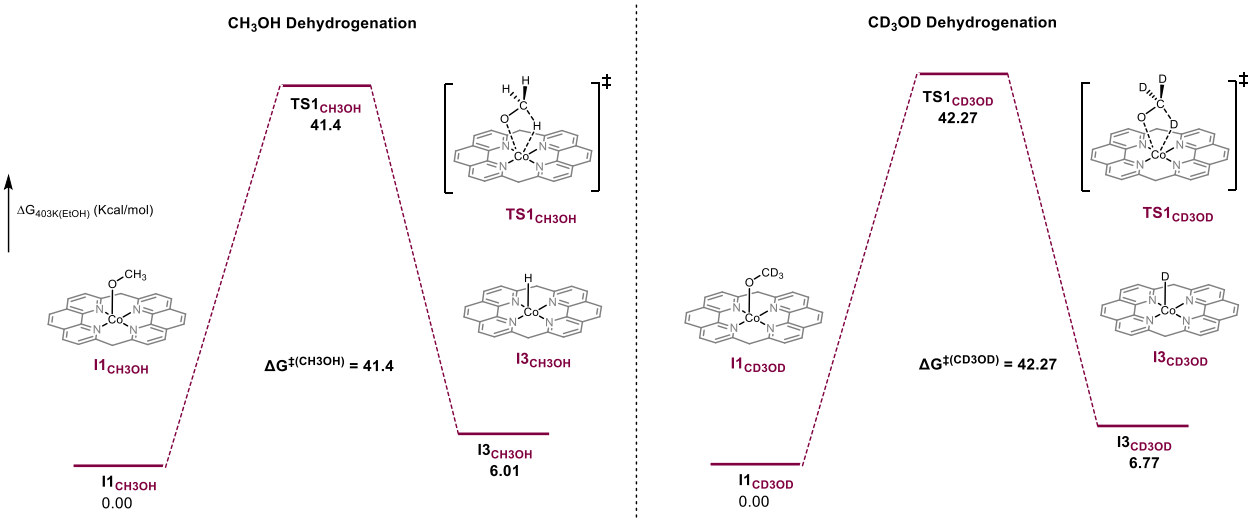


Fig. S18 KIE study on methanol dehydrogenation.

$$k_H/k_D = AExp\ (\Delta G^{\ddagger(CD3OD)}/RT)/AExp\ (\Delta G^{\ddagger(CH3OH)}/RT$$

$$= Exp\,(\Delta G^{\ddagger(CD3OD)} - \Delta G^{\ddagger(CH3OH)})/RT$$

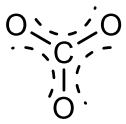
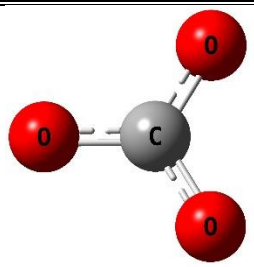
$$= Exp\ (42.27\text{-}41.4/1.9872036\ X\ 10^{-3} X\ 403.15)$$

$$= 2.96$$

$$k_H/k_D = 2.3\ (Experimental)$$

Theoretical found k_H/k_D = 2.96, which is in good agreement with the experimentally determined k_H/k_D = 2.3.

11.3. Cartesian coordinates and statistical thermodynamic analysis data:

St.Pt.	General Structure	Ball & Stick model
CO_3^{2-}		

Cartesian co-ordinate

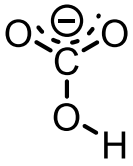
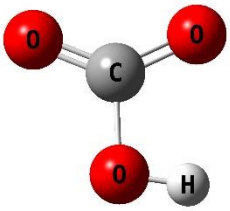
Atoms	X	Y	Z
C	0.00000	0.00000	0.00010
O	0.00000	0.00000	1.30468
O	0.00000	1.12956	-0.65238
O	0.00000	-1.12956	-0.65238

Frequencies

683.1451	684.7635	908.8954
1064.3312	1519.4950	1520.4089

Statistical Thermodynamic Analysis

Temperature=403.15 K	Pressure=1 atm
Zero-point correction= 0.014537	Electronic Energy = -263.493375590
Internal Energy (E)= -263.47407359	Enthalpy (H)= -263.47279659
Gibbs Free Energy (G)=-263.51424659	Gibbs Free Energy of Solvation=-264.0697765

St.Pt.	General Structure	Ball & Stick model
CO_3H^-		

Cartesian co-ordinate

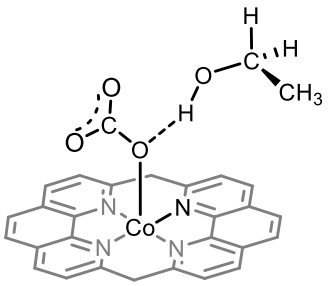
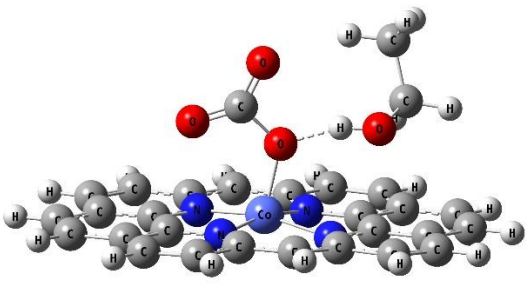
Atoms	X	Y	Z
C	-0.15094	0.07437	-0.00000
O	-1.25093	-0.48684	0.00000
O	0.18499	1.27828	-0.00000
O	0.96662	-0.82251	-0.00000
H	1.70025	-0.19763	0.00003

Frequencies

555.9445	565.6904	658.0212
839.1334	939.8310	1228.8075
1391.8303	1892.5632	3885.3474

Statistical Thermodynamic Analysis

Temperature=403.15 K	Pressure=1 atm
Zero-point correction= 0.027240	Electronic Energy = -264.331402377
Internal Energy (E)= -264.298735377	Enthalpy (H)= -264.297458377
Gibbs Free Energy (G)=-264.340864377	Gibbs Free Energy of Solvation=-264.571242398

St. Pt.	General Structure	Ball & Stick model
$I1_{\beta\text{-}H}$		

Cartesian co-ordinate

Frequencies

Atoms	X	Y	Z
C	1.98201300	3.71994400	-0.51296100
C	3.23090100	3.22340700	-0.71544500
C	3.43278300	1.81694000	-0.89416000
C	2.27390400	1.03342400	-0.85713200
C	0.82107600	2.85616000	-0.46739300
C	4.68774800	1.17677400	-1.07778200
C	2.35871900	-0.38270600	-1.00400700
C	3.60170000	-0.99861100	-1.17514900
C	4.76863600	-0.18858000	-1.21162600
C	3.57380700	-2.42596700	-1.28037100
H	4.50831500	-2.96568300	-1.41171100
C	2.39623100	-3.09581000	-1.19325500
C	1.14316000	-2.40211400	-0.99410800
H	5.58736200	1.78588100	-1.09838200
H	1.82541200	4.78359600	-0.36400100
H	4.09150200	3.88777500	-0.73265600
H	5.73427100	-0.67044600	-1.33888200
H	2.36920900	-4.17939300	-1.24512000
N	1.02462400	1.53506600	-0.66581700
N	1.17860500	-1.05330700	-0.95017300
Co	-0.24242900	0.11654400	-0.4176930
C	-2.90021400	0.66618500	-0.30168200
C	-1.67100500	2.67501900	-0.19780200
C	-2.81355400	-0.75026800	-0.43643600
C	-4.14183900	1.28234800	-0.14351600
C	-2.92411900	3.37160200	-0.01714900
C	-3.96913900	-1.53159000	-0.41137800
C	-5.31427900	0.47331400	-0.12639200
C	-4.10910400	2.70390200	0.00687100
H	-2.89131600	4.44944000	0.10517100
C	-3.76272300	-2.94161000	-0.53393700
C	-5.23034200	-0.88888200	-0.25610400
C	-1.34818600	-2.58111300	-0.70802800

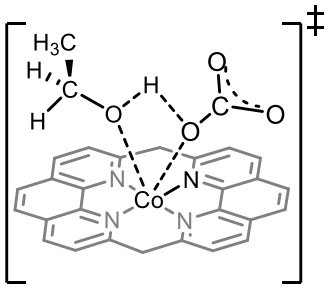
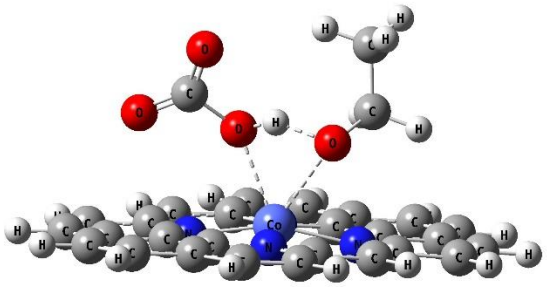
18.4618	32.8223	50.6160
54.1033	61.6389	66.7674
79.6152	91.1307	107.2917
114.6461	127.7864	132.7735
142.9226	160.8234	177.1214
203.7412	213.8029	219.1788
237.3746	248.9135	253.2163
258.5344	276.0505	279.5671
292.6516	308.8673	340.7961
351.1157	352.2569	379.0226
391.6094	406.4994	407.7515
412.3074	447.8813	449.2566
459.6344	470.5324	477.3630
487.2654	492.8454	494.3290
497.1888	537.5428	556.5291
579.5417	586.5008	595.1268
597.0373	599.6729	623.3529
633.7417	679.7265	683.8864
689.2964	691.8959	712.6152
716.2292	717.4330	730.5093
740.3646	742.1147	750.6054
758.4786	760.4295	769.8900
807.3399	817.2832	820.7338
821.6389	823.9215	825.8397
844.0989	854.5677	858.4709
859.6049	863.0397	865.0342
909.6813	920.3572	921.9553
942.3843	943.8344	947.7737
960.6022	960.8070	991.4196
997.8223	1001.1088	1002.6279
1010.3842	1042.5362	1115.2209
1116.8526	1134.8792	1141.2871
1141.8092	1157.0185	1166.9742
1167.4957	1178.7483	1180.3521
1180.7115	1231.6382	1237.5838
1242.5278	1244.8589	1257.0314
1258.8451	1279.1663	1302.4857
1303.3053	1315.8218	1327.8662
1349.5949	1389.5455	1400.1306
1403.5103	1417.5577	1427.2807
1430.7258	1439.0088	1455.8059
1461.0999	1469.8416	1476.9881
1478.9742	1481.5979	1485.1110
1488.4309	1492.0286	1510.8297
1517.9246	1524.5792	1539.1454
1540.4019	1571.4642	1573.3611
1581.1506	1627.2797	1637.8654
1664.2578	1687.6467	1701.3461
1708.3553	1715.3035	1723.6936
1814.7797	3011.9195	3043.4193
3053.5070	3125.6762	3159.9634
3185.5971	3188.2791	3193.7024

H	-6.27996400	0.95555700	-0.00103800
H	-5.04243200	3.24364400	0.14869000
C	-2.50692500	-3.44474600	-0.67356400
H	-4.62202300	-3.60739900	-0.50688400
H	-6.12864600	-1.50003600	-0.23613300
H	-2.34290300	-4.51416200	-0.75831400
N	-1.71878300	1.33620500	-0.34335600
N	-1.56147900	-1.25360000	-0.59286500
O	2.47614100	-1.71003100	1.72466300
C	3.33879800	-0.69668900	2.17864100
H	4.36386600	-1.01913200	1.94410600
H	3.16656800	0.24229700	1.62542000
C	-0.45724300	3.39103500	-0.24158600
H	-0.51938800	4.46401000	-0.09933100
C	-0.05936300	-3.12094900	-0.87973100
H	0.01187200	-4.20116800	-0.93637000
H	1.57585800	-1.33023600	1.78655000
C	3.17482800	-0.43839400	3.67077600
H	3.41222800	-1.34483000	4.23699400
H	3.83415000	0.36985100	4.00966200
H	2.12974500	-0.17611400	3.86332400
O	-0.09369000	-0.48085500	3.43564500
C	-0.68445400	-0.24241500	2.36755100
O	-1.89043500	-0.13348300	2.10006100
O	0.25176600	-0.09167500	1.32378700

3195.1604	3200.4132	3201.4660
3214.6803	3216.2553	3218.0356
3218.5903	3219.5600	3219.9729
3221.4497	3223.3646	3624.8746

Statistical Thermodynamic Analysis

Temperature=403.15 K
Pressure =1 atm
Zero-point correction= 0.440599
Electronic Energy = -1781.63922635
Internal Energy (E)= -1781.14653035
Enthalpy (H)= -1781.14525335
Gibbs Free Energy (G)=-1781.29191235
Gibbs Free Energy of Solvation=-1781.92558115

St.Pt.	General Structure	Ball & Stick model
$TS1_{\beta\text{-}H}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.08919000	-3.66098200	-0.59414400
C	-3.37934900	-3.23440500	-0.58639300
C	-3.67771200	-1.83164500	-0.60556100
C	-2.56138700	-0.98134600	-0.62109300
C	-0.97921500	-2.73120900	-0.61549500
C	-4.96974600	-1.25289300	-0.61098800
C	-2.73578000	0.43510800	-0.64008500
C	-4.02492300	0.99040900	-0.63505800
C	-5.13859700	0.11666700	-0.62489400
C	-4.07782900	2.42134600	-0.64378000
H	-5.04509100	2.91751100	-0.64145600
C	-2.92801200	3.14779800	-0.63633400
C	-1.62872000	2.51281100	-0.62364200
H	-5.83632200	-1.90837500	-0.60013600
H	-1.85707100	-4.72098800	-0.57538600
H	-4.19709500	-3.95031300	-0.56226000
H	-6.13834700	0.54251600	-0.62535300
H	-2.95980600	4.23266100	-0.62339800
N	-1.27790800	-1.40827600	-0.62142600
N	-1.59278300	1.15863700	-0.65858900
Co	-0.05381700	0.03830100	-0.3690630
C	2.61313700	-0.35450300	-0.71428500
C	1.51543300	-2.42260200	-0.71854200

Frequencies

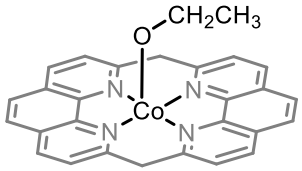
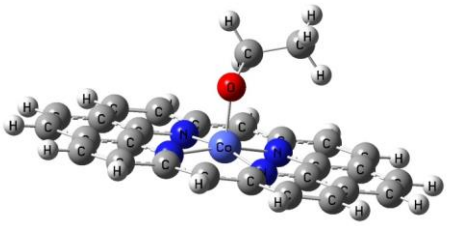
-302.1743	22.4894	37.3146
47.3178	51.6276	62.8059
68.9365	94.3377	106.8843
112.5409	124.8035	140.8861
157.2396	165.7974	175.3826
189.2359	210.4737	216.9521
237.2309	251.4706	256.6869
263.0141	271.7054	275.7796
288.0241	305.3497	331.9377
337.0584	349.4420	361.8875
382.6926	395.6382	405.3702
406.6051	446.0968	455.4988
457.7365	471.9609	479.3368
486.9825	487.1914	492.7092
494.9873	536.0652	552.0764
572.7051	586.3645	590.8555
595.1033	596.0456	616.4035
630.3779	654.0052	672.8328
676.4716	684.5647	705.3501
713.7840	716.4446	738.6335
745.9832	746.3999	759.4451
762.9370	766.5930	801.8634
816.3392	823.7501	825.0518
826.0709	829.2523	839.4303
851.0589	853.5501	857.8687
860.6936	867.5777	889.8971
907.6932	915.3779	921.4408
938.9812	944.5424	952.5181
960.0494	983.2738	989.8136
997.2339	1000.7096	1004.8093
1036.1447	1072.4172	1116.5335
1127.9971	1139.5840	1147.5387
1153.4429	1156.9244	1167.9827
1176.9831	1179.7898	1188.9186
1205.3451	1233.8853	1242.5798
1244.1016	1246.9351	1259.3778
1260.6359	1283.2716	1303.6408
1305.0160	1307.8654	1327.0402

C	2.44506900	1.06043500	-0.65389000
C	3.89615300	-0.91205900	-0.76474400
C	2.80477800	-3.06240900	-0.81566000
C	3.56079100	1.91138300	-0.65191200
C	5.01219900	-0.03769200	-0.76091200
C	3.95215600	-2.33938200	-0.84227600
H	2.83019300	-4.14673800	-0.82622300
C	3.26623200	3.30929700	-0.60469000
C	4.85258200	1.32925100	-0.70551200
C	0.87050500	2.81169500	-0.58193700
H	6.00958800	-0.46710100	-0.79927900
H	4.91935200	-2.83194900	-0.89223700
C	1.97466600	3.74036300	-0.57835800
H	4.08547600	4.02382500	-0.58966000
H	5.72147700	1.98149300	-0.69971900
H	1.74580600	4.80054200	-0.54213000
N	1.46864400	-1.07641900	-0.74412900
N	1.16278600	1.49582500	-0.61496300
O	-0.53107200	1.29528500	1.68693500
C	-1.72125400	1.09030000	2.34544600
H	-2.48727900	1.84770100	2.06128100
H	-2.18049200	0.10471800	2.09629600
C	0.33832100	-3.19747900	-0.66576500
H	0.47254100	-4.27323900	-0.64063100
C	-0.45937600	3.28231800	-0.58952400
H	-0.58831700	4.35913700	-0.55959000
H	0.16539500	0.06015700	1.96306300
C	-1.50694300	1.12040800	3.86230400
H	-1.13818700	2.10604500	4.16357300
H	-2.42912800	0.90190600	4.41618700
H	-0.73666500	0.38481300	4.11735400
O	1.71920700	-0.74363500	3.50904700
C	1.61286200	-1.30143200	2.40769600
O	2.30997900	-2.16495400	1.84562400
O	0.47073100	-0.87971100	1.66068500

1334.6272	1364.0272	1392.3736
1394.1610	1403.0261	1413.3114
1418.7231	1425.3660	1433.8350
1436.8688	1466.3598	1468.0986
1469.4120	1471.1809	1480.8938
1486.0900	1497.3783	1504.9440
1507.6192	1515.5243	1524.8660
1527.7554	1556.7328	1578.1111
1585.5301	1618.1994	1633.7732
1658.0983	1672.2197	1695.9834
1700.4805	1704.9806	1714.9915
1828.5108	2518.2550	2881.3875
2905.4128	3033.9151	3117.7219
3142.4533	3183.8220	3185.4926
3188.0790	3188.8849	3190.8980
3194.5167	3210.5051	3211.3421
3214.4840	3214.8821	3217.2803
3221.7227	3222.5956	3226.8717

Statistical Thermodynamic Analysis

Temperature=403.15 K	Pressure=1 atm
Zero-point correction= 0.436712	Electronic Energy = -1781.63922635
Internal Energy (E)= -1781.15145335	Enthalpy (H)= -1781.15017635
Gibbs Free Energy (G)=-1781.29374335	Gibbs Free Energy of Solvation=-1781.92741215

St. Point.	General Structure	Ball & Stick model
$I2_{\beta\text{-}H}$		

Cartesian coordinate

Atoms	X	Y	Z
C	2.60086	3.45682	-0.02758
C	3.81678	2.84881	-0.05344
C	3.91008	1.42216	-0.14126
C	2.69042	0.74206	-0.20304
C	1.37187	2.697	-0.09249
C	5.11562	0.66861	-0.16736
C	2.66557	-0.67922	-0.2746
C	3.85805	-1.40793	-0.29953
C	5.09138	-0.70239	-0.2466
C	3.71172	-2.82976	-0.37794
H	4.60079	-3.45396	-0.4023
C	2.4744	-3.3937	-0.41919
C	1.27607	-2.58735	-0.38074
H	6.06295	1.19775	-0.12347
H	2.52346	4.5362	0.04884
H	4.72803	3.4385	-0.00256
H	6.01829	-1.26755	-0.26773
H	2.35762	-4.47071	-0.47576

Frequencies

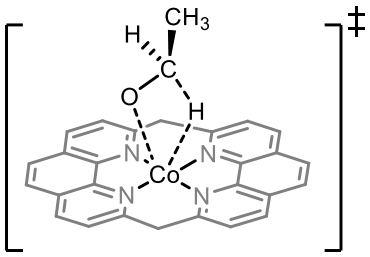
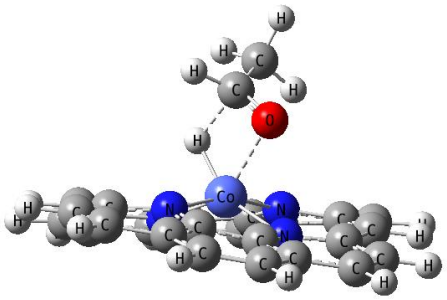
48.0894	60.1269	69.2892
76.7207	95.0908	120.7307
127.2776	132.3114	169.5865
187.4497	210.1555	218.2708
234.2724	249.6663	254.8493
257.7406	274.4765	280.1279
304.5799	318.2987	340.7718
347.4337	354.2285	384.8917
400.9060	406.5439	410.0409
434.7781	449.2930	461.4922
473.2296	478.3070	483.8341
486.3706	495.2656	496.9473
540.2646	557.2857	584.3483
585.9247	596.0417	596.3464
601.3084	608.9938	626.8071
680.6048	687.1125	689.7760
712.7308	716.7610	720.3470
743.8607	744.7817	751.7917
758.4698	766.5429	767.9801
798.4472	815.0668	820.8864
825.9123	829.4720	855.8644
861.6456	864.5572	867.7535
870.9824	878.0582	908.7602
919.5769	922.4538	942.7592
949.2150	971.9395	973.0510
1011.7704	1013.1818	1014.0382
1017.5873	1018.1084	1044.8251
1099.2792	1121.4760	1136.2954
1143.6523	1160.3594	1163.7154
1169.5190	1173.1579	1177.0765
1182.7175	1185.7258	1235.3664
1241.0955	1245.2521	1248.4061

N	1.47585	1.35499	-0.2039
N	1.42712	-1.24659	-0.31732
Co	0.06192	0.07453	-0.08634
C	-2.52924	0.8478	-0.33926
C	-1.13866	2.74769	-0.15121
C	-2.55759	-0.5722	-0.41549
C	-3.72148	1.57732	-0.33906
C	-2.33813	3.55662	-0.14916
C	-3.77562	-1.25274	-0.49145
C	-4.95319	0.87387	-0.42738
C	-3.5745	2.99902	-0.24008
H	-2.22075	4.63198	-0.06683
C	-3.6826	-2.68166	-0.5377
C	-4.98034	-0.49777	-0.502
C	-1.2395	-2.53611	-0.42889
H	-5.8792	1.44103	-0.43163
H	-4.46231	3.62532	-0.2337
C	-2.46866	-3.29405	-0.5085
H	-4.59382	-3.2711	-0.59209
H	-5.92749	-1.02493	-0.56586
H	-2.39347	-4.37575	-0.54007
N	-1.29169	1.40964	-0.26479
N	-1.34024	-1.18809	-0.38463
O	0.08188	0.14414	1.73463
C	-0.15076	-1.02745	2.45524
H	0.51954	-1.00643	3.33048
H	0.12593	-1.933	1.88973
C	0.12712	3.35002	-0.05554
H	0.14686	4.42993	0.03221
C	0.00405	-3.19312	-0.40196
H	-0.01775	-4.276	-0.4378
C	-1.59348	-1.15604	2.93508
H	-1.70859	-2.022	3.59574
H	-1.88367	-0.25702	3.48545
H	-2.28214	-1.27511	2.09322

1258.7366	1259.2478	1279.0274
1301.5028	1304.8074	1322.2752
1330.8892	1388.0743	1391.1005
1398.9677	1420.9177	1421.6173
1428.6937	1435.6525	1455.8844
1460.0989	1466.9856	1476.5086
1482.5175	1483.9766	1485.9878
1487.2218	1495.5119	1499.7403
1515.9426	1521.3595	1536.5409
1571.7394	1573.0089	1578.2092
1628.5736	1637.8713	1663.4661
1684.6426	1703.0731	1705.6853
1713.5316	1723.0758	3003.1851
3036.8011	3061.1295	3138.4145
3155.4073	3200.6954	3202.3947
3207.9390	3208.6529	3215.8406
3217.0286	3218.6167	3219.6409
3224.0022	3227.3139	3230.2840
3233.1601	3233.3698	3234.7155

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.412968	Electronic Energy = -1517.27794481
Internal Energy (E) = -1516.82107581	Enthalpy (H) = -1516.81979881
Gibbs Free Energy (G) = -1516.94483381	Gibbs Free Energy of Solvation = -1516.96123418

St. Point	General Structure	Ball & Stick model
$TS2_{\beta\text{-}H}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-2.34043	-3.40742	-0.70281
C	-3.57295	-2.84741	-0.83355
C	-3.7421	-1.43844	-0.66915
C	-2.57213	-0.715	-0.41533
C	-1.17236	-2.60265	-0.4311
C	-4.98672	-0.74789	-0.72901
C	-2.6445	0.68753	-0.16902
C	-3.86595	1.35893	-0.27538
C	-5.04609	0.60848	-0.54938
C	-3.80953	2.779	-0.11541
H	-4.73015	3.3553	-0.15357
C	-2.60986	3.40422	0.02721
C	-1.37667	2.65418	0.07236
H	-5.88994	-1.31706	-0.92824
H	-2.20567	-4.47977	-0.79763
H	-4.44113	-3.46629	-1.04426

Frequencies

-422.6225	45.8138	59.7434
61.5145	67.5513	97.8821
110.9663	125.2925	153.6859
165.8689	202.1548	203.4776
207.7767	225.9279	247.1280
250.1343	255.0590	267.1302
268.4260	290.7691	323.9920
331.5621	340.2559	374.4936
380.1285	397.5746	403.0641
429.1373	445.1155	457.9594
460.8889	462.3691	470.9448
488.0528	489.7880	493.5863
508.0020	538.1700	554.0692
581.7656	586.3870	591.0206
595.1513	597.8066	611.1024
623.8296	674.0662	682.1631
683.3547	710.9276	712.5432
720.2022	726.7222	737.5890
742.4473	751.6120	757.0217
765.7450	788.6829	807.8828
809.2090	817.1224	820.8962
847.9341	854.3539	857.9835
860.9254	864.7028	871.3842
909.5480	921.6058	928.4424
933.5999	944.6302	964.7155
968.4684	989.6053	1005.3077
1009.1728	1009.9121	1010.2631
1012.3829	1037.9759	1116.6885
1132.0559	1135.9257	1140.7016
1153.5492	1167.0946	1168.3357

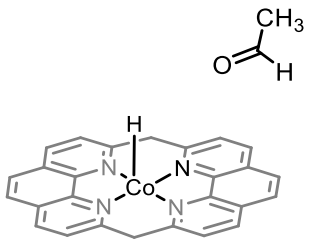
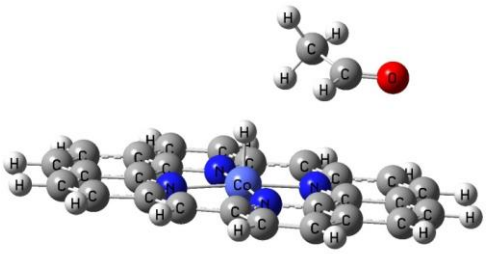
H	-5.99482	1.13282	-0.61471
H	-2.54777	4.48594	0.08139
N	-1.33056	-1.26763	-0.37229
N	-1.46351	1.30974	0.11559
Co	-0.00701	0.04648	0.34604
C	2.59204	-0.6002	-0.28881
C	1.31327	-2.57172	-0.14183
C	2.5154	0.80996	-0.4389
C	3.80778	-1.2616	-0.48403
C	2.55244	-3.31738	-0.25772
C	3.66875	1.55435	-0.69964
C	4.97138	-0.49498	-0.76533
C	3.74954	-2.69263	-0.39981
H	2.48788	-4.40049	-0.2618
C	3.48827	2.97334	-0.76816
C	4.90589	0.87256	-0.86246
C	1.10007	2.70098	-0.27563
H	5.91627	-1.01099	-0.90763
H	4.66577	-3.26895	-0.49661
C	2.26377	3.51769	-0.55068
H	4.34453	3.60856	-0.9784
H	5.79826	1.45332	-1.07557
H	2.1224	4.59291	-0.574
N	1.41701	-1.22798	0.00813
N	1.26764	1.35644	-0.30458
O	-0.79943	-0.82918	2.15518
C	0.0112	-0.06373	2.72844
H	-0.35773	0.89681	3.135
H	0.63821	0.72482	1.51242
C	0.08286	-3.22613	-0.25137
H	0.10683	-4.30637	-0.33183
C	-0.13295	3.31294	-0.00345
H	-0.15074	4.39596	-0.00823
C	1.30788	-0.58646	3.30715
H	2.04438	0.21032	3.43243

1179.5503	1181.9524	1202.9809
1230.6800	1236.2253	1242.6591
1245.7777	1255.9204	1257.4020
1274.1196	1296.8475	1300.3316
1326.9646	1375.8842	1386.0343
1397.0732	1410.7356	1412.3197
1414.0707	1423.0214	1447.5362
1450.8654	1470.6209	1473.6079
1478.5379	1481.7862	1483.4378
1485.3783	1487.0473	1491.2971
1522.3788	1537.5497	1568.8532
1575.9795	1580.3674	1591.9280
1623.0384	1638.9789	1663.3552
1689.7813	1697.2732	1706.7240
1713.7800	1721.0515	1750.0994
3001.2512	3070.9289	3153.8344
3183.6023	3198.2220	3199.1409
3203.0955	3204.5797	3204.7548
3205.0958	3216.1549	3220.7534
3222.4129	3224.2872	3225.3224
3228.1169	3229.9215	3231.1351

H	1.08777	-1.01262	4.29164	
H	1.70646	-1.37295	2.66374	

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.405907
Electronic Energy = -1517.20905031
Internal Energy (E) = -1516.75902531
Enthalpy (H) = -1516.75774931
Gibbs Free Energy (G) = -1516.88349231
Gibbs Free Energy of Solvation = -1516.89740641

St. Point	General Structure	Ball & Stick model
$I3_{\beta\text{-}H}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-2.56816	-2.92756	-0.88582
C	-3.73089	-2.22245	-0.89379
C	-3.71862	-0.80289	-0.70804
C	-2.45849	-0.2296	-0.52906
C	-1.29096	-2.28048	-0.68998
C	-4.86223	0.04266	-0.69101
C	-2.32618	1.17368	-0.335
C	-3.45772	1.9931	-0.3177
C	-4.73618	1.39674	-0.50126
C	-3.20492	3.3878	-0.11195
H	-4.04193	4.08026	-0.0859
C	-1.93259	3.84105	0.05067
C	-0.79799	2.94448	0.02296

Frequencies

33.6697	47.1846	53.3071
60.4957	69.4022	101.8097
109.0813	124.2894	133.4176
157.0282	164.8441	183.9590
220.1171	243.0776	244.7602
249.1575	257.3979	258.9102
263.9101	283.9492	304.3191
338.2252	339.8081	351.1659
384.6871	405.3109	407.5993
410.8968	449.1808	461.9743
462.8057	478.2854	487.6119
487.8725	493.9356	496.3322
509.0317	538.5311	559.6665
584.8715	587.0070	596.6118
599.0151	600.7636	628.0707
680.4137	688.3162	689.2268
712.5953	714.2714	717.5887
723.9746	740.6840	745.2943
750.3327	752.7034	764.2181
766.9818	777.4371	804.2462
818.6019	823.7357	829.3477
832.7708	853.5889	862.3120
865.2542	869.8866	871.1246
877.2976	908.1146	908.6812
921.0509	945.2873	953.1647
977.0981	981.7229	1010.3708

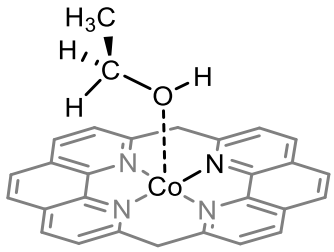
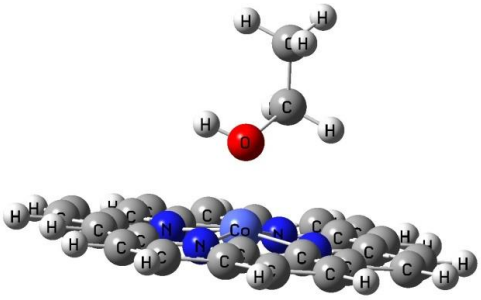
H	-5.84285	-0.4031	-0.82678
H	-2.57375	-4.00421	-1.0171
H	-4.68121	-2.73076	-1.02927
H	-5.61633	2.03259	-0.48868
H	-1.73775	4.8965	0.20883
N	-1.29091	-0.93885	-0.5188
N	-1.05002	1.6305	-0.17595
Co	0.20179	0.19779	-0.18013
C	2.74165	-0.75836	-0.22332
C	1.20943	-2.53541	-0.53696
C	2.87362	0.64695	-0.03981
C	3.87464	-1.57468	-0.2628
C	2.34661	-3.42975	-0.58361
C	4.13795	1.22338	0.10544
C	5.15584	-0.97469	-0.11758
C	3.62049	-2.97247	-0.45294
H	2.15083	-4.487	-0.72827
C	4.14908	2.64493	0.28782
C	5.28328	0.38141	0.06143
C	1.70119	2.69307	0.15838
H	6.03708	-1.60836	-0.15017
H	4.45839	-3.66327	-0.49207
C	2.98378	3.34527	0.31383
H	5.10039	3.15637	0.40727
H	6.26623	0.82973	0.17145
H	2.98876	4.42091	0.45502
N	1.46369	-1.21768	-0.35555
N	1.70606	1.35208	-0.02262
O	-3.1764	-2.01635	2.21475
C	-2.09816	-1.50714	2.40284
H	-1.97388	-0.40548	2.31797
H	0.11901	0.06007	1.19264
C	-0.09841	-3.03277	-0.67908

1011.2123	1012.7877	1013.2323
1013.7848	1043.4386	1117.9448
1134.7707	1139.3416	1145.7254
1152.1422	1158.8126	1171.3189
1172.2337	1183.5293	1185.5747
1233.9789	1238.9365	1243.9897
1247.0458	1259.8455	1260.8899
1277.9152	1300.7340	1303.6246
1330.5753	1384.5289	1392.6889
1396.0283	1417.9498	1424.8402
1429.8596	1438.8823	1453.2942
1460.3436	1467.3510	1472.7303
1478.3675	1480.8884	1481.3187
1483.4483	1483.8922	1486.4864
1520.2996	1534.4093	1572.1185
1573.0963	1579.4002	1627.6667
1636.8778	1658.7008	1684.8405
1699.7046	1707.8297	1712.6988
1720.3997	1888.1332	2147.8499
2972.5244	3070.7866	3146.6925
3187.0051	3200.1926	3200.5840
3204.4762	3210.3872	3215.3983
3219.5130	3222.6196	3223.3297
3226.0656	3227.0370	3228.6185
3230.3999	3231.9371	3236.5863

H	-0.19949	-4.10296	-0.8165
C	0.50959	3.43904	0.18934
H	0.60909	4.50743	0.3409
C	-0.85272	-2.27483	2.75065
H	-0.10566	-2.13173	1.96166
H	-0.42622	-1.88661	3.68138
H	-1.08728	-3.33505	2.85145

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.407941
Electronic Energy = -1517.26912963
Internal Energy (E) = -1516.81587963
Enthalpy (H)= -1516.81460363
Gibbs Free Energy (G) = -1516.94483463
Gibbs Free Energy of Solvation=-1516.95870052

St. Point	General Structure	Ball & Stick model
$I1_{MLC}$		

Cartesian coordinate

Atoms	X	Y	Z
C	2.42045	3.52614	-0.15707
C	3.65098	2.95293	-0.23736
C	3.77933	1.5289	-0.3343
C	2.57614	0.80905	-0.34714
C	1.21443	2.73089	-0.16835
C	4.99524	0.80923	-0.41948
C	2.58457	-0.60833	-0.43867

Frequencies

26.9069	47.8395	55.9897
63.3606	90.3622	94.7301
119.4298	129.2714	160.9827
173.2442	182.6471	207.6631
214.2182	248.3156	252.9137
254.9044	255.2832	273.1618
275.5314	294.9600	312.7221
334.7043	343.1989	353.2920
384.5808	406.9965	408.6448
410.6131	447.5699	455.2321
460.6829	486.2095	487.0598
488.6215	492.6474	495.6068
541.0466	541.6933	556.5407
579.7173	584.3679	586.6097
587.3271	594.5713	597.9705
623.3227	678.2511	686.1919

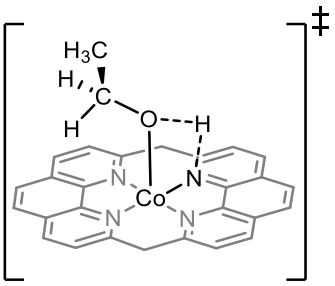
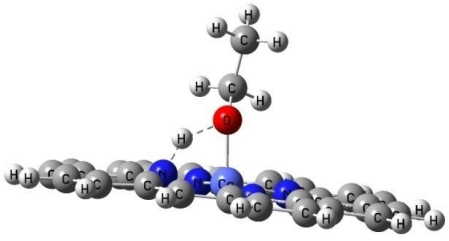
C	3.79764	-1.30803	-0.51149
C	5.00416	-0.56751	-0.50449
C	3.68868	-2.7346	-0.59255
H	4.59156	-3.33464	-0.65555
C	2.46532	-3.32857	-0.58871
C	1.24923	-2.55353	-0.50367
H	5.93058	1.35979	-0.42001
H	2.31474	4.60276	-0.08173
H	4.54554	3.56831	-0.22849
H	5.94684	-1.10129	-0.5718
H	2.37346	-4.40747	-0.64786
N	1.34392	1.38424	-0.27793
N	1.35904	-1.20244	-0.44451
Co	-0.0255	0.06687	-0.11188
C	-2.63766	0.77117	-0.29701
C	-1.30452	2.71108	-0.14873
C	-2.62788	-0.64749	-0.37957
C	-3.85081	1.47264	-0.26012
C	-2.51911	3.48925	-0.1134
C	-3.83144	-1.36461	-0.43026
C	-5.05863	0.73434	-0.3193
C	-3.743	2.89723	-0.16895
H	-2.42788	4.56719	-0.03857
C	-3.70459	-2.7879	-0.51271
C	-5.04928	-0.64125	-0.40233
C	-1.26888	-2.57278	-0.46967
H	-6.00156	1.27154	-0.30172
H	-4.64639	3.49908	-0.1423
C	-2.47267	-3.36572	-0.53145
H	-4.59997	-3.40053	-0.5586
H	-5.98486	-1.18935	-0.45056
H	-2.36669	-4.44316	-0.59269
N	-1.41521	1.36573	-0.2615

686.7584	715.6645	716.4481
718.8304	745.9621	747.6736
763.4168	767.0974	791.2613
793.9336	821.2797	822.2796
826.2571	832.6694	851.4743
862.8580	863.8911	865.2955
884.2825	885.1649	896.3315
907.3625	909.0267	922.3285
943.1804	950.2278	992.1144
992.4453	1009.8314	1023.9169
1025.7198	1028.0556	1029.8753
1040.4670	1079.6512	1101.2464
1125.3948	1133.3507	1147.9907
1148.3144	1162.4681	1165.7377
1179.7335	1187.4677	1191.0890
1238.7853	1244.7738	1251.0983
1254.4930	1265.5767	1266.2281
1283.4596	1287.9366	1304.6472
1307.9333	1337.9583	1369.4294
1391.9511	1400.8360	1415.0790
1420.7092	1429.1647	1431.1828
1444.0940	1449.2134	1460.1518
1464.9166	1465.6368	1470.0044
1479.3743	1485.0064	1496.7882
1500.4396	1508.8058	1515.6642
1520.0271	1530.7743	1554.7111
1576.2170	1583.2033	1624.1229
1628.0655	1660.0225	1673.0654
1698.8236	1701.4656	1705.8268
1717.4608	3074.9482	3083.9933
3148.8662	3165.6914	3178.7246
3211.9626	3213.0428	3222.8350
3225.9001	3226.6142	3226.6704
3228.9681	3229.1102	3230.8111
3233.9235	3241.9186	3242.9249
3244.8313	3245.9007	3845.5872

N	-1.39701	-1.22576	-0.40593
O	-0.07866	0.01952	1.85916
C	0.52584	-1.09621	2.55894
H	0.09711	-1.98296	2.08569
H	1.60609	-1.08884	2.37434
C	-0.0475	3.34205	-0.07622
H	-0.05502	4.42202	0.01436
C	-0.003	-3.19033	-0.48454
H	0.00477	-4.27308	-0.53334
H	0.23506	0.85522	2.23468
C	0.19467	-1.0246	4.03301
H	0.61191	-0.12187	4.48955
H	-0.88598	-1.03169	4.18675
H	0.62682	-1.88572	4.54789

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.426341
Electronic Energy = -1517.69317386
Internal Energy (E) = -1517.22187286
Enthalpy (H) = -1517.22059586
Gibbs Free Energy (G) = -1517.34955186
Gibbs Free Energy of Solvation = -1517.40472741

St. Point	General Structure	Ball & Stick model
$TS1_{MLC}$		

Cartesian coordinate

Atoms	X	Y	Z
C	2.47214	3.50404	-0.24889
C	3.68318	2.9018	-0.29408

Frequencies

-491.0748	44.9927	51.5402
62.8253	70.0469	94.0549
113.6647	127.9371	159.3376
163.9387	210.5636	213.7695
220.7964	242.5285	252.2019
253.2344	257.3910	271.8173
279.1342	297.6389	322.0262

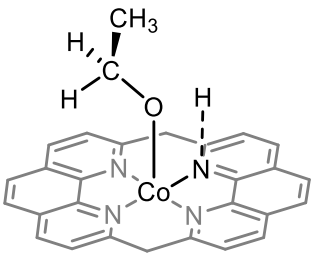
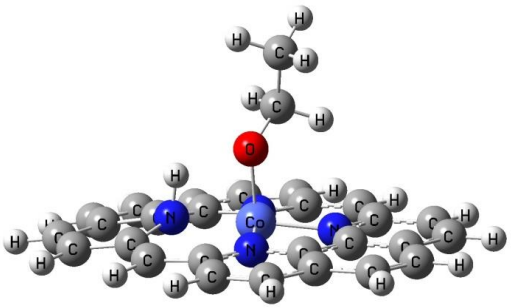
C	3.80672	1.45351	-0.3211
C	2.62879	0.7354	-0.21314
C	1.23461	2.74681	-0.16121
C	5.01041	0.73072	-0.49418
C	2.59119	-0.65874	-0.34856
C	3.79039	-1.37466	-0.47905
C	5.0015	-0.64878	-0.54851
C	3.66302	-2.80265	-0.55026
H	4.55786	-3.41109	-0.64084
C	2.4377	-3.38476	-0.49521
C	1.22525	-2.59973	-0.39853
H	5.94563	1.27388	-0.58314
H	2.38989	4.58446	-0.29547
H	4.58586	3.50165	-0.35718
H	5.93284	-1.19326	-0.66733
H	2.33431	-4.46328	-0.53474
N	1.38181	1.35645	0.04485
N	1.34433	-1.25053	-0.36458
Co	-0.04079	0.00135	-0.12664
C	-2.64005	0.75796	-0.30234
C	-1.29293	2.67977	-0.22691
C	-2.63886	-0.66339	-0.34094
C	-3.84461	1.47247	-0.30917
C	-2.48209	3.47163	-0.23266
C	-3.83907	-1.36708	-0.39658
C	-5.06716	0.73929	-0.36235
C	-3.7209	2.88709	-0.27026
H	-2.38207	4.55053	-0.20162
C	-3.72535	-2.79575	-0.43343
C	-5.06095	-0.63029	-0.40492
C	-1.28552	-2.609	-0.36133
H	-6.00505	1.28473	-0.37192
H	-4.61539	3.5029	-0.27056

336.8191	346.3038	349.1275
386.1981	399.1407	403.7877
411.2154	444.9578	453.9754
469.5332	476.1675	482.1740
486.4392	491.4827	497.2441
538.9705	549.4366	575.3480
578.9817	588.4550	595.6707
598.4126	600.9950	620.5088
657.3699	680.5948	687.4683
694.2124	714.1347	715.8364
722.5252	745.5437	753.8112
760.2971	764.7071	783.6736
795.0081	816.5443	824.6253
826.3734	832.9875	851.1275
855.7326	862.8708	865.4404
881.2042	886.2388	895.7849
902.8532	916.6682	929.3797
946.9239	953.8886	988.3785
998.8949	1001.0131	1020.6742
1022.7650	1027.5533	1033.1827
1038.4732	1099.3066	1115.7732
1127.5357	1142.3852	1148.5968
1159.2917	1174.6699	1181.9426
1184.4390	1185.7441	1191.0385
1227.5162	1244.2107	1246.3394
1248.8670	1260.2507	1261.1774
1273.9742	1279.8847	1299.9716
1314.6613	1328.3930	1350.1050
1391.2200	1400.9583	1415.3406
1420.5853	1425.8011	1431.3503
1445.4386	1450.5681	1457.0329
1460.2832	1475.5999	1481.1184
1485.0744	1496.9248	1508.9162
1509.8453	1525.9334	1531.0899
1535.9675	1548.8839	1569.7074
1578.8896	1618.3327	1637.1828
1653.8501	1674.1611	1691.3697
1702.5312	1705.4017	1715.7942
1726.9570	1880.9654	3041.3487
3081.8958	3091.6948	3169.2147
3175.3325	3212.8066	3215.3451
3218.6329	3224.6507	3226.3540
3226.7241	3228.1929	3229.4186
3233.7395	3234.1548	3241.2360
3241.4528	3243.1463	3246.8826

C	-2.50091	-3.38748	-0.41663
H	-4.6263	-3.40034	-0.47392
H	-5.99698	-1.1783	-0.44493
H	-2.4069	-4.46728	-0.44444
N	-1.41664	1.34828	-0.27149
N	-1.40909	-1.26094	-0.32527
O	0.0313	0.25829	1.7054
C	0.42304	-0.85876	2.49538
H	-0.10947	-1.75656	2.15233
H	1.50083	-1.04813	2.38796
C	0.00099	3.32953	-0.20279
H	-0.02211	4.4127	-0.24522
C	-0.02703	-3.23518	-0.36293
H	-0.02377	-4.31788	-0.39423
H	1.02601	1.07894	1.1007
C	0.07339	-0.55488	3.94204
H	0.60068	0.33858	4.28356
H	-1.00048	-0.38628	4.04429
H	0.3614	-1.39492	4.57937

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.422434
Electronic Energy = -1517.64298742
Internal Energy (E) = -1517.17689042
Enthalpy (H) = -1517.17561342
Gibbs Free Energy (G) =-1517.30055442
Gibbs Free Energy of Solvation = -1517.35591974

St. Point	General Structure	Ball & Stick model
$I2_{MLC}$		

Cartesian coordinate

Atoms	X	Y	Z
C	2.53906	3.51767	-0.18831
C	3.74282	2.9044	-0.21472
C	3.85225	1.4506	-0.24198
C	2.67907	0.73338	-0.10879
C	1.29185	2.7736	-0.09769
C	5.04608	0.72864	-0.46731
C	2.62148	-0.6525	-0.27919
C	3.81401	-1.37033	-0.46964
C	5.02531	-0.65019	-0.55305
C	3.67769	-2.7947	-0.59164
H	4.56816	-3.40295	-0.71926
C	2.44995	-3.37072	-0.55007
C	1.24228	-2.58203	-0.41512
H	5.9807	1.26888	-0.57638
H	2.46638	4.59779	-0.25705
H	4.65214	3.49336	-0.28145
H	5.94927	-1.19671	-0.7143
H	2.33877	-4.44551	-0.63998
N	1.42859	1.37301	0.20615
N	1.37248	-1.23907	-0.29098
Co	-0.00816	0.01666	-0.04631
C	-2.59714	0.80496	-0.30551
C	-1.24527	2.71238	-0.20229
C	-2.60327	-0.61784	-0.38542
C	-3.79674	1.53174	-0.34285
C	-2.41771	3.51766	-0.23622
C	-3.8076	-1.30583	-0.4985
C	-5.02482	0.80962	-0.44353
C	-3.66367	2.9412	-0.29389

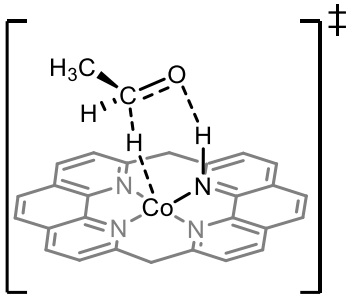
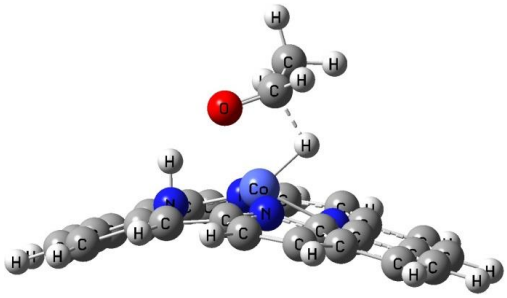
Frequencies

45.6291	52.0657	61.3413
70.7177	95.2555	101.8566
125.4697	150.3844	161.2192
201.0247	209.1187	214.3410
223.0085	242.3295	248.2169
253.2277	267.5305	275.3698
293.2668	308.5214	325.1853
336.9462	343.7421	353.6238
381.0793	396.4399	404.9290
412.9313	448.6113	452.1819
461.2986	477.7629	482.3426
484.4714	490.7069	507.9662
536.2247	550.9550	567.0044
583.4337	588.3446	593.5570
600.4676	619.7382	653.6330
670.3900	679.9190	689.4738
708.2268	710.7482	718.4901
724.4277	744.0048	758.8174
764.0992	774.1669	787.5950
812.5651	824.3850	831.1091
832.2180	845.3061	849.9695
860.8619	863.7925	876.4844
880.7716	884.1641	914.1749
915.1072	924.8032	943.1715
951.9960	975.5430	988.4840
1000.8250	1003.4063	1017.2025
1019.5465	1023.6257	1031.8831
1034.2564	1089.0501	1109.6828
1124.6340	1145.6593	1157.0158
1158.0425	1174.5692	1180.8100
1182.4999	1190.1857	1190.6343
1222.8462	1237.7703	1243.6038
1246.7353	1260.0978	1261.5158
1270.5675	1273.5862	1295.9680
1313.3443	1325.0235	1343.0520
1385.2759	1400.7875	1408.4903
1411.7006	1419.4734	1420.6715
1442.3304	1444.4869	1449.8218
1455.9146	1459.2516	1478.0470
1480.6680	1488.8296	1493.5903
1511.4978	1514.6104	1532.7658
1541.0209	1548.2815	1571.1847
1581.6393	1629.6713	1644.2237
1656.9634	1681.5721	1693.9909
1700.6652	1709.1011	1717.6238
1733.6900	3012.7164	3068.9877
3080.3147	3168.9524	3171.1748
3209.4400	3211.9023	3212.7049
3215.2125	3220.0866	3221.2104
3225.2951	3226.2511	3230.9140
3233.4460	3237.9151	3241.9963

H	-2.30931	4.59596	-0.21311	3242.6770	3245.0667	3245.9249
C	-3.70604	-2.73259	-0.58834			
C	-5.02458	-0.55698	-0.51757			
C	-1.26702	-2.57035	-0.45349			
H	-5.95795	1.36246	-0.46744			
H	-4.55283	3.56445	-0.31252			
C	-2.48676	-3.33511	-0.5686			
H	-4.61109	-3.32656	-0.67293			
H	-5.96286	-1.09705	-0.59736			
H	-2.401	-4.41389	-0.63677			
N	-1.37538	1.38577	-0.2266			
N	-1.38123	-1.22494	-0.36745			
O	-0.17067	0.09081	1.7631			
C	0.11393	-1.09142	2.47646			
H	-0.37454	-1.96204	2.01463			
H	1.19671	-1.29393	2.49391			
C	0.06868	3.34959	-0.19009			
H	0.05354	4.42994	-0.29273			
C	-0.01341	-3.20829	-0.44456			
H	-0.01727	-4.28791	-0.53065			
H	1.2486	1.25951	1.22394			
C	-0.40773	-0.90474	3.89483			
H	0.06828	-0.04158	4.36513			
H	-1.48723	-0.74151	3.88106			
H	-0.19007	-1.79317	4.4933			

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.426055
Electronic Energy = -1517.64521591
Internal Energy (E) = -1517.17476191
Enthalpy (H) = -1517.17348591
Gibbs Free Energy (G) = -1517.30003791
Gibbs Free Energy of Solvation = -1517.35699537

St. Point	General Structure	Ball & Stick model
$TS2_{MLC}$		

Cartesian coordinate

Atoms	X	Y	Z
C	2.22961	3.60613	-0.60976
C	3.4277	3.03296	-0.86607
C	3.63147	1.5985	-0.73926
C	2.56446	0.84612	-0.2789
C	1.09558	2.82913	-0.15092
C	4.82526	0.9261	-1.08231
C	2.59527	-0.5528	-0.20687
C	3.79045	-1.21171	-0.55798
C	4.90249	-0.4464	-0.97145
C	3.75361	-2.64506	-0.53817
H	4.66416	-3.2034	-0.73358
C	2.57325	-3.28545	-0.35079
C	1.34381	-2.54907	-0.14698
H	5.67503	1.49889	-1.43867
H	2.07568	4.66849	-0.76463
H	4.25734	3.64127	-1.21278
H	5.81764	-0.96396	-1.24174
H	2.50873	-4.36619	-0.41253
N	1.35687	1.464	0.16933
N	1.4271	-1.22062	0.0991
Co	-0.07039	-0.0585	0.52123

Frequencies

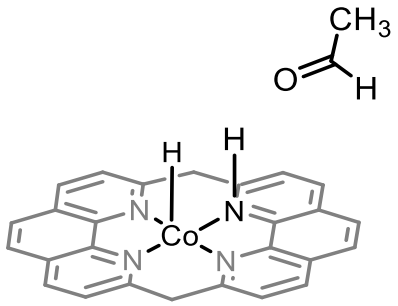
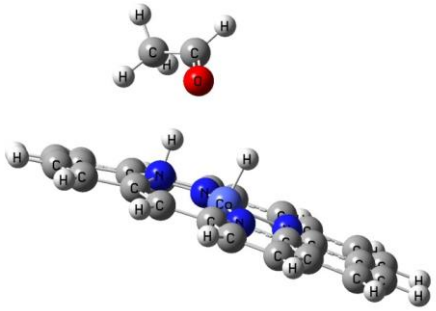
-396.4084	46.5312	53.7100
57.7334	74.1757	94.8006
114.3984	126.7765	144.6178
169.8674	199.6672	205.3921
213.2953	220.7477	236.0631
241.8393	251.3341	260.6167
269.9634	289.0643	320.8748
328.3707	335.3726	350.8343
381.8266	395.1608	397.7623
437.3878	442.0980	445.4839
458.6071	461.4549	472.1662
482.6448	485.6088	487.6987
497.1213	531.3851	545.3669
568.2948	577.2518	586.5172
588.1961	593.7234	595.0088
619.5030	652.1101	666.3433
678.5731	704.1935	707.3941
714.9348	718.9647	731.7122
753.2962	760.9753	770.0711
782.6888	784.3466	805.8839
821.6482	822.3717	835.4108
845.1884	852.9244	860.2266
872.6674	878.9294	881.6408
905.0770	914.9868	917.5290
942.2464	944.2455	981.3027
987.6541	998.6506	998.7851
1017.8048	1020.5324	1023.1019
1026.5993	1027.6339	1058.8892
1106.5062	1132.9831	1135.9678
1141.7808	1151.3902	1173.9131
1180.7891	1183.1549	1190.0308
1224.7558	1233.2596	1240.1209
1245.6183	1250.4412	1260.9447
1262.2282	1275.6099	1275.9698
1297.2499	1324.1744	1344.7335
1374.5739	1391.8229	1393.5517
1401.1008	1414.4898	1423.1949
1432.4325	1440.1317	1445.1293
1457.0510	1463.8627	1471.6909

C	-2.6419	0.68773	-0.17018
C	-1.40232	2.63131	0.18243
C	-2.54612	-0.69948	-0.473
C	-3.85751	1.36892	-0.34366
C	-2.60856	3.38987	0.06746
C	-3.68395	-1.41093	-0.85497
C	-5.01086	0.62776	-0.7304
C	-3.81127	2.77441	-0.14902
H	-2.5437	4.47039	0.12736
C	-3.49611	-2.81096	-1.09214
C	-4.92298	-0.71816	-0.96905
C	-1.12587	-2.59283	-0.5131
H	-5.95565	1.14835	-0.84527
H	-4.72293	3.35904	-0.23033
C	-2.27313	-3.37458	-0.91505
H	-4.34338	-3.41754	-1.39738
H	-5.80406	-1.27873	-1.26545
H	-2.12414	-4.43741	-1.06946
N	-1.47916	1.2944	0.20453
N	-1.3036	-1.25542	-0.37314
O	0.47846	0.54248	2.43817
C	-0.21322	-0.45978	2.80871
H	-1.23358	-0.26352	3.18061
H	-0.75935	-0.95946	1.51422
C	-0.14286	3.34624	0.07117
H	-0.24047	4.42181	-0.03285
C	0.11448	-3.21199	-0.2967
H	0.15236	-4.28424	-0.4421
H	1.3933	1.44448	1.19576
C	0.45314	-1.72237	3.29228
H	0.70225	-1.57206	4.34817
H	-0.21189	-2.58453	3.21677
H	1.37367	-1.90048	2.73481

1471.9070	1479.5629	1483.4237
1486.9651	1507.0740	1530.3455
1536.5976	1571.6367	1573.6291
1579.0210	1612.8378	1635.3431
1649.4898	1675.0218	1685.9335
1697.9603	1703.5042	1714.8606
1726.5522	1734.4623	3060.2666
3076.4491	3160.8342	3193.4542
3215.2072	3217.1838	3220.5337
3220.8005	3222.2071	3226.2306
3227.7587	3230.2241	3237.3596
3237.9368	3238.6919	3241.8526
3243.4078	3244.2952	3362.5059

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.419634	Electronic Energy = -1517.57993126
Internal Energy (E) = -1517.11583326	Enthalpy (H) = -1517.11455726
Gibbs Free Energy (G) =-1517.24105826	Gibbs Free Energy of Solvation = -1517.29455297

St. Point	General Structure	Ball & Stick model
$I3_{MLC}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-2.1414	-3.49698	-0.6084
C	-3.34291	-2.90499	-0.78537
C	-3.48166	-1.45335	-0.7747
C	-2.35374	-0.72087	-0.45724
C	-0.93607	-2.73192	-0.32448
C	-4.65692	-0.74543	-1.11739
C	-2.31538	0.67547	-0.52972
C	-3.49312	1.37642	-0.84605
C	-4.66202	0.63738	-1.12869
C	-3.37936	2.80871	-0.8663
H	-4.25889	3.40751	-1.08379
C	-2.18214	3.40287	-0.63135
C	-0.97927	2.63056	-0.38345
H	-5.55366	-1.29862	-1.37653
H	-2.03558	-4.57252	-0.70354

Frequencies

32.9647	38.0711	53.5433
64.3766	74.4267	91.6692
102.7363	123.8873	144.7224
149.8913	158.0577	189.0358
211.9229	220.6222	239.1235
247.0716	248.0548	254.2074
266.1930	275.8071	313.0521
327.4416	338.0065	344.9099
375.4063	393.6290	400.7625
407.7793	447.0732	453.8710
458.9729	473.2078	481.2571
484.3658	491.8303	503.2080
519.5413	536.1897	552.7512
565.8753	584.0177	589.8366
594.0656	602.3433	622.3925
659.0343	671.2826	686.2934
705.0923	711.6131	717.4178
722.7801	734.4668	742.4916
757.7636	766.2319	772.1669
780.3497	790.1878	811.4758
823.9789	827.9661	835.6794
846.6690	852.2770	863.9178
866.3129	882.8855	884.0798
885.6634	914.2924	916.8740
918.5342	927.9476	953.8815
992.7229	993.6618	999.6509
1017.9335	1023.0034	1027.1365
1030.3943	1033.6696	1098.2260

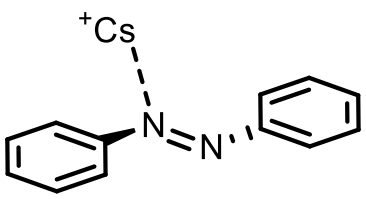
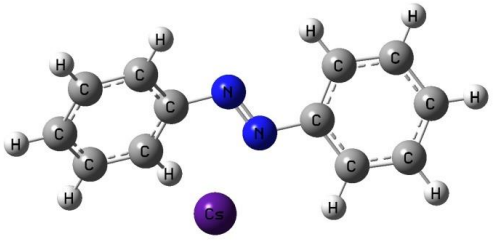
H	-4.21953	-3.50711	-1.00282
H	-5.5709	1.17355	-1.38415
H	-2.08783	4.48292	-0.65561
N	-1.14769	-1.34945	0.02402
N	-1.09924	1.28226	-0.32066
Co	0.2849	0.02461	-0.06645
C	2.91011	-0.68726	-0.01843
C	1.59763	-2.62202	-0.13196
C	2.89038	0.73966	-0.03908
C	4.12515	-1.38982	0.01066
C	2.78593	-3.40317	-0.10389
C	4.08564	1.45245	-0.01086
C	5.34096	-0.64165	0.05
C	4.01924	-2.80211	-0.02249
H	2.70098	-4.48285	-0.15095
C	3.95769	2.87947	-0.04301
C	5.31522	0.72719	0.04219
C	1.5189	2.66342	-0.15051
H	6.285	-1.1753	0.07972
H	4.92046	-3.40771	0.002
C	2.72706	3.45541	-0.1077
H	4.85157	3.49535	-0.01748
H	6.24462	1.28765	0.06941
H	2.62357	4.53453	-0.13349
N	1.69678	-1.29304	-0.06469
N	1.65881	1.31745	-0.1132
O	-1.67201	-0.54467	2.67308
C	-2.51501	0.18392	3.15659
H	-2.29123	0.70373	4.10607
H	0.32332	0.1249	1.3039
C	0.30303	-3.28006	-0.29396
H	0.35528	-4.35348	-0.44745
C	0.25785	3.27854	-0.25568

1113.9755	1133.6420	1142.8712
1145.2922	1151.7643	1157.3882
1174.9498	1181.3287	1181.9173
1190.5385	1222.5914	1235.9326
1243.5348	1246.8086	1260.8894
1261.1756	1270.1650	1272.5484
1297.5789	1325.6935	1346.3990
1384.6244	1388.9764	1395.8881
1406.2237	1420.1269	1423.9564
1444.1805	1450.6855	1452.7206
1458.9532	1461.9640	1465.1875
1479.8573	1481.8680	1488.1415
1490.9707	1514.1474	1533.6415
1545.2828	1572.0571	1580.9913
1626.8200	1641.5877	1653.8678
1679.5725	1693.2524	1698.9328
1708.2781	1718.6062	1732.1315
1859.9628	2185.6777	3048.6305
3071.3563	3148.8491	3177.7594
3189.9812	3214.5629	3214.9068
3219.7045	3221.9602	3226.2241
3228.1798	3229.1642	3231.7986
3234.5550	3238.8388	3239.4179
3240.8308	3242.9746	3246.0857

H	0.24863	4.36049	-0.30189
H	-1.2588	-1.31678	1.05961
C	-3.85832	0.45249	2.55654
H	-4.63401	0.32291	3.31691
H	-3.89517	1.50221	2.24073
H	-4.0495	-0.19501	1.69899

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.421361
Electronic Energy = -1517.64147783
Internal Energy (E) = -1517.17445983
Enthalpy (H) = -1517.17318283
Gibbs Free Energy (G) = -1517.30439283
Gibbs Free Energy of Solvation = -1517.35936556

St. Point	General Structure	Ball & Stick model
Azobenzene (Cs+-coordinated)		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740

Frequencies

20.3361	26.0580	44.2393
67.4118	84.2364	100.9353
138.0764	211.7141	275.5489
304.0300	348.8699	418.0200
426.2119	481.8267	537.8891
546.1306	570.2543	622.5548
628.3696	679.7735	704.5196
719.3472	791.7370	807.7348
845.6634	876.1587	883.7976
944.9427	968.9584	971.1331
1015.7359	1016.7883	1018.6400
1020.5555	1039.0971	1043.0367
1060.5521	1061.2220	1112.8193
1118.6075	1183.7213	1187.5108
1189.3245	1190.6384	1233.1986
1283.9727	1337.3521	1346.7028
1364.5180	1377.2852	1505.1091
1512.9817	1533.2716	1543.8296
1636.6340	1673.4380	1684.6879
1691.6255	1701.0727	3211.2236

C	2.97003	1.36227	1.45493	3215.6732	3219.1797	3224.5687
H	0.92854	1.09680	2.12790	3226.6006	3234.5784	3235.9959
C	3.23170	1.99738	-0.86467	3242.5091	3246.0618	3264.7983
H	1.38538	2.24928	-1.97212			
C	3.79323	1.68392	0.37297			
H	3.40717	1.16948	2.42960			
H	3.86928	2.27642	-1.69672			
H	4.86928	1.72260	0.50506			
Cs	1.13863	-1.78685	-0.24190			
C	-2.47342	3.43093	-0.00949			
C	-3.82339	-1.41770	-0.02924			
C	-5.04390	0.68674	-0.04268			
C	-3.70087	2.84513	-0.02388			
H	-2.37687	4.51148	-0.00260			
C	-3.70086	-2.84511	-0.02396			
C	-5.04390	-0.68672	-0.04268			
C	-1.25756	-2.64674	0.00047			
H	-5.98116	1.23509	-0.05313			
H	-4.60015	3.45511	-0.02958			
C	-2.47341	-3.43094	-0.00962			
H	-4.60014	-3.45510	-0.02964			
H	-5.98117	-1.23506	-0.05312			
H	-2.37687	-4.51149	-0.00276			
N	-1.38780	1.30028	-0.01186			
N	-1.38782	-1.30028	-0.01191			
H	0.00022	-0.00008	1.45530			
C	-0.00001	3.27742	0.01504			
H	-0.00000	4.36099	0.02340			
C	-0.00000	-3.27741	0.01489			
H	0.00001	-4.36099	0.02318			

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.193762

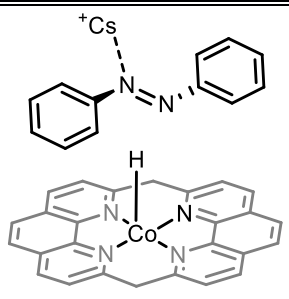
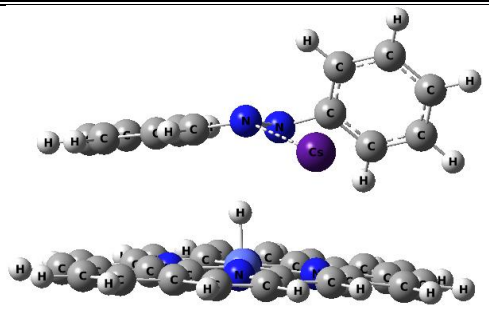
Electronic Energy = -592.212277481

Internal Energy (E) = -591.996024481

Enthalpy (H) = -591.994747481

Gibbs Free Energy (G) =-592.085083481

Gibbs Free Energy of Solvation =-592.168642489

St. Point	General Structure	Ball & Stick model
I2$^{Hyd(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672
H	4.86928	1.72260	0.50506
Cs	1.13863	-1.78685	-0.24190
C	-2.47342	3.43093	-0.00949
C	-3.82339	-1.41770	-0.02924
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964
H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

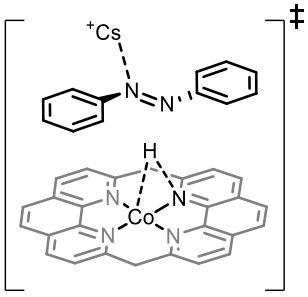
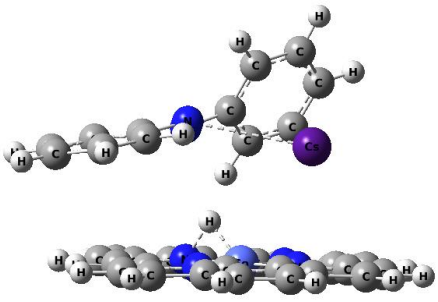
Frequencies

16.1886	19.5992	30.9713
41.6992	48.6996	53.5664
61.0114	63.6412	78.9196
81.0216	86.4280	92.4177
99.1701	99.7323	123.9895
139.4520	156.9871	162.6380
180.0154	201.3417	228.7421
242.9894	251.1213	257.8106
261.6035	265.2048	282.7451
283.3273	302.3088	302.9966
339.6396	342.2815	350.2256
380.1152	384.6101	405.4388
409.1494	411.0294	412.1062
426.5366	448.8458	458.8658
463.3402	463.7381	477.3346
484.8039	485.7680	493.8750
496.4880	536.1127	537.9858
550.5720	558.5225	571.5014
584.8184	587.1317	595.5571
598.5088	600.5177	622.8991
627.9863	628.2926	677.7712
679.5634	688.4206	689.6013
693.6914	698.3051	711.9259
715.3481	719.5109	720.8185
743.7384	747.6604	751.7160
763.4314	768.2910	772.0732
784.4668	786.3290	796.1572
820.6387	823.0694	829.4558
833.2895	843.3488	850.6712
858.7031	862.1430	868.2969
869.7120	876.1387	882.0651
883.8364	907.7568	920.1849
935.6151	942.7283	945.5219
951.7396	970.2310	981.2232
987.2637	988.4210	1009.2898
1012.5681	1017.1480	1017.6477
1019.4744	1020.7415	1021.3596
1021.9830	1025.5861	1030.0482
1043.9416	1059.8190	1061.3269
1108.5472	1115.2966	1119.1106
1135.5000	1142.0201	1159.7775
1168.8236	1173.2430	1178.8091
1182.4539	1183.1288	1185.6766
1186.7548	1187.0126	1231.2380
1232.0332	1241.8836	1243.4103
1246.6784	1255.1657	1257.8797
1274.5009	1280.7894	1298.1675
1302.3568	1329.3783	1331.6490
1340.8717	1361.7096	1374.6574
1383.1205	1394.8484	1416.8378
1421.2954	1431.7755	1450.6874
1457.4196	1465.9054	1469.6592
1476.5117	1478.6585	1483.9665

	1486.5821	1500.9334	1509.4216
	1516.7356	1532.5834	1533.2911
	1542.0748	1565.6504	1569.5503
	1573.3629	1625.3069	1635.3830
	1648.6960	1657.5747	1671.1077
	1680.3908	1686.3188	1691.8888
	1698.9287	1702.3399	1704.2117
	1709.7051	1719.2949	2141.0449
	3200.4055	3204.3389	3206.2260
	3206.8383	3208.2652	3210.7272
	3213.7408	3214.8775	3215.2496
	3219.1976	3219.7978	3220.5367
	3225.9534	3228.9732	3229.4317
	3232.9518	3233.2965	3233.5489
	3234.3753	3235.2840	3236.1287
	3237.6567	3237.7069	3258.0009

Statistical Thermodynamic Analysis

Temperature = 403.15 K
Pressure = 1 atm
Zero-point correction = 0.544432
Electronic Energy = -1955.76051398
Internal Energy (E) = -1955.15388998
Enthalpy (H) = -1955.15261398
Gibbs Free Energy (G) = -1955.32276798
Gibbs Free Energy of Solvation = -1955.390835

St. Point	General Structure	Ball & Stick model
TS1$^{Hyd(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713

Frequencies

-1211.7879	19.3397	24.6616
34.6775	41.6588	47.6085
53.5586	58.2169	72.9999
81.9955	85.6695	88.5574
98.3436	104.6805	108.9823
127.7003	141.3948	161.0756
163.0545	180.7915	202.4008
230.9652	238.5698	242.8680
250.6699	262.0975	265.5529
282.0188	284.1693	299.4834
302.0018	340.5283	346.1235
355.1161	379.3844	381.8970
405.4311	407.9228	410.4750

C	-5.08375	0.18956	-0.06765	417.4960	428.0093	447.5431
H	-5.00017	1.84900	-1.43752	460.7187	464.6349	468.3809
H	-4.87690	-1.41985	1.34743	478.7743	485.1076	486.9784
H	-6.15469	0.05672	-0.17966	493.9093	496.4860	534.8229
C	1.03275	1.60972	0.04286	537.2614	552.9267	559.4307
C	1.58869	1.31970	1.29532	570.6039	583.7261	584.5610
C	1.84875	1.98202	-1.02740	593.9945	597.5379	601.8667
C	2.97003	1.36227	1.45493	621.2642	625.8140	628.2226
H	0.92854	1.09680	2.12790	675.7249	677.6392	686.1341
C	3.23170	1.99738	-0.86467	687.6002	699.8092	711.5534
H	1.38538	2.24928	-1.97212	714.3414	720.2738	723.7996
C	3.79323	1.68392	0.37297	740.8411	742.9754	754.6874
H	3.40717	1.16948	2.42960	765.8701	768.6118	772.7690
H	3.86928	2.27642	-1.69672	787.5388	801.5735	814.0607
H	4.86928	1.72260	0.50506	818.7231	824.4063	834.4182
Cs	1.13863	-1.78685	-0.24190	843.6472	854.4404	856.9460
C	-2.47342	3.43093	-0.00949	863.0585	864.7319	868.1693
C	-3.82339	-1.41770	-0.02924	876.9316	881.9860	886.7396
C	-5.04390	0.68674	-0.04268	902.1006	915.6667	937.8249
C	-3.70087	2.84513	-0.02388	941.7732	948.8682	954.1909
H	-2.37687	4.51148	-0.00260	974.0706	981.6770	982.7704
C	-3.70086	-2.84511	-0.02396	983.1270	1001.0941	1011.2790
C	-5.04390	-0.68672	-0.04268	1013.3705	1016.4351	1016.8908
C	-1.25756	-2.64674	0.00047	1017.9616	1020.5212	1021.1910
H	-5.98116	1.23509	-0.05313	1021.7341	1025.0594	1036.2276
H	-4.60015	3.45511	-0.02958	1046.7399	1059.6774	1060.4257
C	-2.47341	-3.43094	-0.00962	1112.4856	1114.1733	1120.4781
H	-4.60014	-3.45510	-0.02964	1134.0590	1140.9502	1159.2913
H	-5.98117	-1.23506	-0.05312	1170.1461	1173.5701	1180.6729
H	-2.37687	-4.51149	-0.00276	1181.6421	1183.2365	1185.0169
N	-1.38780	1.30028	-0.01186	1185.1563	1189.7594	1229.3155
N	-1.38782	-1.30028	-0.01191	1230.3243	1236.3827	1240.2434
H	0.00022	-0.00008	1.45530	1244.5255	1256.4752	1257.8219
C	-0.00001	3.27742	0.01504	1269.8818	1280.4042	1289.4282
H	-0.00000	4.36099	0.02340	1298.8794	1323.7714	1334.7467
C	-0.00000	-3.27741	0.01489	1342.9418	1364.0926	1373.1070
H	0.00001	-4.36099	0.02318	1377.0020	1393.0813	1411.5410
				1416.8327	1433.2380	1449.8890
				1452.7639	1461.9400	1471.9898
				1475.5612	1477.9980	1481.7677
				1490.1568	1502.7049	1509.5158
				1517.4580	1521.7383	1532.1134
				1541.7223	1565.9377	1568.1473
				1577.8196	1622.2583	1637.9606
				1642.0770	1655.7409	1672.3696
				1678.2723	1685.0650	1689.4358
				1696.0079	1700.4175	1701.7761
				1707.0684	1717.9543	1866.4109
				3203.2935	3204.2456	3204.9031
				3206.2249	3208.3278	3208.4767
				3208.5540	3211.2299	3213.6162
				3217.8337	3223.7930	3224.7371
				3225.1668	3226.5212	3226.6296
				3226.8342	3227.7438	3227.9506

	3231.4542	3233.6364	3243.1953
	3243.5400	3256.9128	3261.0160

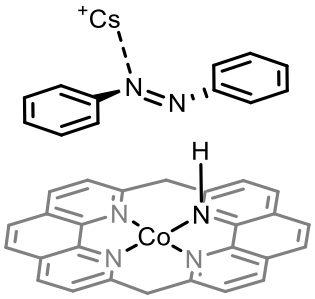
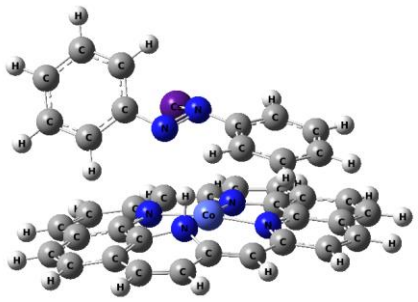
Statistical Thermodynamic Analysis

Temperature = 403.15 K — Pressure = 1 atm

Zero-point correction = 0.542628 — Electronic Energy = -1955.73859903

Internal Energy (E) = -1955.13425203 — Enthalpy (H) = -1955.13297603

Gibbs Free Energy (G) = -1955.30139303 — Gibbs Free Energy of Solvation = -1955.36795181

St. Point	General Structure	Ball & Stick model
$I3^{Hyd(Spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672

Frequencies

16.6981	24.4283	27.3806
33.0649	41.4118	45.5332
52.4172	55.0044	66.9501
75.6046	89.8118	91.9969
100.0517	102.7922	120.0549
136.8538	152.8329	165.3827
179.9798	207.4949	223.5079
232.0909	235.2116	241.5448
249.5086	257.4604	265.2142
288.5523	293.5324	297.3585
319.2358	340.3852	344.2942
365.6314	371.5490	381.4601
390.5941	404.4503	416.2061
426.0088	435.3637	443.2499
454.7636	467.4870	470.9229
478.0321	482.1971	487.2246
492.6701	529.6536	539.6676
545.4279	552.3079	560.5963
564.8906	574.1963	582.9631
592.4989	599.8486	616.3173
624.0227	629.7763	649.9554
655.0886	674.9909	680.3601
693.1212	699.2717	706.9245
712.6924	715.5989	717.8017
728.8363	751.8030	756.2793
763.8595	778.9907	779.5007
797.5079	805.2352	817.5095

H	4.86928	1.72260	0.50506	823.4684	836.3652	844.4004
Cs	1.13863	-1.78685	-0.24190	845.0711	851.4940	853.8454
C	-2.47342	3.43093	-0.00949	855.9754	862.3879	871.1245
C	-3.82339	-1.41770	-0.02924	872.8333	878.0433	908.8083
C	-5.04390	0.68674	-0.04268	909.9656	913.1582	940.6026
C	-3.70087	2.84513	-0.02388	942.0969	944.2023	949.8301
H	-2.37687	4.51148	-0.00260	970.4657	989.1859	990.2950
C	-3.70086	-2.84511	-0.02396	991.3506	996.1339	1007.1116
C	-5.04390	-0.68672	-0.04268	1008.4663	1013.7525	1014.0830
C	-1.25756	-2.64674	0.00047	1016.1024	1017.5251	1019.5129
H	-5.98116	1.23509	-0.05313	1020.5027	1023.0524	1032.6696
H	-4.60015	3.45511	-0.02958	1061.4265	1065.3131	1098.9901
C	-2.47341	-3.43094	-0.00962	1117.9493	1120.2566	1122.0819
H	-4.60014	-3.45510	-0.02964	1134.9156	1145.1623	1167.2844
H	-5.98117	-1.23506	-0.05312	1173.6205	1178.5113	1182.3669
H	-2.37687	-4.51149	-0.00276	1182.5199	1186.8752	1192.0287
N	-1.38780	1.30028	-0.01186	1194.4447	1218.6118	1226.0003
N	-1.38782	-1.30028	-0.01191	1234.0357	1235.1119	1239.9113
H	0.00022	-0.00008	1.45530	1256.4551	1257.0075	1263.8926
C	-0.00001	3.27742	0.01504	1264.4577	1279.4234	1283.2040
H	-0.00000	4.36099	0.02340	1313.7050	1336.8756	1344.7907
C	-0.00000	-3.27741	0.01489	1347.7220	1372.2262	1375.7736
H	0.00001	-4.36099	0.02318	1382.5717	1382.9361	1394.1544
				1407.8809	1420.3893	1436.6180
				1445.4072	1453.4512	1461.2259
				1468.8378	1476.1727	1486.1987
				1499.3668	1503.7291	1507.8286
				1512.1156	1530.5706	1533.7211
				1544.3718	1567.4206	1570.9843
				1613.0014	1624.7257	1628.9945
				1640.3854	1668.0682	1675.4645
				1681.5500	1683.9139	1692.2339
				1692.8744	1699.3571	1700.5231
				1707.1523	1722.3080	3201.6284
				3201.9391	3203.6681	3204.7901
				3206.4715	3206.6489	3207.2261
				3211.7550	3214.7372	3214.9270
				3218.4289	3219.4635	3220.3857
				3224.5697	3226.4997	3226.9641
				3228.5330	3232.8356	3234.1647
				3236.4831	3236.9005	3239.2984
				3240.9731	3243.0252	3296.5530

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.546626

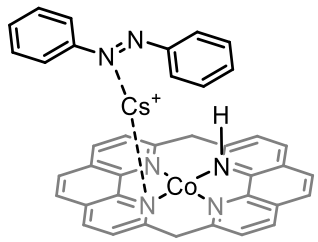
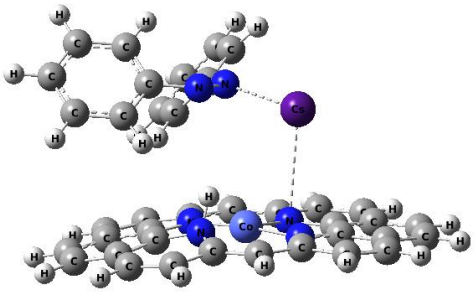
Electronic Energy = -1955.74882591

Internal Energy (E) = -1955.13955491

Enthalpy (H) = -1955.13827791

Gibbs Free Energy (G) = -1955.31047191

Gibbs Free Energy of Solvation = -1955.37733413

St. Point	General Structure	Ball & Stick model
I4$^{Hyd(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672
H	4.86928	1.72260	0.50506
Cs	1.13863	-1.78685	-0.24190
C	-2.47342	3.43093	-0.00949
C	-3.82339	-1.41770	-0.02924
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962

Frequencies

12.7580	15.0972	20.1212
25.3914	29.4230	40.5219
45.3640	52.7118	62.4395
66.4686	69.6727	76.3877
93.9076	103.4659	110.6788
134.1057	145.9641	163.8683
174.2675	193.6027	209.5176
229.5612	235.0212	240.4907
249.3250	258.6620	268.5786
282.4258	285.8291	308.4220
319.0784	339.2089	346.7022
363.6371	380.2255	392.5476
402.7508	413.3644	419.2791
422.7380	443.8516	449.7144
454.3360	463.0920	466.9782
477.7497	482.4146	485.9729
491.4428	518.1310	527.6412
545.2108	551.8622	559.2213
571.1457	582.7794	592.1032
597.6084	613.4566	614.3988
626.4522	627.8262	636.3342
655.1245	677.5778	683.3208
705.4884	706.7410	711.7629
713.1692	716.6245	728.9545
730.4726	746.0114	758.3200
764.1527	772.8694	781.8484
790.6734	799.8911	807.7784
809.1430	813.1058	819.0343
843.3793	846.1493	856.0491
856.5298	865.0467	867.0365
872.8545	878.8610	897.1851
902.7138	912.4544	915.5398
930.3657	944.1884	954.1765
964.5736	983.9067	989.0104
996.3502	997.8163	998.1705
1012.4123	1015.7819	1017.0388
1018.2405	1020.7346	1021.1411
1024.4167	1026.3649	1030.7112
1063.2593	1071.2773	1100.5010
1116.8038	1123.8521	1127.4513

H	-4.60014	-3.45510	-0.02964	1135.8484	1145.9868	1167.8295
H	-5.98117	-1.23506	-0.05312	1177.2881	1180.9868	1182.7957
H	-2.37687	-4.51149	-0.00276	1183.9986	1185.7644	1193.5007
N	-1.38780	1.30028	-0.01186	1198.5089	1216.0807	1222.2069
N	-1.38782	-1.30028	-0.01191	1229.9084	1234.5780	1239.5383
H	0.00022	-0.00008	1.45530	1240.5447	1255.4837	1257.5165
C	-0.00001	3.27742	0.01504	1261.8308	1272.2278	1285.0463
H	-0.00000	4.36099	0.02340	1315.7477	1337.0772	1337.5812
C	-0.00000	-3.27741	0.01489	1347.4195	1360.6533	1370.0330
H	0.00001	-4.36099	0.02318	1375.5096	1388.0313	1396.8134
				1415.1537	1433.5323	1440.6667
				1448.3076	1458.7334	1461.1956
				1473.0189	1477.1384	1486.9436
				1496.0927	1505.1433	1507.8249
				1511.9457	1530.7784	1534.4654
				1545.0078	1567.8482	1569.4037
				1602.5961	1630.8780	1634.2393
				1662.9173	1672.6748	1676.5085
				1678.1531	1686.8296	1691.0803
				1692.3218	1694.7465	1705.4389
				1715.1136	1724.9321	3194.3802
				3200.9270	3205.0002	3205.3255
				3209.3800	3209.8440	3211.0850
				3211.2149	3214.3741	3215.0780
				3215.8391	3217.0945	3221.7913
				3225.4684	3226.1387	3226.4758
				3227.2563	3228.4438	3229.5216
				3230.9769	3233.8523	3238.8257
				3242.8308	3242.8918	3249.7283

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.546075

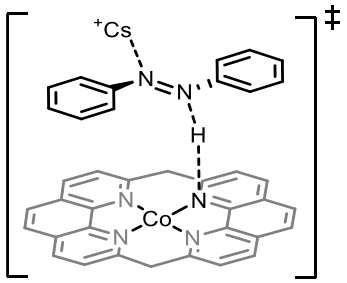
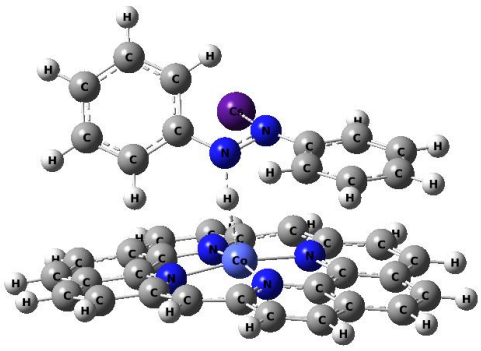
Electronic Energy = -1955.72160439

Internal Energy (E) = -1955.11256639

Enthalpy (H) = -1955.11129039

Gibbs Free Energy (G) = -1955.28755039

Gibbs Free Energy of Solvation = -1955.35455308

St. Point	General Structure	Ball & Stick model
TS2$^{Hyd(spill)}$		

Cartesian co-ordinate			
Atoms	**X**	**Y**	**Z**
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672
H	4.86928	1.72260	0.50506
Cs	1.13863	-1.78685	-0.24190
C	-2.47342	3.43093	-0.00949
C	-3.82339	-1.41770	-0.02924
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964
H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

Frequencies		
-333.6079	16.9603	22.0985
29.4019	39.1899	45.0560
48.5082	54.1221	67.7966
73.9706	85.2266	90.4980
107.1269	111.2283	119.4727
132.2038	167.1769	172.0154
193.1428	213.4524	222.5890
226.1802	240.0786	242.0772
247.0934	256.0590	270.2057
280.8440	297.8805	322.5358
330.4582	341.8011	348.2322
367.9433	385.6964	394.7549
398.7671	410.0163	420.9072
436.0557	441.9097	456.1462
458.5709	472.1744	475.8817
476.5638	484.4685	488.8415
496.0291	517.7624	531.6480
545.5905	552.1430	564.2979
577.9018	582.7521	590.6445
593.7651	601.4912	620.9181
624.0652	626.2863	653.4318
678.3547	683.5739	704.2571
706.5495	711.8037	713.1768
717.7773	729.5792	731.1723
740.6075	745.7782	752.5681
759.9808	763.4278	789.4188
790.5699	800.0127	808.0743
812.5726	821.0347	835.1798
840.4766	854.3558	855.0597
865.2448	866.7114	870.1886
873.5182	884.7797	888.9164
908.7168	914.7136	921.7825
945.2328	946.8623	954.7675
964.6093	977.2776	979.8877
998.5853	1003.5360	1006.8809
1010.4433	1013.0574	1014.6675
1017.2043	1017.4260	1019.1006
1024.5632	1033.1815	1037.8368
1065.3238	1069.7670	1110.8422
1119.4486	1122.2904	1124.0345
1137.3802	1148.2474	1167.2512
1169.9127	1174.4450	1180.2118
1181.3388	1185.3580	1186.6102
1202.0782	1213.0980	1217.8438
1234.6758	1239.5859	1241.3158
1252.9156	1254.7367	1259.8427
1264.8004	1279.8455	1292.9024
1315.2412	1330.4950	1334.6926
1351.7603	1358.5657	1363.7566
1371.5169	1387.9209	1401.0509
1407.1478	1425.8970	1443.9043
1444.9106	1455.0361	1461.2057
1472.6671	1476.6034	1480.0289

	1490.0773	1502.1137	1504.4020
	1506.5205	1516.1772	1525.8012
	1535.6322	1537.4636	1562.5696
	1570.4460	1586.4153	1627.2420
	1632.1866	1654.5949	1663.8658
	1670.8056	1671.8967	1685.1139
	1686.8179	1688.5062	1691.4343
	1707.9150	1717.2250	1762.9330
	3180.2445	3197.3998	3199.6253
	3199.9037	3200.3300	3206.1671
	3206.9475	3207.5920	3209.4290
	3209.6193	3209.9544	3215.9906
	3216.2957	3219.1386	3219.7809
	3221.0035	3222.5131	3226.7822
	3226.8398	3227.1136	3230.5910
	3237.4170	3238.3415	3239.0369

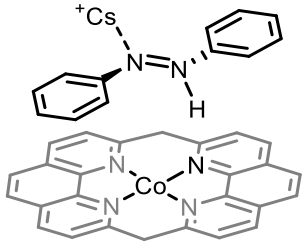
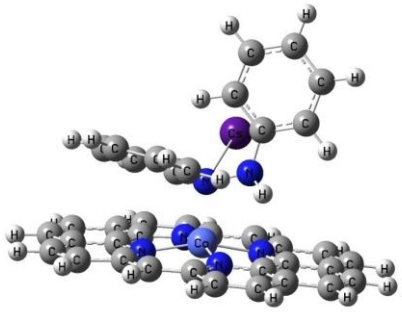
Statistical Thermodynamic Analysis

Temperature = 403.15 K Pressure = 1 atm

Zero-point correction = 0.542687 Electronic Energy = -1955.70068110

Internal Energy (E) = -1955.0968191 Enthalpy (H) = -1955.0955431

Gibbs Free Energy (G) = -1955.2632231 Gibbs Free Energy of Solvation = -1955.33947791

St. Point	General Structure	Ball & Stick model
$I5^{Hyd(Spill)}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822

Frequencies

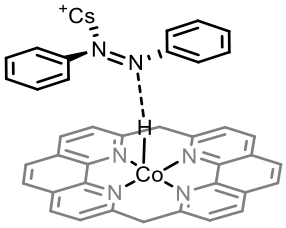
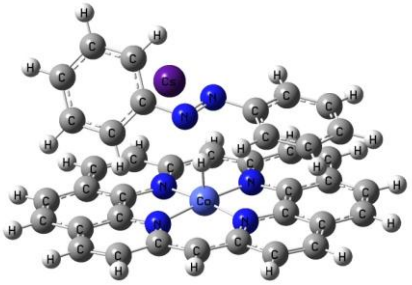
6.6710	27.2933	28.5098
33.7402	43.8958	49.7448
61.5893	65.3341	69.7420
81.8326	89.2178	96.5332
109.0701	124.8288	129.6393
170.7010	176.7027	191.9832
207.4067	221.7654	238.3499
247.1232	251.6913	256.4804
272.9346	275.0323	277.6443
292.1482	305.2130	323.2354
339.4637	350.2416	353.6125
382.0306	402.2135	406.2930

H	-2.41579	-1.08523	1.60713	407.6228	420.8013	422.8827
C	-5.08375	0.18956	-0.06765	447.2330	457.3818	464.3835
H	-5.00017	1.84900	-1.43752	472.7248	476.9137	485.9154
H	-4.87690	-1.41985	1.34743	491.1614	493.3341	496.6127
H	-6.15469	0.05672	-0.17966	505.3049	526.9945	535.8142
C	1.03275	1.60972	0.04286	552.0065	556.7560	566.2377
C	1.58869	1.31970	1.29532	585.6608	586.3006	593.8073
C	1.84875	1.98202	-1.02740	594.4328	599.9409	624.1825
C	2.97003	1.36227	1.45493	626.4797	627.8905	659.3229
H	0.92854	1.09680	2.12790	674.6712	683.7279	688.0851
C	3.23170	1.99738	-0.86467	699.9299	712.3576	713.4711
H	1.38538	2.24928	-1.97212	717.1368	720.4415	722.2928
C	3.79323	1.68392	0.37297	744.2749	745.8080	755.5384
H	3.40717	1.16948	2.42960	764.0446	773.0223	775.4924
H	3.86928	2.27642	-1.69672	775.8177	805.6097	815.4743
H	4.86928	1.72260	0.50506	819.5127	823.5469	836.7992
Cs	1.13863	-1.78685	-0.24190	850.5275	856.3735	858.2430
C	-2.47342	3.43093	-0.00949	859.0408	860.5427	863.0754
C	-3.82339	-1.41770	-0.02924	871.0754	875.9986	883.5131
C	-5.04390	0.68674	-0.04268	885.4349	907.2378	919.1542
C	-3.70087	2.84513	-0.02388	920.1378	937.4685	941.5923
H	-2.37687	4.51148	-0.00260	945.7965	982.2735	989.2332
C	-3.70086	-2.84511	-0.02396	991.3402	993.2394	1007.7200
C	-5.04390	-0.68672	-0.04268	1010.0881	1012.6353	1015.2182
C	-1.25756	-2.64674	0.00047	1016.0555	1017.3832	1018.0080
H	-5.98116	1.23509	-0.05313	1019.0967	1022.1572	1040.9104
H	-4.60015	3.45511	-0.02958	1064.5179	1068.1473	1090.9992
C	-2.47341	-3.43094	-0.00962	1117.1184	1121.1802	1128.3787
H	-4.60014	-3.45510	-0.02964	1133.8884	1142.7172	1157.1361
H	-5.98117	-1.23506	-0.05312	1166.9847	1175.2281	1178.3813
H	-2.37687	-4.51149	-0.00276	1182.6442	1183.2151	1187.2224
N	-1.38780	1.30028	-0.01186	1196.1028	1203.4370	1231.3727
N	-1.38782	-1.30028	-0.01191	1240.1440	1244.9762	1246.5510
H	0.00022	-0.00008	1.45530	1248.9576	1258.7413	1259.9295
C	-0.00001	3.27742	0.01504	1275.7297	1293.9552	1298.5548
H	-0.00000	4.36099	0.02340	1303.7383	1330.2031	1333.8281
C	-0.00000	-3.27741	0.01489	1344.6872	1361.4041	1371.0899
H	0.00001	-4.36099	0.02318	1384.6857	1395.5542	1418.7726
				1422.9577	1435.7536	1452.6494
				1454.8768	1457.2089	1460.5037
				1468.8870	1470.4979	1479.0932
				1479.7716	1486.2763	1507.7817
				1515.3393	1522.5651	1527.1028
				1537.7995	1548.9943	1561.0545
				1569.7794	1576.2107	1624.4963
				1631.5311	1656.0408	1671.0498
				1672.7089	1676.8411	1687.6613
				1696.5947	1697.7581	1702.4595
				1708.3989	1715.4896	3187.1101
				3191.6662	3204.2140	3204.4095
				3207.6628	3208.1096	3209.1034
				3210.8704	3210.9698	3212.5720
				3217.6878	3218.2458	3221.3663
				3223.8466	3225.3278	3225.8509
				3226.9903	3229.4383	3229.9844

	3231.3644	3235.3782	3238.5665
	3240.6221	3240.9900	3502.3630

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.547990	Electronic Energy = -1955.77280451
Internal Energy (E) = -1955.16444651	Enthalpy (H) = -1955.16316951
Gibbs Free Energy (G) = -1955.32657851	Gibbs Free Energy of Solvation = -1955.39490889

St. Pt.	General Structure	Ball & Stick model
$I2^{Hyd}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672

Frequencies

14.2341	24.6861	29.5044
40.2388	51.3154	52.1005
55.8797	63.7921	69.6399
78.2514	88.2091	97.2984
105.3787	116.7530	123.3358
136.3745	146.6586	168.3592
175.8305	200.0686	221.4465
242.6964	250.1965	260.1420
262.3191	267.8039	282.5353
283.5246	301.4575	307.6297
338.9002	341.8447	350.5119
381.8385	384.2844	405.4213
406.6023	410.9878	418.3530
426.3696	448.7444	460.3736
461.6046	465.9814	477.5745
484.6703	487.8298	491.6864
495.8610	536.5291	537.3104
553.8738	558.2369	571.8766
585.1280	586.6431	595.4320
598.0853	600.5377	623.6905
628.2068	628.9335	678.7112
679.4681	687.8328	689.9671
701.4143	711.4944	715.2305
718.7608	721.5449	725.3767
742.8576	749.6610	754.5383
760.2828	766.5059	769.9978
774.2134	785.8169	796.6709

H	4.86928	1.72260	0.50506	816.1990	820.9822	830.0080
Cs	1.13863	-1.78685	-0.24190	835.0177	844.8820	855.4805
C	-2.47342	3.43093	-0.00949	859.9429	861.4263	866.4479
C	-3.82339	-1.41770	-0.02924	868.2900	872.8347	875.0272
C	-5.04390	0.68674	-0.04268	880.5289	907.4315	919.1741
C	-3.70087	2.84513	-0.02388	936.1143	942.2026	951.3704
H	-2.37687	4.51148	-0.00260	953.3713	968.8929	977.9309
C	-3.70086	-2.84511	-0.02396	982.2994	1000.6082	1005.5861
C	-5.04390	-0.68672	-0.04268	1010.2106	1011.3258	1013.0126
C	-1.25756	-2.64674	0.00047	1018.2036	1018.3027	1018.5966
H	-5.98116	1.23509	-0.05313	1020.9706	1026.0707	1026.8896
H	-4.60015	3.45511	-0.02958	1043.1962	1060.3700	1061.2472
C	-2.47341	-3.43094	-0.00962	1109.4587	1115.2560	1117.7599
H	-4.60014	-3.45510	-0.02964	1137.1979	1143.5158	1159.0328
H	-5.98117	-1.23506	-0.05312	1170.0093	1174.1197	1180.9949
H	-2.37687	-4.51149	-0.00276	1182.5340	1183.1943	1186.0996
N	-1.38780	1.30028	-0.01186	1187.3483	1187.7269	1232.0715
N	-1.38782	-1.30028	-0.01191	1232.8768	1241.1002	1243.8109
H	0.00022	-0.00008	1.45530	1246.9702	1256.9077	1257.2735
C	-0.00001	3.27742	0.01504	1273.8749	1283.1134	1298.4245
H	-0.00000	4.36099	0.02340	1301.4289	1329.2608	1333.4732
C	-0.00000	-3.27741	0.01489	1342.2546	1363.1721	1377.4699
H	0.00001	-4.36099	0.02318	1382.8039	1395.1480	1417.0467
				1421.7967	1431.1412	1451.0568
				1456.5818	1465.9423	1470.9407
				1475.7107	1478.5228	1483.7019
				1485.5104	1502.6243	1509.9378
				1518.9482	1531.2217	1531.5483
				1541.5020	1565.2168	1568.7592
				1573.3749	1622.0828	1637.0252
				1650.5078	1655.4298	1673.5933
				1681.2303	1685.2059	1690.5890
				1696.8156	1704.1055	1704.7171
				1708.9550	1716.8349	2180.4132
				3201.8871	3202.6159	3204.9732
				3206.2595	3207.1266	3208.1967
				3209.1888	3213.4581	3214.5433
				3215.3459	3220.2980	3221.7057
				3222.0071	3222.3321	3223.3743
				3226.3731	3226.6505	3226.7457
				3229.2274	3231.3570	3237.2439
				3239.6404	3245.3386	3256.5327

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.544434

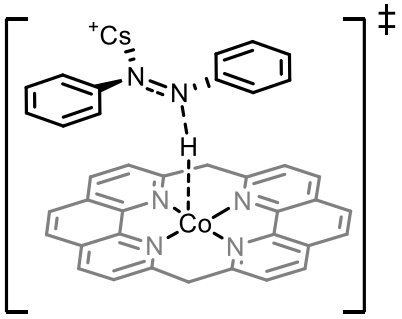
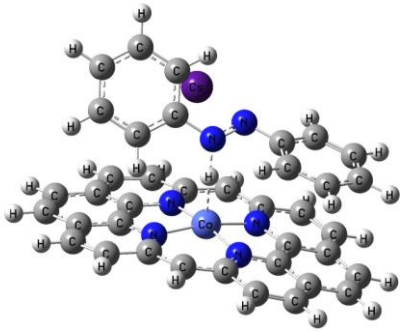
Electronic Energy = -1955.76165576

Internal Energy (E) = -1955.15504876

Enthalpy (H)= -1955.15377176

Gibbs Free Energy (G) = -1955.32386176

Gibbs Free Energy of Solvation = -1955.39202528

St. Point	General Structure	Ball & Stick model
TS1^{Hyd}		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672
H	4.86928	1.72260	0.50506
Cs	1.13863	-1.78685	-0.24190
C	-2.47342	3.43093	-0.00949
C	-3.82339	-1.41770	-0.02924
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313

Frequencies

-713.6423	9.8729	25.8497
28.5252	39.7924	50.5448
54.1918	62.4594	69.8988
77.0474	97.4742	104.3999
108.8623	114.9102	128.5425
139.7552	161.9888	165.5346
178.3697	206.3680	213.3269
221.3672	245.6592	247.0890
261.8036	264.7102	270.4847
277.5364	301.3189	307.8430
337.5945	342.4677	351.4730
364.2098	378.2011	387.1523
402.9772	405.1126	406.6595
426.2320	432.7669	445.1495
461.5510	463.3214	472.3148
481.5588	485.9094	489.7265
492.3358	528.4799	534.0252
543.0274	548.1491	556.0428
584.3807	587.8725	590.3771
593.9477	598.9039	601.9684
620.4400	628.0745	631.6404
675.4468	676.0546	683.1680
688.8198	691.0311	711.0664
712.3852	714.2980	725.5709
732.6501	744.7709	755.1496
756.8621	766.2415	771.9065
780.3338	787.2608	816.2264
819.0098	824.1680	829.5089
841.9506	853.9786	855.4129
857.3411	861.9852	864.8240
871.0891	873.5452	880.1206
905.8908	918.9185	930.9491
940.1284	947.4639	950.4019
959.8977	980.4387	981.4622
992.1079	1006.3772	1008.5412
1011.5502	1012.2399	1013.9406
1015.2913	1018.4538	1020.2418
1020.3967	1030.1176	1032.5794

H	-4.60015	3.45511	-0.02958	1058.2159	1062.6424	1103.7170
C	-2.47341	-3.43094	-0.00962	1113.8980	1117.7663	1131.8018
H	-4.60014	-3.45510	-0.02964	1136.7437	1141.1824	1153.6924
H	-5.98117	-1.23506	-0.05312	1166.9493	1172.4594	1178.5623
H	-2.37687	-4.51149	-0.00276	1179.0801	1183.6397	1187.2635
N	-1.38780	1.30028	-0.01186	1187.7903	1192.2525	1227.5195
N	-1.38782	-1.30028	-0.01191	1236.6725	1240.7077	1241.5360
H	0.00022	-0.00008	1.45530	1254.9176	1256.5950	1259.3290
C	-0.00001	3.27742	0.01504	1265.2435	1292.2657	1298.6266
H	-0.00000	4.36099	0.02340	1300.4291	1324.5372	1329.6343
C	-0.00000	-3.27741	0.01489	1345.9614	1365.5445	1381.3824
H	0.00001	-4.36099	0.02318	1386.5153	1395.8996	1405.6641
				1407.4355	1414.4942	1426.4488
				1450.8482	1454.8905	1463.6842
				1468.2565	1471.4149	1477.8295
				1481.7009	1484.5079	1505.6331
				1511.6051	1516.6484	1520.7470
				1532.9323	1540.5266	1542.0754
				1553.9608	1563.2169	1574.1403
				1614.5088	1630.7424	1648.8634
				1656.9219	1672.6380	1675.9165
				1686.9200	1688.9713	1691.0878
				1699.9359	1704.0076	1711.4984
				3186.5187	3190.7228	3202.9988
				3203.1564	3205.9014	3206.3048
				3207.0165	3209.5779	3214.0308
				3214.7501	3215.0096	3218.3441
				3219.5972	3222.6703	3222.8392
				3224.5536	3227.9742	3229.0613
				3232.3504	3233.5837	3233.9358
				3237.2237	3239.1069	3300.2057

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.541630

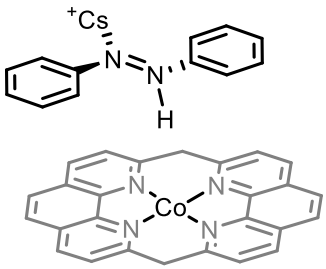
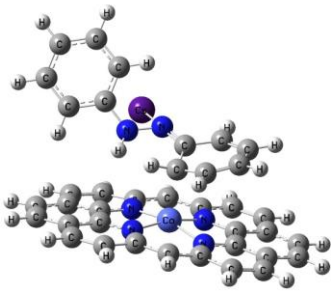
Electronic Energy = -1955.73132475

Internal Energy (E) = -1955.12836375

Enthalpy (H) = -1955.12708675

Gibbs Free Energy (G) =-1955.29476775

Gibbs Free Energy of Solvation = -1955.36959807

St. Pt.	General Structure	Ball & Stick model
I3^{Hyd}		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.36540	1.54303	-0.20810
N	-0.94090	0.62812	0.41698
C	-2.34640	0.54230	0.21341
C	-3.06482	1.38661	-0.64205
C	-2.99530	-0.46633	0.92784
C	-4.43204	1.20114	-0.77872
H	-2.54390	2.17073	-1.17886
C	-4.36764	-0.64278	0.78822
H	-2.41579	-1.08523	1.60713
C	-5.08375	0.18956	-0.06765
H	-5.00017	1.84900	-1.43752
H	-4.87690	-1.41985	1.34743
H	-6.15469	0.05672	-0.17966
C	1.03275	1.60972	0.04286
C	1.58869	1.31970	1.29532
C	1.84875	1.98202	-1.02740
C	2.97003	1.36227	1.45493
H	0.92854	1.09680	2.12790
C	3.23170	1.99738	-0.86467
H	1.38538	2.24928	-1.97212
C	3.79323	1.68392	0.37297
H	3.40717	1.16948	2.42960
H	3.86928	2.27642	-1.69672
H	4.86928	1.72260	0.50506
Cs	1.13863	-1.78685	-0.24190
C	-2.47342	3.43093	-0.00949
C	-3.82339	-1.41770	-0.02924
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964
H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

Frequencies

19.4448	27.5809	37.6813
46.4756	53.3023	54.4404
57.4807	64.2098	68.5664
87.9497	104.7702	110.1909
130.4363	135.9887	139.4374
167.2438	177.1036	192.3232
209.8241	221.4669	239.2424
248.1260	255.2523	258.9256
272.8016	279.9726	297.3053
300.3534	315.4089	325.2468
342.1474	353.9038	354.7152
366.6329	381.0447	403.1229
406.6160	408.3249	425.6365
438.1048	447.7895	458.7892
464.3681	470.5991	477.0089
486.4072	490.3234	492.8506
496.2691	526.5252	529.2807
535.4169	554.1306	556.5724
580.7449	584.7728	585.9245
594.3136	596.7576	599.3381
600.8014	626.2231	627.9081
651.7595	676.7700	684.0313
687.5130	710.4803	712.5688
718.4098	721.3430	723.1960
729.8228	744.6903	751.1661
759.2960	766.2599	767.3850
780.2872	780.7813	807.2966
815.9928	821.6906	824.6265
831.5377	832.9381	851.2268
858.5656	862.1785	864.1504
872.4430	874.3499	881.5130
897.5756	907.2640	920.0598
929.1493	936.1214	939.8330
947.4483	978.6598	982.5593
988.9373	999.3196	1001.3202
1003.1748	1004.2579	1009.8309
1010.8798	1011.1105	1015.8632
1016.9554	1019.5178	1024.4819
1039.5908	1064.3848	1083.3171
1108.9148	1115.4438	1133.5234
1141.2259	1155.9429	1166.3137
1171.0251	1171.8581	1173.1990
1176.6120	1180.0382	1184.6219
1193.9958	1196.9477	1228.2613
1240.6690	1243.5724	1246.4158
1256.3803	1258.4592	1273.9354
1291.0597	1298.0789	1300.2135
1316.0754	1327.1688	1343.3337
1363.2199	1383.1963	1386.4858
1398.5637	1413.6703	1420.2327
1422.8050	1432.3891	1451.1962
1458.0621	1462.1537	1467.2399
1470.2349	1473.7316	1477.8819

	1480.1419	1487.2797	1488.6408
	1516.8862	1526.1338	1531.5446
	1556.7004	1561.9613	1567.7288
	1575.1054	1620.8366	1621.8035
	1633.6930	1654.5416	1655.8259
	1673.0314	1677.5969	1696.3379
	1696.5241	1700.8270	1707.1695
	1716.5439	1721.8045	3139.5768
	3179.6592	3185.6548	3203.4031
	3203.8010	3204.3398	3204.8511
	3205.7454	3208.7829	3210.6993
	3210.9809	3211.9441	3212.9052
	3217.9081	3221.0286	3223.1561
	3223.8528	3226.0206	3226.4067
	3227.3408	3229.1182	3229.4038
	3234.0933	3243.5165	3598.6290

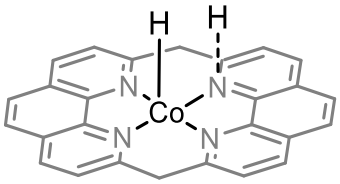
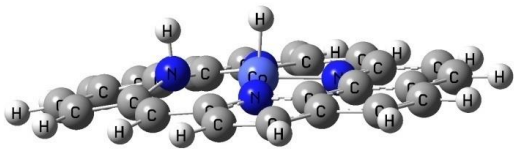
Statistical Thermodynamic Analysis

Temperature = 403.15 K — Pressure = 1 atm

Zero-point correction = 0.547634 — Electronic Energy = -1955.76038242

Internal Energy (E) = -1955.15108942 — Enthalpy (H) = -1955.14981242

Gibbs Free Energy (G)=-1955.31663442 — Gibbs Free Energy of Solvation = -1955.39078054

St. Pt.	General Structure	Ball & Stick model
$I2^{Hyd1(MLC)}$/ $I2^{Hyd2(MLC)}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-2.51797	-3.44611	-0.08264
C	-3.72170	-2.83222	-0.09791
C	-3.83259	-1.37874	-0.05431
C	-2.66670	-0.66553	0.14755
C	-1.27352	-2.70648	0.06602
C	-5.02076	-0.65011	-0.28282
C	-2.60569	0.72710	0.05641
C	-3.79629	1.44958	-0.14051
C	-5.00019	0.73223	-0.30016
C	-3.65977	2.87854	-0.18581
H	-4.54724	3.49193	-0.30971
C	-2.43457	3.45160	-0.08165
C	-1.22795	2.65855	0.04657

Frequencies

48.3606	60.8641	95.6061
122.4633	150.3820	160.1210
208.4525	235.6481	238.4646
246.9020	249.3949	260.5137
275.2453	301.8042	318.5522
335.0754	342.6053	374.7917
391.8667	400.5610	406.4440
445.2387	449.2125	454.6019
471.6689	479.0623	483.7753
489.6753	500.0564	535.8009
551.6620	558.9286	583.0300
583.9880	592.4817	600.2536
617.4134	655.5121	664.7998
685.1051	699.3269	708.4269
710.5393	717.7293	724.2741
741.9330	756.3664	765.4903
771.8345	783.3393	810.1790

H	-5.94928	-1.18576	-0.45009	823.8249	831.0816	839.3393
H	-2.44271	-4.52063	-0.21132	845.6314	848.6022	862.6935
H	-4.62903	-3.41684	-0.21310	864.0477	876.5505	879.8093
H	-5.92035	1.28442	-0.46457	884.3302	914.0536	918.1334
H	-2.32333	4.52945	-0.12041	926.6151	953.1062	986.1771
N	-1.42115	-1.32580	0.48729	988.6093	1000.7480	1011.6319
N	-1.36214	1.31242	0.12679	1016.5833	1023.6270	1026.1495
Co	0.01679	0.03428	0.23511	1026.9085	1032.6729	1108.5792
C	2.62000	-0.72395	-0.00624	1121.8028	1144.7370	1156.7634
C	1.27032	-2.63453	-0.02095	1174.3392	1178.6941	1180.8917
C	2.62225	0.70242	-0.00950	1189.8560	1220.0782	1231.4138
C	3.81972	-1.44756	-0.11029	1244.0492	1246.7917	1260.2380
C	2.43874	-3.43571	-0.12938	1261.8212	1269.2849	1271.9589
C	3.82628	1.39527	-0.09170	1298.0884	1324.4185	1344.8002
C	5.04592	-0.71999	-0.18079	1369.6127	1381.4063	1403.2579
C	3.68573	-2.85612	-0.15703	1417.9569	1420.2785	1443.3501
H	2.32963	-4.51250	-0.19077	1449.5876	1457.5633	1461.3041
C	3.72116	2.82537	-0.09574	1479.3420	1480.4654	1488.8436
C	5.04215	0.64935	-0.16783	1513.8433	1534.2196	1546.8072
C	1.27913	2.64979	0.02889	1572.1227	1582.1696	1630.3410
H	5.97926	-1.26824	-0.25207	1643.3274	1653.1732	1680.9419
H	4.57397	-3.47685	-0.23081	1692.1175	1698.6150	1709.4171
C	2.50038	3.42118	-0.03734	1718.7862	1733.9352	2133.9869
H	4.62414	3.42615	-0.14688	3211.1675	3211.7269	3211.7846
H	5.97941	1.19435	-0.22462	3214.6858	3217.7410	3224.5460
H	2.41296	4.50196	-0.04125	3224.7111	3226.0426	3230.1973
N	1.39837	-1.30919	0.06494	3234.8347	3236.7915	3239.2728
N	1.39857	1.30012	0.04294	3240.8027	3244.7530	3379.6427
H	0.19989	0.13900	1.59991			
C	-0.04820	-3.26690	-0.06233			
H	-0.03262	-4.33522	-0.25561			
C	0.02703	3.28554	0.04759			
H	0.03107	4.36759	0.00562			
H	-1.39197	-1.36276	1.51537			

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction= 0.362846

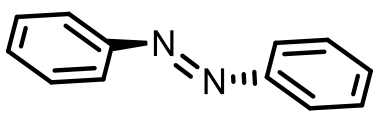
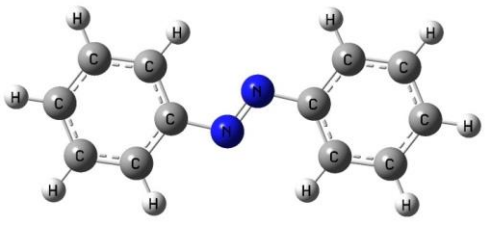
Electronic Energy = -1363.86036414

Internal Energy (E)= -1363.46913114

Enthalpy (H)= -1363.46801314

Gibbs Free Energy (G)=-1363.55647714

Gibbs Free Energy of Solvation=-1363.61478036

St. Pt.	General Structure	Ball & Stick model
Azobenzene		

Cartesian co-ordinate

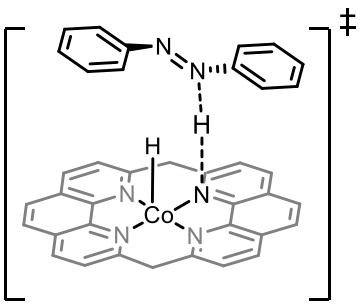
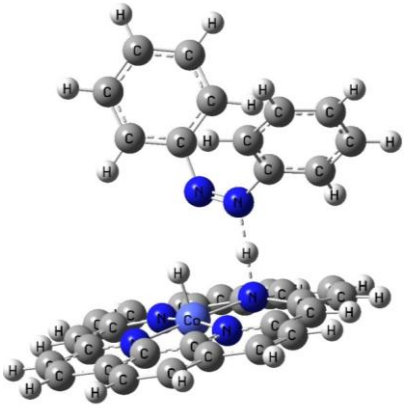
Atoms	X	Y	Z
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029
C	4.51876	-0.20015	-0.00010
H	4.06571	-2.30567	0.00068
H	4.66732	1.94739	-0.00073
H	5.59301	-0.35476	-0.00022
C	-1.76545	-0.18454	-0.00036
C	-2.28245	1.11551	-0.00005
C	-2.62311	-1.28332	-0.00051
C	-3.65737	1.30009	0.00033
H	-1.59539	1.95358	-0.00014
C	-4.00089	-1.09118	-0.00009
H	-2.18588	-2.27650	-0.00086
C	-4.51869	0.20052	0.00038
H	-4.06519	2.30595	0.00055
H	-4.66771	-1.94697	-0.00020
H	-5.59292	0.35526	0.00068
C	3.81972	-1.44756	-0.11029
C	2.43874	-3.43571	-0.12938
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889
H	5.97926	-1.26824	-0.25207
H	4.57397	-3.47685	-0.23081
C	2.50038	3.42118	-0.03734
H	4.62414	3.42615	-0.14688
H	5.97941	1.19435	-0.22462
H	2.41296	4.50196	-0.04125
N	1.39837	-1.30919	0.06494
N	1.39857	1.30012	0.04294
H	0.19989	0.13900	1.59991
C	-0.04820	-3.26690	-0.06233
H	-0.03262	-4.33522	-0.25561
C	0.02703	3.28554	0.04759
H	0.03107	4.36759	0.00562
H	-1.39197	-1.36276	1.51537

Frequencies

16.9448	62.0504	84.4054
100.8773	229.7836	259.8431
308.8900	312.3335	418.7603
421.5302	490.6024	535.0013
547.9514	563.8987	623.9784
630.4536	683.0236	704.4025
710.6771	786.6123	807.4848
847.9017	874.2953	875.0459
951.5498	960.9928	965.8592
1008.8559	1009.0403	1020.7389
1022.3690	1026.1828	1026.3066
1062.1989	1062.2752	1109.6373
1113.3389	1179.7828	1181.0265
1183.1966	1184.6324	1226.9590
1278.1210	1335.5058	1342.8464
1370.1954	1373.4340	1509.8878
1511.9310	1535.4371	1546.6110
1648.7542	1682.2422	1692.1464
1699.8227	1711.8268	3199.7222
3199.8030	3210.5688	3210.6082
3216.5711	3216.6016	3231.2453
3231.4265	3242.8675	3242.9861

Statistical Thermodynamic Analysis

Temperature = 353.15 K	Pressure = 1 atm
Zero-point correction = 0.192808	Electronic Energy = -572.525521298
Internal Energy (E) = -572.317828298	Enthalpy (H) = -572.316710298
Gibbs Free Energy (G) = -572.381131298	Gibbs Free Energy of Solvation = -572.386355339

St. Pt.	General Structure	Ball & Stick model
TS1$^{Hyd1(MLC)}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029
C	4.51876	-0.20015	-0.00010
H	4.06571	-2.30567	0.00068
H	4.66732	1.94739	-0.00073
H	5.59301	-0.35476	-0.00022
C	-1.76545	-0.18454	-0.00036
C	-2.28245	1.11551	-0.00005
C	-2.62311	-1.28332	-0.00051
C	-3.65737	1.30009	0.00033
H	-1.59539	1.95358	-0.00014
C	-4.00089	-1.09118	-0.00009
H	-2.18588	-2.27650	-0.00086
C	-4.51869	0.20052	0.00038
H	-4.06519	2.30595	0.00055

Frequencies

-666.0071	11.3531	16.5783
25.8128	38.7576	44.1879
51.4598	57.1238	63.4135
71.7880	77.3432	103.2822
120.8424	134.9565	157.7035
165.0465	200.2714	211.4236
215.3743	240.5628	246.9180
253.2002	255.0447	270.9319
280.1272	286.5473	303.9710
320.8081	337.3559	347.7053
371.9716	380.9165	399.1432
403.4036	408.7577	412.8884
419.4791	447.4673	450.5032
457.3156	468.0117	472.1510
479.2158	485.1075	489.6548
491.2162	510.4744	530.2146
537.1852	555.2847	573.3440
582.1232	585.1553	593.2898
597.9193	611.1140	614.6087
623.8860	625.6914	635.7988
671.4223	678.2471	684.6263
692.3949	705.0578	708.3166
711.3228	717.2734	721.0587
735.6271	741.2756	745.8826
754.9070	763.4629	771.7775
781.5155	787.0236	793.4566

H	-4.66771	-1.94697	-0.00020	797.8030	814.5556	820.3684
H	-5.59292	0.35526	0.00068	825.3549	833.3865	847.3669
C	3.81972	-1.44756	-0.11029	853.3899	860.9032	866.0132
C	2.43874	-3.43571	-0.12938	870.1845	875.6904	878.7197
C	3.82628	1.39527	-0.09170	883.8619	895.5861	897.6619
C	5.04592	-0.71999	-0.18079	916.9032	930.2455	941.2365
C	3.68573	-2.85612	-0.15703	953.1656	967.1883	979.8411
H	2.32963	-4.51250	-0.19077	987.4143	999.0664	1004.8574
C	3.72116	2.82537	-0.09574	1006.9249	1012.0558	1014.5572
C	5.04215	0.64935	-0.16783	1021.1176	1023.4092	1023.5028
C	1.27913	2.64979	0.02889	1026.3843	1027.4390	1032.6685
H	5.97926	-1.26824	-0.25207	1036.7221	1039.1649	1066.2380
H	4.57397	-3.47685	-0.23081	1067.7968	1112.9133	1121.2118
C	2.50038	3.42118	-0.03734	1125.2598	1128.3309	1143.7793
H	4.62414	3.42615	-0.14688	1155.8502	1170.4489	1172.9921
H	5.97941	1.19435	-0.22462	1182.5440	1186.0604	1187.2863
H	2.41296	4.50196	-0.04125	1189.0823	1195.7465	1200.9769
N	1.39837	-1.30919	0.06494	1222.8464	1224.9099	1241.8114
N	1.39857	1.30012	0.04294	1243.4681	1245.5800	1246.6438
H	0.19989	0.13900	1.59991	1254.6014	1262.0045	1270.7467
C	-0.04820	-3.26690	-0.06233	1278.8861	1298.0032	1320.9324
H	-0.03262	-4.33522	-0.25561	1327.5633	1346.0564	1348.7964
C	0.02703	3.28554	0.04759	1358.8760	1364.1475	1375.0200
H	0.03107	4.36759	0.00562	1392.7002	1411.3939	1418.9673
H	-1.39197	-1.36276	1.51537	1431.2596	1443.0647	1449.2288
				1460.4004	1463.8270	1479.4997
				1481.7964	1484.9287	1507.1731
				1510.0872	1512.0648	1532.4158
				1537.5891	1538.5353	1541.4203
				1572.5367	1576.6299	1616.0086
				1633.0218	1637.9732	1651.2968
				1671.1866	1673.0820	1675.3809
				1684.8254	1687.7462	1689.6903
				1700.9326	1705.0745	1715.0415
				1724.5179	1728.9111	2170.0152
				3205.2048	3206.2694	3211.9348
				3212.5704	3214.7400	3214.8060
				3216.2194	3220.4373	3222.7207
				3223.4204	3223.7653	3225.2508
				3226.2580	3226.4739	3228.7955
				3231.8367	3237.2024	3237.7969
				3238.4670	3239.1115	3240.9208
				3245.4038	3251.5416	3262.1338

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction = 0.551917

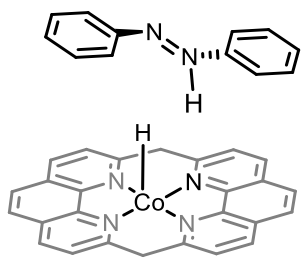
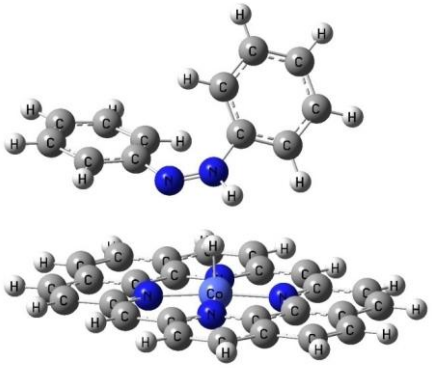
Electronic Energy = -1936.39019315

Internal Energy (E) = -1935.79316715

Enthalpy (H) = -1935.79204815

Gibbs Free Energy (G) =-1935.92150215

Gibbs Free Energy of Solvation = -1935.97318967

St. Pt.	General Structure	Ball & Stick model
$I2^{Hyd1(MLC)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029
C	4.51876	-0.20015	-0.00010
H	4.06571	-2.30567	0.00068
H	4.66732	1.94739	-0.00073
H	5.59301	-0.35476	-0.00022
C	-1.76545	-0.18454	-0.00036
C	-2.28245	1.11551	-0.00005
C	-2.62311	-1.28332	-0.00051
C	-3.65737	1.30009	0.00033
H	-1.59539	1.95358	-0.00014
C	-4.00089	-1.09118	-0.00009
H	-2.18588	-2.27650	-0.00086
C	-4.51869	0.20052	0.00038
H	-4.06519	2.30595	0.00055
H	-4.66771	-1.94697	-0.00020
H	-5.59292	0.35526	0.00068
C	3.81972	-1.44756	-0.11029
C	2.43874	-3.43571	-0.12938
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889

Frequencies

18.1218	28.9544	33.2073
41.5992	49.4314	58.8651
63.6069	71.9940	78.8198
95.7954	102.2133	118.9448
139.8833	163.1413	171.2855
186.1619	212.4416	220.5648
241.3052	250.7175	259.2827
260.6071	266.5373	278.5986
281.8122	296.1818	307.1399
337.9287	339.1830	350.2399
384.1976	405.9325	406.2034
406.4416	410.4934	415.0320
417.8131	447.7329	460.6103
462.2507	468.6182	476.8901
485.2696	487.9026	492.7527
494.5756	512.3833	535.7415
538.1853	557.7894	584.0756
585.2408	588.6728	594.3103
596.0402	598.9333	618.3504
623.2085	628.3542	678.2769
684.5920	686.3039	687.8981
695.3028	703.2232	712.0498
714.9204	722.7840	733.9654
741.2468	747.2384	755.5883
764.2851	767.1409	774.3392
776.7977	782.8614	788.3418
804.7201	812.0346	816.9275
831.4487	833.6672	852.9384
856.7003	861.4982	861.6657
868.2890	869.3525	873.5118
876.4565	884.4244	906.1346
907.9581	919.2704	943.0535
952.4696	968.5873	971.8417
978.1618	988.1263	1008.0757
1010.3465	1012.1966	1013.1282
1014.7150	1015.0118	1017.3568
1023.2051	1024.7739	1035.6810

H	5.97926	-1.26824	-0.25207	1042.3437	1044.5141	1064.9163
H	4.57397	-3.47685	-0.23081	1066.8899	1117.7275	1128.7765
C	2.50038	3.42118	-0.03734	1131.2335	1137.1833	1143.0043
H	4.62414	3.42615	-0.14688	1159.3249	1167.4967	1173.9437
H	5.97941	1.19435	-0.22462	1182.6884	1186.1213	1187.8571
H	2.41296	4.50196	-0.04125	1191.2703	1192.8806	1206.4220
N	1.39837	-1.30919	0.06494	1224.9543	1231.3683	1238.3270
N	1.39857	1.30012	0.04294	1243.4036	1246.9290	1253.7309
H	0.19989	0.13900	1.59991	1257.6313	1258.7708	1275.8257
C	-0.04820	-3.26690	-0.06233	1300.6323	1303.4922	1331.5460
H	-0.03262	-4.33522	-0.25561	1348.4311	1356.0230	1369.6792
C	0.02703	3.28554	0.04759	1383.1198	1386.9782	1397.5228
H	0.03107	4.36759	0.00562	1417.0657	1422.4673	1433.0898
H	-1.39197	-1.36276	1.51537	1451.8443	1456.5310	1461.9981
				1470.3951	1474.9578	1479.3693
				1480.4016	1487.1887	1504.3788
				1511.2046	1516.4257	1526.7160
				1529.6192	1542.8817	1552.1389
				1566.7350	1568.4404	1577.1638
				1604.5136	1616.3316	1639.2671
				1654.4278	1659.7471	1677.0964
				1681.9251	1686.3884	1695.8148
				1698.0281	1702.8593	1708.5271
				1717.1012	2068.2866	3201.0912
				3203.5940	3203.7980	3207.0150
				3207.5889	3208.1541	3209.7395
				3216.5364	3219.4073	3225.8707
				3227.3334	3227.3883	3229.4847
				3230.7098	3231.1917	3231.3318
				3232.0987	3236.1719	3242.1989
				3247.1960	3248.6964	3251.4232
				3255.7470	3258.5132	3394.4564

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction = 0.557150

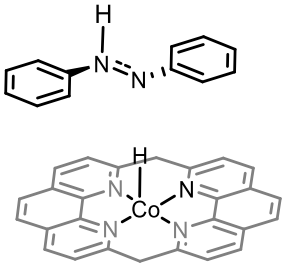
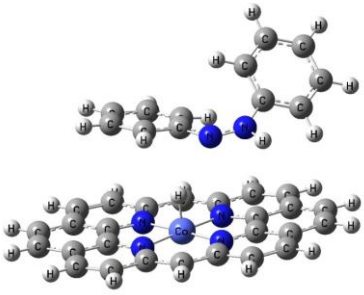
Electronic Energy = -1936.41057117

Internal Energy (E) = -1935.80815017

Enthalpy (H) = -1935.80703217

Gibbs Free Energy (G) = -1935.93456917

Gibbs Free Energy of Solvation = -1935.99093972

St. Point	General Structure	Ball & Stick model
$I3^{Hyd1(MLC)}$		

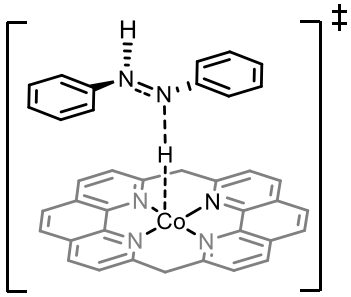
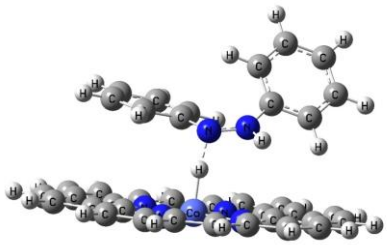
Cartesian coordinate			
Atoms	**X**	**Y**	**Z**
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029
C	4.51876	-0.20015	-0.00010
H	4.06571	-2.30567	0.00068
H	4.66732	1.94739	-0.00073
H	5.59301	-0.35476	-0.00022
C	-1.76545	-0.18454	-0.00036
C	-2.28245	1.11551	-0.00005
C	-2.62311	-1.28332	-0.00051
C	-3.65737	1.30009	0.00033
H	-1.59539	1.95358	-0.00014
C	-4.00089	-1.09118	-0.00009
H	-2.18588	-2.27650	-0.00086
C	-4.51869	0.20052	0.00038
H	-4.06519	2.30595	0.00055
H	-4.66771	-1.94697	-0.00020
H	-5.59292	0.35526	0.00068
C	3.81972	-1.44756	-0.11029
C	2.43874	-3.43571	-0.12938
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889
H	5.97926	-1.26824	-0.25207
H	4.57397	-3.47685	-0.23081
C	2.50038	3.42118	-0.03734
H	4.62414	3.42615	-0.14688
H	5.97941	1.19435	-0.22462
H	2.41296	4.50196	-0.04125
N	1.39837	-1.30919	0.06494
N	1.39857	1.30012	0.04294
H	0.19989	0.13900	1.59991
C	-0.04820	-3.26690	-0.06233
H	-0.03262	-4.33522	-0.25561
C	0.02703	3.28554	0.04759
H	0.03107	4.36759	0.00562
H	-1.39197	-1.36276	1.51537

Frequencies		
31.1607	33.1570	40.0874
43.2839	52.6526	60.5361
73.3689	79.8647	95.1561
108.0867	113.9586	138.0017
139.6030	159.8553	167.9283
185.9321	212.4604	231.3946
241.9960	250.4744	257.0463
258.9070	266.1700	272.1911
284.0949	297.1456	308.1735
338.7804	339.1362	353.4966
384.5352	399.1381	406.1455
409.6372	409.9060	420.0620
426.1417	448.6867	457.2970
462.7641	474.1949	481.2938
487.3703	489.1667	492.5477
495.8253	512.8656	535.5256
538.9590	559.4769	570.1513
583.8830	585.9661	595.3548
596.3689	599.2854	617.1871
624.4320	626.7629	671.3362
680.5604	686.9032	687.8423
689.2854	706.1534	712.9492
715.4191	719.7090	728.1459
740.9852	744.0567	748.9364
750.2021	757.5746	769.2241
773.9988	775.6215	778.2912
801.6542	806.4143	814.0750
817.0683	829.5457	834.5474
843.3203	856.0795	861.1539
869.7344	870.8215	875.8187
876.1593	884.4316	902.7695
908.1815	921.8111	945.1172
953.0755	958.8450	969.7011
976.2452	985.8374	999.7415
1009.1456	1011.3700	1014.2246
1015.1200	1017.5885	1018.2014
1019.3145	1022.1480	1027.8204
1038.9577	1042.0311	1061.5360
1070.3961	1119.9662	1131.7728
1133.8296	1140.0615	1145.4788
1159.8676	1171.7609	1174.6443
1180.5735	1185.3015	1187.1790
1193.8370	1196.0198	1205.2003
1226.6114	1237.1806	1243.1275
1245.4551	1246.6225	1258.8665
1260.6130	1263.4892	1272.4608
1298.3671	1302.5618	1328.7542
1345.8633	1356.1148	1372.7430
1382.0876	1389.6580	1399.0198
1415.2387	1421.3938	1433.0715
1452.2334	1458.3351	1465.7970
1471.9279	1477.7674	1479.8581
1483.7182	1490.9524	1497.7839

1507.0269	1514.2266	1519.0414
1527.1326	1537.0935	1545.4659
1565.9493	1567.1655	1574.3473
1588.9606	1621.4036	1634.0814
1639.5508	1657.9102	1675.2242
1682.1485	1685.8752	1694.0688
1695.9200	1702.7448	1705.2181
1719.5471	2249.0576	3199.6997
3200.3206	3208.6026	3209.1524
3212.2947	3215.8716	3218.4257
3218.5747	3218.8240	3221.8139
3225.0746	3227.2771	3227.7197
3228.6611	3230.8406	3234.1111
3234.9477	3235.3838	3239.1855
3241.0881	3247.6173	3250.7019
3257.6046	3259.7405	3518.1342

Statistical Thermodynamic Analysis

Temperature = 353.15 K
Pressure = 1 atm
Zero-point correction = 0.557664
Electronic Energy = -1936.40851433
Internal Energy (E) = -1935.80573933
Enthalpy (H) = -1935.80462033
Gibbs Free Energy (G) = -1935.93014833
Gibbs Free Energy of Solvation = -1935.98701898

St. Pt.	General Structure	Ball & Stick model
TS2$^{Hyd1(MLC)}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029

Frequencies

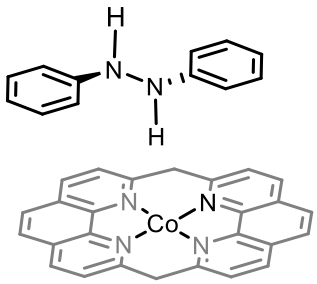
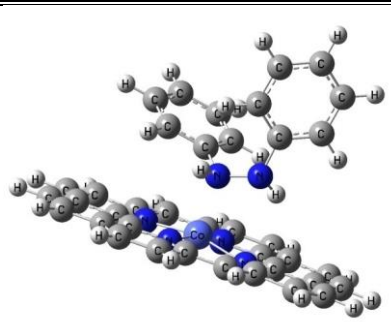
-849.9495	22.0438	30.7946
38.5460	45.8870	55.9739
62.0262	68.6720	74.0029
79.7364	106.1964	122.1954
133.4944	154.7033	163.7467
164.1962	189.1081	216.8029
231.7628	241.1125	249.9601
258.0443	265.0051	266.7090
278.7151	297.1168	305.2679
316.7623	335.3625	337.4558
356.2527	379.7081	404.7338
405.6264	407.6589	420.1606
437.5966	443.6819	456.9931

C	4.51876	-0.20015	-0.00010	460.2910	462.6156	478.8746
H	4.06571	-2.30567	0.00068	479.9311	485.3730	487.1899
H	4.66732	1.94739	-0.00073	490.6073	508.5719	520.7170
H	5.59301	-0.35476	-0.00022	531.2266	534.3611	557.3763
C	-1.76545	-0.18454	-0.00036	577.6541	583.0106	584.2658
C	-2.28245	1.11551	-0.00005	589.0546	595.3560	595.7552
C	-2.62311	-1.28332	-0.00051	610.6514	620.3055	624.9664
C	-3.65737	1.30009	0.00033	633.0487	677.7186	684.5392
H	-1.59539	1.95358	-0.00014	686.3914	699.4967	710.1587
C	-4.00089	-1.09118	-0.00009	711.6770	715.7859	716.3417
H	-2.18588	-2.27650	-0.00086	735.4103	743.4431	746.6183
C	-4.51869	0.20052	0.00038	759.7126	765.9381	774.9063
H	-4.06519	2.30595	0.00055	779.2135	784.1360	788.2332
H	-4.66771	-1.94697	-0.00020	806.6618	818.5704	821.2116
H	-5.59292	0.35526	0.00068	828.6103	842.2204	857.0561
C	3.81972	-1.44756	-0.11029	859.9107	865.7437	872.2479
C	2.43874	-3.43571	-0.12938	873.4667	875.1367	878.7688
C	3.82628	1.39527	-0.09170	888.2435	903.2706	909.2636
C	5.04592	-0.71999	-0.18079	910.2556	921.3793	945.1521
C	3.68573	-2.85612	-0.15703	952.1354	962.1644	973.1493
H	2.32963	-4.51250	-0.19077	976.0693	993.0715	1009.4133
C	3.72116	2.82537	-0.09574	1010.8533	1013.8242	1014.5981
C	5.04215	0.64935	-0.16783	1014.9842	1015.6243	1018.8271
C	1.27913	2.64979	0.02889	1019.4424	1022.5672	1027.0178
H	5.97926	-1.26824	-0.25207	1032.6437	1033.5793	1065.3425
H	4.57397	-3.47685	-0.23081	1069.0553	1120.4002	1127.8288
C	2.50038	3.42118	-0.03734	1130.6918	1131.7533	1139.1913
H	4.62414	3.42615	-0.14688	1140.3883	1155.9998	1158.0241
H	5.97941	1.19435	-0.22462	1178.2415	1181.5464	1187.4743
H	2.41296	4.50196	-0.04125	1187.7979	1189.3581	1200.6919
N	1.39837	-1.30919	0.06494	1207.4150	1225.2021	1232.5856
N	1.39857	1.30012	0.04294	1241.5009	1245.1708	1246.4370
H	0.19989	0.13900	1.59991	1255.1796	1259.3628	1261.1558
C	-0.04820	-3.26690	-0.06233	1277.4984	1292.6839	1305.0278
H	-0.03262	-4.33522	-0.25561	1330.7174	1344.4891	1353.2067
C	0.02703	3.28554	0.04759	1369.6629	1377.1259	1395.6835
H	0.03107	4.36759	0.00562	1400.4183	1405.3249	1411.7191
H	-1.39197	-1.36276	1.51537	1422.1110	1437.4147	1439.9795
				1461.4012	1462.5364	1469.4991
				1473.6258	1477.7818	1486.1516
				1495.9089	1502.3839	1511.1878
				1515.2988	1517.6208	1528.6776
				1536.4835	1544.4723	1568.4035
				1576.9077	1580.3945	1605.4475
				1620.9800	1650.4281	1652.8822
				1660.2600	1682.0648	1684.8966
				1687.8376	1688.6580	1692.9687
				1697.6880	1710.2741	3201.8787
				3208.1984	3209.8829	3211.7423
				3213.2832	3215.5586	3216.2823
				3217.4121	3218.0575	3220.4928
				3221.0864	3222.5722	3222.6202
				3228.3582	3228.9804	3230.7854
				3231.6727	3235.8974	3237.6570

	3237.6992	3242.6738	3242.8864
	3249.3440	3253.1638	3550.8419

Statistical Thermodynamic Analysis

Temperature = 353.15 K	Pressure = 1 atm
Zero-point correction = 0.553355	Electronic Energy = -1936.39831071
Internal Energy (E) = -1935.80010371	Enthalpy (H) = -1935.79898571
Gibbs Free Energy (G) = -1935.92445371	Gibbs Free Energy of Solvation = -1935.97735028

St. Pt.	General Structure	Ball & Stick model
I4$^{Hyd1(MLC)}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	-0.37540	-0.49712	-0.00066
N	0.37532	0.49678	0.00042
C	1.76540	0.18428	0.00020
C	2.28268	-1.11567	0.00052
C	2.62286	1.28323	-0.00014
C	3.65764	-1.29991	0.00039
H	1.59580	-1.95391	0.00087
C	4.00071	1.09144	-0.00036
H	2.18529	2.27626	-0.00029
C	4.51876	-0.20015	-0.00010
H	4.06571	-2.30567	0.00068
H	4.66732	1.94739	-0.00073
H	5.59301	-0.35476	-0.00022
C	-1.76545	-0.18454	-0.00036
C	-2.28245	1.11551	-0.00005
C	-2.62311	-1.28332	-0.00051
C	-3.65737	1.30009	0.00033
H	-1.59539	1.95358	-0.00014
C	-4.00089	-1.09118	-0.00009
H	-2.18588	-2.27650	-0.00086
C	-4.51869	0.20052	0.00038
H	-4.06519	2.30595	0.00055

Frequencies

-17.6522	25.5789	28.0367
41.7139	47.9439	61.8288
65.3623	83.4470	88.3408
98.6831	103.5785	128.6043
153.7812	167.9630	184.8492
195.7755	216.4606	230.2787
248.0924	252.2502	255.3021
263.5521	275.4594	277.9176
288.1629	303.0727	334.3010
346.4800	352.7944	356.9843
386.2347	408.8669	409.3418
413.1752	414.4539	418.2877
448.0857	454.1572	460.4233
466.2541	482.5498	486.6498
487.3726	491.7659	496.1500
507.0136	527.2982	540.5481
555.8059	563.2996	575.0740
582.8615	585.8240	587.3206
594.6087	596.3146	622.2509
623.7360	630.2092	673.9146
677.4598	684.5717	685.9924
704.8219	712.5861	715.1856
715.9234	717.3958	722.9052
744.5109	745.7673	758.4223
765.9277	780.3759	783.4295
785.0558	787.4438	813.4189
821.1255	825.8091	837.5816

H	-4.66771	-1.94697	-0.00020	840.0622	845.6028	851.7650
H	-5.59292	0.35526	0.00068	859.4777	862.9646	863.3542
C	3.81972	-1.44756	-0.11029	879.6425	881.7648	882.1104
C	2.43874	-3.43571	-0.12938	892.2643	908.7031	914.7334
C	3.82628	1.39527	-0.09170	921.7044	932.6184	941.5967
C	5.04592	-0.71999	-0.18079	948.6197	984.7645	987.0151
C	3.68573	-2.85612	-0.15703	987.6782	987.8209	1008.5031
H	2.32963	-4.51250	-0.19077	1015.1116	1016.4064	1018.8087
C	3.72116	2.82537	-0.09574	1021.1428	1021.3929	1022.0645
C	5.04215	0.64935	-0.16783	1022.5177	1023.0419	1041.2692
C	1.27913	2.64979	0.02889	1058.3518	1067.1537	1080.3945
H	5.97926	-1.26824	-0.25207	1113.8697	1123.3081	1128.0225
H	4.57397	-3.47685	-0.23081	1136.1529	1147.6767	1161.9074
C	2.50038	3.42118	-0.03734	1167.1569	1174.7656	1184.6628
H	4.62414	3.42615	-0.14688	1185.6264	1186.8909	1191.0672
H	5.97941	1.19435	-0.22462	1196.6384	1199.1616	1213.8717
H	2.41296	4.50196	-0.04125	1233.2605	1234.4053	1241.3603
N	1.39837	-1.30919	0.06494	1251.5026	1255.3203	1263.5126
N	1.39857	1.30012	0.04294	1264.6419	1285.1862	1292.5142
H	0.19989	0.13900	1.59991	1304.6481	1311.3677	1337.1188
C	-0.04820	-3.26690	-0.06233	1338.7641	1347.9485	1366.2881
H	-0.03262	-4.33522	-0.25561	1369.8074	1389.9625	1398.7026
C	0.02703	3.28554	0.04759	1420.6495	1430.1896	1432.9024
H	0.03107	4.36759	0.00562	1433.4577	1443.7844	1460.5766
H	-1.39197	-1.36276	1.51537	1462.2560	1464.9609	1468.5811
				1479.9319	1486.8391	1495.3600
				1501.0406	1515.2238	1524.2754
				1531.5409	1545.3399	1555.9675
				1557.6857	1565.4401	1576.5374
				1581.7121	1626.1324	1627.1294
				1660.2851	1673.1052	1692.7839
				1695.2462	1699.1455	1700.4143
				1703.0282	1705.7810	1707.1783
				1716.9189	3175.6188	3181.2960
				3201.5876	3206.7615	3207.7928
				3211.7070	3215.2047	3216.0813
				3217.8510	3219.6151	3220.8211
				3220.8624	3220.9011	3222.8318
				3223.0942	3224.2713	3225.6226
				3227.6918	3239.5658	3240.4170
				3240.5779	3245.9413	3247.8513
				3248.8113	3500.9540	3575.4312

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction = 0.562389

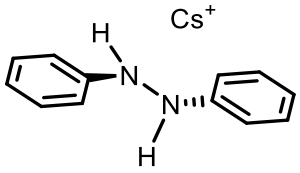
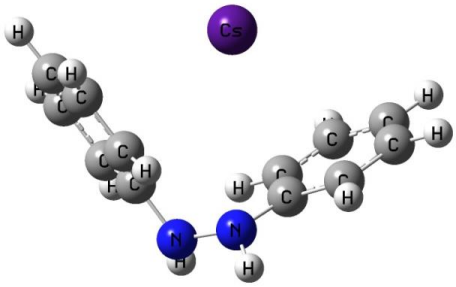
Electronic Energy = -1936.47746412

Internal Energy (E) = -1935.87143412

Enthalpy (H) = -1935.87031612

Gibbs Free Energy (G) = -1935.99242912

Gibbs Free Energy of Solvation = -1936.04759042

St. Pt.	General Structure	Ball & Stick model
Hydrazobenzene (Cs⁺-coordinated)		

Cartesian co-ordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964

Frequencies

29.2412	39.6213	43.3109
62.2534	100.9270	110.7705
175.9298	214.4776	251.0566
327.0320	396.4422	420.8715
423.5349	454.8735	478.1922
527.9849	531.2374	594.3131
624.1514	629.0093	661.8544
712.5827	713.9675	766.0431
786.4989	792.8066	852.1004
862.8007	868.3576	877.3254
919.3970	929.0565	999.5661
1000.7311	1009.1618	1010.3103
1019.8123	1023.4213	1063.9766
1069.7219	1111.8962	1125.7243
1176.9051	1186.5460	1198.1817
1201.6196	1214.0833	1281.2209
1322.9463	1340.3414	1351.4336
1360.6387	1372.6873	1462.7916
1479.1599	1526.8517	1535.8371
1554.1096	1556.5407	1671.7775
1678.6381	1692.3932	1699.2944
3190.8341	3209.1996	3211.3112
3215.5966	3219.8443	3225.1768
3229.2065	3234.5222	3235.2384
3242.1098	3520.6391	3631.4036

H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.218343

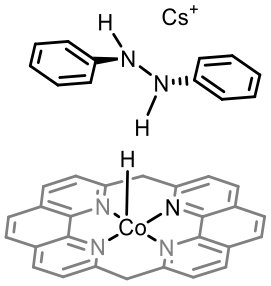
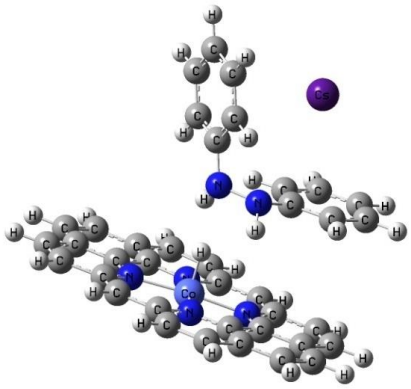
Electronic Energy = -593.434389987

Internal Energy (E) = -593.192797987

Enthalpy (H) = -593.191520987

Gibbs Free Energy (G) = -593.281147987

Gibbs Free Energy of Solvation = -593.361060111

St. Pt.	General Structure	Ball & Stick model
I2$^{\text{Hyd2(spill)}}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583

Frequencies

13.8271	20.3766	22.5781
26.2347	43.4408	45.4681
48.4922	53.9949	56.5788
66.4660	72.7185	97.3163
110.7590	113.6621	119.6405
139.5463	163.2853	169.7066
196.5289	217.8244	232.8507
242.4713	248.6808	257.2763
258.0857	264.6861	267.0677
282.1914	305.8551	338.4345

H	-1.75333	1.79240	2.17372	339.4514	348.6568	351.7180
C	-2.96423	0.07010	-1.07621	385.5111	407.9080	408.5428
H	-1.56292	1.36600	-2.09154	410.8868	414.1270	423.0692
C	-3.51235	-0.30873	0.15241	430.2692	449.1763	460.1837
H	-3.50543	0.05370	2.27510	461.5406	478.9797	485.0492
H	-3.33006	-0.37886	-1.99522	486.0454	488.5880	493.8993
H	-4.29697	-1.05644	0.19757	495.1548	531.9434	535.7534
C	1.55284	1.51899	-0.26755	536.9581	545.9328	558.9439
C	2.57342	1.03639	-1.10339	585.7968	586.5736	596.0953
C	1.52644	1.11662	1.07431	598.1054	598.8223	608.7432
C	3.53929	0.17265	-0.60458	625.8695	629.0783	630.5169
H	2.59701	1.34604	-2.14455	669.0208	679.3440	688.8093
C	2.50452	0.24790	1.56385	690.6683	710.4199	712.0250
H	0.75747	1.48483	1.74416	715.0602	715.8416	725.5868
C	3.50750	-0.23907	0.73169	732.8584	748.7240	751.1911
H	4.32665	-0.18078	-1.26264	754.0172	764.1211	770.6820
H	2.48615	-0.03088	2.61352	771.1741	779.3029	785.0860
H	4.27156	-0.90311	1.12010	797.6077	803.0022	816.6104
H	0.84940	3.04753	-1.46726	823.5940	831.1682	833.6307
H	-0.31192	3.11093	0.83413	857.7510	860.3059	861.3582
Cs	-0.01646	-1.68112	-0.13529	868.6957	868.8119	871.1788
C	-5.04390	0.68674	-0.04268	873.5722	874.3388	882.3388
C	-3.70087	2.84513	-0.02388	886.2683	907.8410	912.7775
H	-2.37687	4.51148	-0.00260	920.5868	929.8828	943.1706
C	-3.70086	-2.84511	-0.02396	951.4555	976.2696	979.5196
C	-5.04390	-0.68672	-0.04268	995.0402	1001.2520	1007.5970
C	-1.25756	-2.64674	0.00047	1010.5893	1011.9280	1014.1764
H	-5.98116	1.23509	-0.05313	1015.4586	1016.2479	1017.9738
H	-4.60015	3.45511	-0.02958	1019.5777	1020.2896	1042.4615
C	-2.47341	-3.43094	-0.00962	1066.7582	1067.6557	1115.7446
H	-4.60014	-3.45510	-0.02964	1117.8117	1124.5034	1138.4382
H	-5.98117	-1.23506	-0.05312	1145.4041	1158.4571	1170.7955
H	-2.37687	-4.51149	-0.00276	1172.1011	1178.2742	1182.7559
N	-1.38780	1.30028	-0.01186	1183.4860	1186.8354	1199.3878
N	-1.38782	-1.30028	-0.01191	1204.7314	1208.7459	1236.6233
H	0.00022	-0.00008	1.45530	1241.6355	1243.7588	1246.2322
C	-0.00001	3.27742	0.01504	1259.2440	1259.7794	1276.7449
H	-0.00000	4.36099	0.02340	1288.5388	1299.7185	1303.9122
C	-0.00000	-3.27741	0.01489	1323.8913	1330.5933	1347.0241
H	0.00001	-4.36099	0.02318	1351.3270	1367.2971	1374.1674
				1384.3446	1396.0154	1415.3927
				1421.2270	1428.4651	1451.8544
				1458.1874	1461.6298	1469.0460
				1471.8868	1478.0418	1480.5349
				1482.9150	1484.1657	1486.8871
				1518.6285	1525.5500	1532.0278
				1537.1292	1552.9868	1560.4203
				1568.3217	1572.1524	1576.1941
				1625.7119	1633.9660	1656.5682
				1670.9551	1674.8748	1681.4528
				1693.2240	1696.7107	1699.4692
				1704.8608	1709.2951	1719.1881
				2123.1118	3195.7734	3199.2152
				3199.5760	3206.0078	3208.1606
				3209.7111	3212.1161	3212.8071

	3213.2648	3213.7789	3214.1751
	3220.5554	3222.5971	3226.8241
	3227.3400	3228.2107	3230.2601
	3230.7116	3233.6698	3233.6942
	3236.1545	3238.8052	3238.9457
	3245.2017	3537.9562	3543.8599

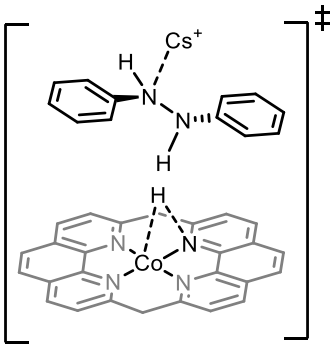
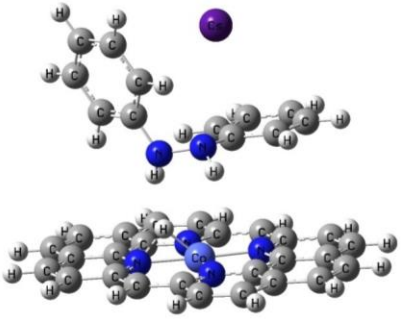
Statistical Thermodynamic Analysis

Temperature = 403.15 K — Pressure = 1 atm

Zero-point correction = 0.569786 — Electronic Energy = -1956.96386558

Internal Energy (E) = -1956.33119458 — Enthalpy (H)= -1956.32991758

Gibbs Free Energy (G) = -1956.50358058 — Gibbs Free Energy of Solvation = -1956.58227248

St. Pt.	General Structure	Ball & Stick model
TS1$^{\text{Hyd2(spill)}}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455

Frequencies

-1083.2170	9.4802	18.5701
20.3095	25.3218	25.6899
34.9723	45.5456	55.6538
58.1433	65.2052	71.5419
96.9243	100.3832	109.0321
120.5234	135.6660	161.2958
167.0215	195.0990	215.4456
230.9862	239.4907	241.5734
250.8787	259.1873	263.7488
273.4057	282.4345	301.6842
319.1887	337.7094	343.7338
355.8336	383.1358	402.5473
405.9779	407.1226	410.7808
419.9268	425.0906	447.5014
458.4065	466.7658	479.3554
483.2752	489.3987	493.8369
497.2289	498.3172	521.0546
534.8538	536.4488	558.7400
560.9050	581.8591	583.6206
594.7505	597.8062	600.6738
602.0685	625.6219	626.7678
631.8562	677.0865	683.4104

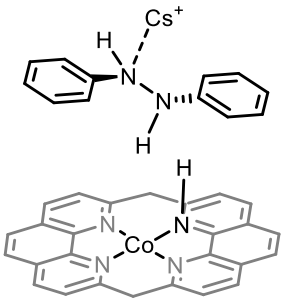
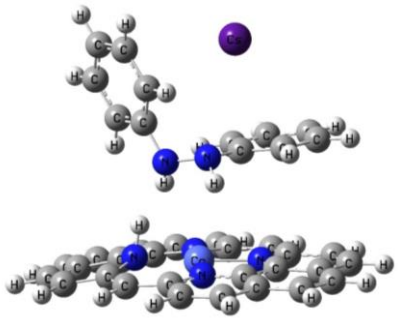
C	2.50452	0.24790	1.56385	687.1828	690.1052	706.1066
H	0.75747	1.48483	1.74416	710.7242	714.5867	718.6714
C	3.50750	-0.23907	0.73169	721.5533	736.4772	746.3041
H	4.32665	-0.18078	-1.26264	753.3468	765.0727	766.7684
H	2.48615	-0.03088	2.61352	774.1054	777.6953	788.7352
H	4.27156	-0.90311	1.12010	796.3111	802.9633	816.1316
H	0.84940	3.04753	-1.46726	826.0400	834.8895	846.5780
H	-0.31192	3.11093	0.83413	856.6342	857.4102	865.3693
	-0.01646	-1.68112	-0.13529	870.0265	871.1561	874.0781
C	-5.04390	0.68674	-0.04268	878.5317	885.6121	901.9616
C	-3.70087	2.84513	-0.02388	904.1974	907.0207	917.0123
H	-2.37687	4.51148	-0.00260	931.3005	937.9658	949.5569
C	-3.70086	-2.84511	-0.02396	971.4989	984.0937	986.2994
C	-5.04390	-0.68672	-0.04268	996.3287	1001.7171	1004.9418
C	-1.25756	-2.64674	0.00047	1012.6505	1013.6393	1014.4942
H	-5.98116	1.23509	-0.05313	1014.9163	1016.1984	1023.5321
H	-4.60015	3.45511	-0.02958	1024.1926	1027.7824	1055.9434
C	-2.47341	-3.43094	-0.00962	1068.1433	1068.6080	1115.5231
H	-4.60014	-3.45510	-0.02964	1124.0503	1124.7295	1132.1037
H	-5.98117	-1.23506	-0.05312	1139.0822	1161.6511	1168.8197
H	-2.37687	-4.51149	-0.00276	1175.2486	1180.0966	1180.7077
N	-1.38780	1.30028	-0.01186	1186.1355	1188.6644	1198.4489
N	-1.38782	-1.30028	-0.01191	1207.6328	1209.7054	1229.7773
H	0.00022	-0.00008	1.45530	1236.7406	1242.1507	1245.6689
C	-0.00001	3.27742	0.01504	1254.8106	1255.1355	1273.7226
H	-0.00000	4.36099	0.02340	1287.8770	1294.5209	1299.0236
C	-0.00000	-3.27741	0.01489	1324.2290	1326.0988	1346.1102
H	0.00001	-4.36099	0.02318	1350.4016	1370.8756	1376.1084
				1378.6362	1395.3215	1410.7833
				1416.2382	1431.8756	1448.2977
				1454.4049	1462.4283	1466.0306
				1473.2480	1479.0649	1480.3236
				1483.3968	1489.4435	1494.4268
				1519.1004	1525.1386	1534.1163
				1540.7488	1553.2304	1563.8959
				1567.5624	1570.8803	1579.1260
				1620.6550	1641.5777	1654.7874
				1673.3880	1676.8467	1680.1005
				1694.6772	1695.3877	1700.1733
				1701.9908	1708.4488	1718.4833
				1886.7953	3186.9889	3197.7886
				3203.0683	3205.4009	3206.3740
				3208.5781	3209.5102	3210.5491
				3214.6343	3217.4754	3219.7078
				3221.1692	3221.8272	3222.2566
				3222.7259	3226.7786	3227.9266
				3230.1069	3233.1690	3234.0685
				3237.9671	3238.6241	3239.0812
				3246.6754	3517.6099	3537.7915

Statistical Thermodynamic Analysis

Temperature = 403.15 K Pressure = 1 atm

Zero-point correction = 0.567505 Electronic Energy = -1956.93909238

Internal Energy (E) = -1956.30879938	Enthalpy (H)= -1956.30752238
Gibbs Free Energy (G) = -1956.48294638	Gibbs Free Energy of Solvation = -1956.56145611

St. Pt.	General Structure	Ball & Stick model
$I3^{Hyd2(spill)}$		

Cartesian co-ordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260

Frequencies

9.5430	15.9379	24.3918
25.9351	34.8880	39.5021
42.7461	58.4464	60.1874
65.8414	70.7727	96.4209
100.0190	108.7134	118.2872
129.3801	152.7403	161.9348
194.7158	213.8416	226.8360
229.8801	235.5921	239.5362
247.9296	257.2056	268.8008
274.2089	291.3365	318.5299
326.0172	337.2729	346.3207
365.6299	386.1482	391.1961
403.1911	409.2118	421.5191
426.2789	435.1487	442.0762
452.1768	468.4219	477.0905
481.5697	486.6884	492.4956
497.0483	521.4530	528.3279
536.3642	548.1147	561.3582
573.9991	581.7234	582.2470
592.6348	598.6628	606.1366
617.6695	625.3572	631.6324
645.6258	652.1660	678.0389
685.9998	697.6370	703.5735
708.0930	713.5717	714.8684
724.0509	728.9022	734.0772
750.4734	762.1082	767.1423
787.2726	797.5459	798.8987
804.3427	813.8747	818.6539
823.0515	838.8081	847.7541
849.2218	853.8247	857.0908
867.6004	870.9632	879.1056
882.0299	899.7088	902.8557
910.7943	912.0934	934.3929
935.9074	946.2246	951.0911

C	-3.70086	-2.84511	-0.02396	978.4561	984.3571	985.6458
C	-5.04390	-0.68672	-0.04268	997.8774	1003.7938	1004.6704
C	-1.25756	-2.64674	0.00047	1007.4773	1008.1604	1009.5169
H	-5.98116	1.23509	-0.05313	1013.5255	1013.6778	1014.3810
H	-4.60015	3.45511	-0.02958	1021.5423	1024.9851	1066.6486
C	-2.47341	-3.43094	-0.00962	1069.4176	1099.6252	1113.7446
H	-4.60014	-3.45510	-0.02964	1122.1790	1125.6893	1134.1873
H	-5.98117	-1.23506	-0.05312	1145.8542	1164.8116	1171.4786
H	-2.37687	-4.51149	-0.00276	1175.4712	1178.2525	1180.4978
N	-1.38780	1.30028	-0.01186	1187.0011	1193.6947	1205.3873
N	-1.38782	-1.30028	-0.01191	1214.2729	1216.2394	1228.3455
H	0.00022	-0.00008	1.45530	1236.4478	1239.4203	1254.2319
C	-0.00001	3.27742	0.01504	1255.8066	1265.2914	1266.8298
H	-0.00000	4.36099	0.02340	1284.1310	1285.9466	1314.8589
C	-0.00000	-3.27741	0.01489	1322.5059	1341.3375	1345.0020
H	0.00001	-4.36099	0.02318	1350.4917	1368.5961	1373.2153
				1384.7541	1388.1277	1395.0697
				1410.1791	1430.7406	1438.8992
				1442.7105	1457.2110	1457.9115
				1464.7836	1471.2925	1475.9017
				1487.8993	1491.4244	1505.2633
				1507.8614	1527.6487	1532.9284
				1538.8790	1551.8113	1561.4546
				1567.3828	1569.2962	1612.2102
				1625.2911	1640.5060	1662.5695
				1673.4131	1675.4358	1680.8646
				1692.4898	1694.3851	1695.1019
				1700.6503	1705.0869	1720.6091
				3189.7891	3199.5842	3199.8026
				3200.5293	3203.1136	3203.6055
				3204.1358	3208.4232	3209.1153
				3211.1776	3211.6099	3213.4099
				3216.0550	3218.8709	3219.4942
				3223.8521	3223.9758	3224.7102
				3225.0661	3227.9376	3228.8998
				3229.6301	3233.7505	3246.4720
				3262.5058	3428.6663	3505.2292

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.571107

Electronic Energy = -1956.94875510

Internal Energy (E) = -1956.3142021

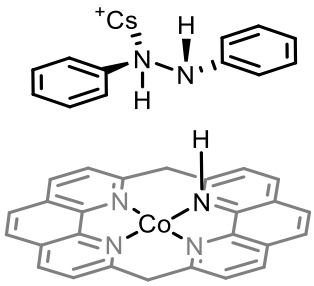
Enthalpy (H) = -1956.3129251

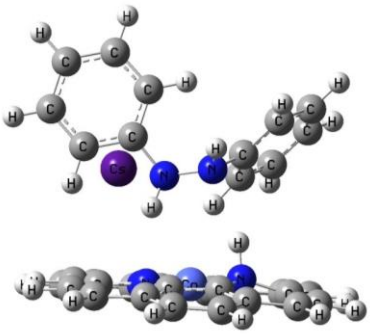
Gibbs Free Energy (G) = -1956.4891671

Gibbs Free Energy of Solvation = -1956.56826114

St. Pt.	General Structure	Ball & Stick model

I4[Hyd2(spill)]





Cartesian co-ordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964

Frequencies

11.0390	19.6496	24.7503
32.3097	35.6816	42.6149
48.4134	52.0157	56.8605
70.2975	78.0930	89.2647
100.5273	105.4812	123.6460
133.2044	150.7662	160.0560
191.6208	207.3241	213.5531
229.1245	235.0726	240.2171
251.6738	261.0257	268.6947
278.0209	293.1823	306.5219
316.8388	339.9137	344.3346
367.1305	383.2132	384.9534
392.0605	403.9129	420.0248
428.3811	440.0567	443.0074
454.1561	467.3776	479.5863
481.1304	486.2126	492.8663
501.9607	525.9834	529.8888
531.8262	548.0775	564.1212
574.8792	581.8898	588.9678
591.9960	600.4719	615.8729
619.8139	628.3364	641.9121
653.5846	656.6585	676.0336
689.6192	704.7468	710.0166
712.7193	714.5591	721.6651
728.3099	730.2608	742.6527
757.9260	760.8051	772.7544
787.5428	794.6565	795.0482
802.0273	804.6695	815.9977
822.9134	838.4877	849.5618
852.7554	857.7926	867.1738
868.8964	874.6799	876.3456
877.6939	893.3778	895.1788
906.0879	910.6115	925.4785
938.8583	944.2143	948.7480
981.5683	984.5027	1000.9392
1002.5554	1004.0313	1006.8510
1010.4636	1011.1932	1011.3930
1015.3352	1016.8883	1018.8610
1024.0901	1027.4974	1064.8973
1072.4699	1102.3789	1110.1001
1124.7411	1127.1188	1133.8282

H	-5.98117	-1.23506	-0.05312	1144.2727	1168.2513	1178.7039
H	-2.37687	-4.51149	-0.00276	1180.0943	1181.0997	1183.6158
N	-1.38780	1.30028	-0.01186	1185.0679	1187.0580	1197.4246
N	-1.38782	-1.30028	-0.01191	1217.2643	1217.5053	1224.8509
H	0.00022	-0.00008	1.45530	1236.5921	1239.5508	1252.0085
C	-0.00001	3.27742	0.01504	1256.6815	1261.1876	1269.8041
H	-0.00000	4.36099	0.02340	1278.9923	1283.8728	1313.0355
C	-0.00000	-3.27741	0.01489	1329.7830	1333.7362	1347.6746
H	0.00001	-4.36099	0.02318	1352.9333	1362.7282	1370.3063
				1386.6312	1393.1139	1393.8960
				1415.0342	1435.5798	1440.0604
				1448.9718	1456.8593	1463.3007
				1471.3543	1475.1060	1476.5896
				1488.1125	1491.5306	1494.9131
				1506.2278	1528.4599	1543.2677
				1548.4753	1556.3763	1564.2091
				1565.9965	1568.7831	1601.5529
				1629.4583	1633.4354	1662.6025
				1675.1817	1678.9039	1688.5748
				1690.9207	1692.8119	1695.7103
				1700.5250	1702.9854	1723.9349
				3193.5642	3195.4182	3197.5898
				3199.2220	3199.7996	3201.6259
				3206.3580	3207.2385	3207.2989
				3209.1509	3211.7060	3214.6802
				3214.9903	3217.0575	3222.6541
				3223.6763	3225.1851	3225.7535
				3226.5046	3229.1557	3230.7164
				3233.0640	3236.6421	3241.6673
				3252.1437	3493.0666	3544.1576

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.571634

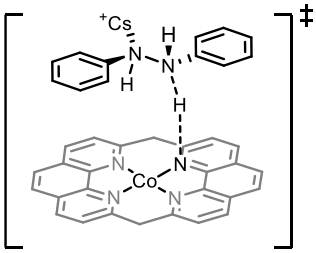
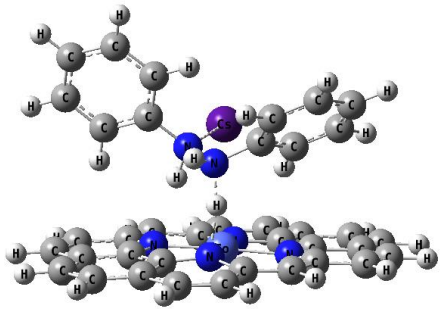
Electronic Energy = -1956.96259833

Internal Energy (E) = -1956.32758033

Enthalpy (H) = -1956.32630333

Gibbs Free Energy (G) = -1956.50130633

Gibbs Free Energy of Solvation = -1956.57019094

St. Pt.	General Structure	Ball & Stick model
TS2$^{Hyd2(spill)}$		

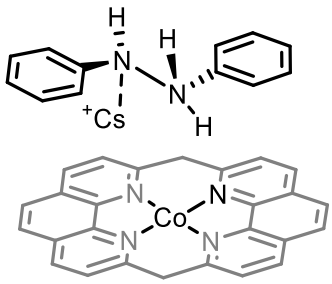
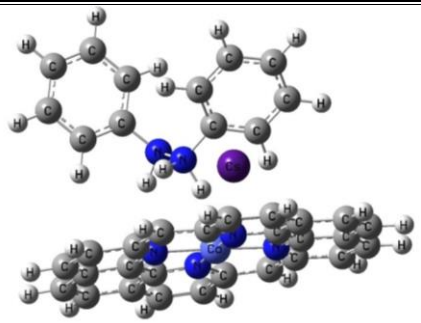
Cartesian co-ordinate			
Atoms	**X**	**Y**	**Z**
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964
H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

Frequencies		
-521.5742	6.9572	15.8399
21.8779	25.0691	35.0751
41.6904	51.6869	53.3731
56.3514	71.7063	76.1304
89.3282	104.2173	113.5133
134.7975	145.6647	164.2075
169.8271	188.4342	203.3284
220.3709	238.0387	243.6405
252.4587	260.5104	267.2497
272.3570	280.4543	317.1553
329.8996	344.1044	349.5949
367.1101	378.4029	392.0123
403.3103	407.3107	419.2379
426.2138	431.7683	444.1693
460.0713	464.2250	470.9343
482.0847	483.6392	488.6139
493.4237	505.1669	531.2609
533.8198	552.2673	565.9872
582.0881	586.0063	593.6576
598.0129	601.9426	612.8399
624.2772	625.5835	631.2594
667.4421	674.6516	682.3378
699.7561	708.3210	711.6498
719.9792	720.3905	723.2848
732.8866	746.3848	749.8539
761.8766	768.0088	772.1889
785.7706	793.0245	805.6782
814.6882	818.6566	822.6985
829.0380	850.4273	855.7216
857.2064	862.1532	865.2642
868.1369	872.2348	872.9255
880.7703	904.7179	915.2897
933.1714	941.8665	943.8295
948.5300	975.0282	977.0739
982.2802	999.0420	1003.9854
1009.8483	1010.3634	1010.7860
1015.2394	1015.4974	1016.3681
1022.0660	1022.4685	1031.9327
1032.7866	1052.7482	1065.8473
1069.1689	1108.4692	1109.7416
1120.0210	1131.0593	1137.3402
1147.0481	1155.6604	1167.9427
1175.9923	1180.2775	1182.5919
1183.4589	1186.8902	1199.7546
1204.0973	1219.2777	1228.3658
1237.8934	1241.5382	1249.6116
1253.6720	1255.6223	1262.4720
1280.7828	1285.1947	1292.9745
1314.5633	1332.6690	1348.6669
1362.7599	1366.7351	1370.2386
1387.4278	1402.6399	1407.9889
1421.0048	1441.7298	1445.3363
1449.0162	1458.8382	1460.8998

	1471.9560	1472.9251	1473.8692
	1476.7104	1497.2228	1503.5949
	1512.4743	1521.5930	1531.2060
	1550.2630	1550.8419	1558.9574
	1566.0750	1578.0952	1586.6307
	1613.9337	1625.6643	1644.5379
	1657.8162	1671.5008	1688.9244
	1689.4881	1696.2961	1697.6645
	1698.9574	1701.6440	1704.6967
	1712.8829	3198.3008	3199.3980
	3200.5882	3203.0750	3203.5571
	3204.1974	3204.3035	3207.2945
	3208.0512	3210.0275	3211.2376
	3217.6278	3218.6829	3219.5767
	3219.6679	3220.6792	3223.4373
	3226.5939	3227.4881	3229.2103
	3230.1786	3234.5898	3237.6524
	3241.3235	3319.1730	3425.5781

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.567859	Electronic Energy = -1956.94564937
Internal Energy (E) = -1956.31551037	Enthalpy (H) = -1956.31423337
Gibbs Free Energy (G) = -1956.48807637	Gibbs Free Energy of Solvation = -1956.5656291

St. Pt.	General Structure	Ball & Stick model
I5$^{Hyd2(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372

Frequencies

14.3941	25.3150	30.1505
36.1624	39.8454	46.0883
49.9528	54.0599	59.7365
73.3754	82.9318	91.7929
99.3336	117.9722	133.6674
137.9004	151.8804	169.2410
172.5749	184.5108	224.9342
239.0055	246.5543	254.7092
258.1793	260.4951	264.6600
275.7222	308.5673	335.8759
342.9830	352.5257	355.3010

C	-2.96423	0.07010	-1.07621	375.0528	393.7565	403.1196
H	-1.56292	1.36600	-2.09154	406.9792	421.4396	429.4991
C	-3.51235	-0.30873	0.15241	437.3845	444.9823	448.4670
H	-3.50543	0.05370	2.27510	453.7477	463.5450	473.7246
H	-3.33006	-0.37886	-1.99522	483.3871	486.9206	489.0528
H	-4.29697	-1.05644	0.19757	492.8789	494.3479	525.2817
C	1.55284	1.51899	-0.26755	534.2464	555.3082	582.5154
C	2.57342	1.03639	-1.10339	586.8430	589.2463	595.0754
C	1.52644	1.11662	1.07431	595.6132	601.0816	620.2104
C	3.53929	0.17265	-0.60458	626.6832	630.8281	634.5010
H	2.59701	1.34604	-2.14455	673.2373	682.3906	693.4325
C	2.50452	0.24790	1.56385	710.6365	711.9258	719.0315
H	0.75747	1.48483	1.74416	722.7954	724.3191	732.5950
C	3.50750	-0.23907	0.73169	741.1068	746.7453	753.4188
H	4.32665	-0.18078	-1.26264	760.4912	764.8199	774.7375
H	2.48615	-0.03088	2.61352	800.9097	809.4837	812.7531
H	4.27156	-0.90311	1.12010	815.7835	820.6774	823.4264
H	0.84940	3.04753	-1.46726	834.3797	855.1654	856.3242
H	-0.31192	3.11093	0.83413	861.5314	862.6259	871.6375
Cs	-0.01646	-1.68112	-0.13529	873.2647	877.8254	884.0055
C	-5.04390	0.68674	-0.04268	901.4054	916.0860	935.5637
C	-3.70087	2.84513	-0.02388	946.5121	951.3370	960.6296
H	-2.37687	4.51148	-0.00260	979.7332	983.6351	986.2196
C	-3.70086	-2.84511	-0.02396	1007.8530	1008.6242	1009.6116
C	-5.04390	-0.68672	-0.04268	1010.8143	1011.1762	1013.8770
C	-1.25756	-2.64674	0.00047	1015.4294	1021.3052	1021.7372
H	-5.98116	1.23509	-0.05313	1022.6257	1025.0163	1041.0400
H	-4.60015	3.45511	-0.02958	1042.2312	1066.1628	1070.6182
C	-2.47341	-3.43094	-0.00962	1096.3733	1113.9919	1126.0304
H	-4.60014	-3.45510	-0.02964	1129.0491	1135.0864	1139.3846
H	-5.98117	-1.23506	-0.05312	1150.3833	1168.4421	1174.7735
H	-2.37687	-4.51149	-0.00276	1181.5116	1186.7836	1190.3115
N	-1.38780	1.30028	-0.01186	1196.6443	1206.3546	1209.4944
N	-1.38782	-1.30028	-0.01191	1220.3806	1226.8000	1237.2974
H	0.00022	-0.00008	1.45530	1240.1621	1244.0689	1251.2518
C	-0.00001	3.27742	0.01504	1254.2457	1256.5976	1260.1687
H	-0.00000	4.36099	0.02340	1283.0438	1292.5425	1318.1080
C	-0.00000	-3.27741	0.01489	1321.6931	1346.6502	1365.7071
H	0.00001	-4.36099	0.02318	1367.1730	1373.5572	1384.8262
				1394.2692	1402.1006	1406.1415
				1416.5308	1432.8966	1446.7022
				1449.7229	1463.6993	1465.3540
				1471.5687	1475.4105	1479.8034
				1484.6877	1499.8922	1506.6132
				1520.7168	1523.7273	1540.8297
				1544.6206	1556.1383	1560.3293
				1561.2346	1569.4585	1591.1332
				1611.5319	1623.1472	1646.0762
				1672.6432	1690.2342	1690.5569
				1691.5573	1698.3341	1698.7386
				1700.1200	1704.4423	1711.8319
				2304.4671	3193.3421	3195.8938
				3197.1619	3198.8327	3199.4056
				3201.4901	3202.1825	3208.2985
				3210.7479	3215.1197	3216.7403

	3219.8089	3219.8189	3220.8478
	3223.0703	3226.1528	3228.7050
	3232.9609	3233.1917	3233.2773
	3236.9179	3242.7236	3243.5109
	3247.2419	3253.6842	3422.1388

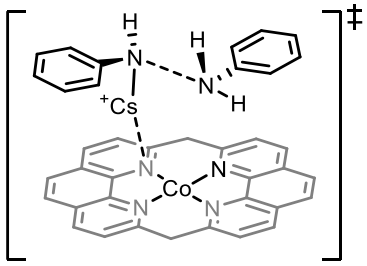
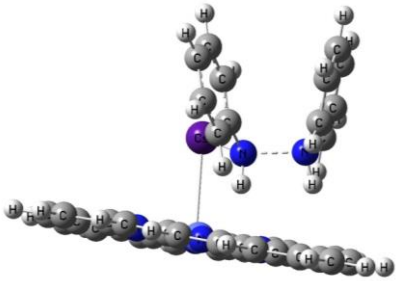
Statistical Thermodynamic Analysis

Temperature = 403.15 K Pressure = 1 atm

Zero-point correction = 0.571971 Electronic Energy = -1956.95641784

Internal Energy (E) = -1956.32193784 Enthalpy (H) = -1956.32066184

Gibbs Free Energy (G) =-1956.49249984 Gibbs Free Energy of Solvation =-1956.56778224

St. Pt.	General Structure	Ball & Stick model
$TS3^{Hyd2(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169

Frequencies

-493.8226	13.9739	20.4283
27.0399	34.9271	38.7580
46.1595	50.9769	55.1533
65.0698	67.4656	81.6345
85.7556	94.6111	104.7548
118.9777	127.6591	135.7616
156.0796	166.2179	177.6264
218.7053	239.2085	241.4438
250.1069	258.4180	262.5340
267.5497	277.5436	308.1484
313.4141	334.6703	343.1422
352.6426	374.7836	388.1524
399.7888	403.5494	406.3234
418.4559	425.2720	433.2347
443.9396	455.7512	462.4733
472.3659	483.5813	484.1859
490.2987	493.7938	517.9003
529.2314	534.0022	545.2107
550.1260	555.9402	581.7444
587.0379	594.0941	596.7006
599.6862	625.8952	627.5615
628.5635	673.8673	683.4974
689.7228	703.3136	708.3466
710.2431	713.2385	721.9428
728.8755	731.6604	739.0338

H	4.32665	-0.18078	-1.26264	745.0388	749.5377	762.6784
H	2.48615	-0.03088	2.61352	764.4740	784.8867	801.7526
H	4.27156	-0.90311	1.12010	802.0881	809.8432	815.2906
H	0.84940	3.04753	-1.46726	825.4336	826.2920	852.4699
H	-0.31192	3.11093	0.83413	856.9517	857.5489	860.8547
Cs	-0.01646	-1.68112	-0.13529	861.5459	865.3613	870.1509
C	-5.04390	0.68674	-0.04268	872.8785	876.7665	903.2671
C	-3.70087	2.84513	-0.02388	917.0776	936.2339	936.8370
H	-2.37687	4.51148	-0.00260	946.1412	954.4257	964.4890
C	-3.70086	-2.84511	-0.02396	976.8506	981.2057	1002.8892
C	-5.04390	-0.68672	-0.04268	1005.1158	1009.6630	1011.2087
C	-1.25756	-2.64674	0.00047	1011.8380	1013.7933	1013.9105
H	-5.98116	1.23509	-0.05313	1015.2204	1015.5629	1027.8577
H	-4.60015	3.45511	-0.02958	1030.2869	1034.0715	1037.9181
C	-2.47341	-3.43094	-0.00962	1062.5384	1068.3562	1101.1405
H	-4.60014	-3.45510	-0.02964	1111.7399	1116.5534	1133.2232
H	-5.98117	-1.23506	-0.05312	1136.0924	1146.9563	1151.3583
H	-2.37687	-4.51149	-0.00276	1164.6674	1165.9325	1173.8184
N	-1.38780	1.30028	-0.01186	1178.4860	1181.2778	1186.7361
N	-1.38782	-1.30028	-0.01191	1192.1826	1194.1072	1212.8669
H	0.00022	-0.00008	1.45530	1222.7910	1233.8117	1236.3835
C	-0.00001	3.27742	0.01504	1238.7278	1253.6131	1254.3283
H	-0.00000	4.36099	0.02340	1263.4167	1265.6388	1287.7800
C	-0.00000	-3.27741	0.01489	1295.2065	1296.1800	1316.6912
H	0.00001	-4.36099	0.02318	1352.4530	1371.0798	1373.9262
				1375.5327	1383.1637	1392.1853
				1400.3918	1406.7224	1412.1561
				1444.3492	1455.3032	1463.0829
				1466.0476	1468.6037	1477.2424
				1479.2062	1483.0733	1508.0620
				1511.6254	1515.3790	1527.4221
				1532.8506	1549.0701	1554.0246
				1560.3645	1566.5564	1611.4771
				1624.0408	1626.6135	1643.5188
				1660.4201	1668.9661	1679.4149
				1685.6739	1688.2198	1689.9346
				1693.1831	1699.0434	1709.5219
				3181.1238	3198.1482	3201.7401
				3202.0912	3202.2995	3205.1334
				3206.3495	3208.7972	3208.9940
				3209.3004	3219.8499	3220.0355
				3221.2509	3222.6133	3222.8731
				3222.9702	3223.1977	3225.8376
				3227.2591	3229.4454	3232.5673
				3233.8256	3244.9964	3249.2941
				3455.4315	3504.4028	3588.5354

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.569037

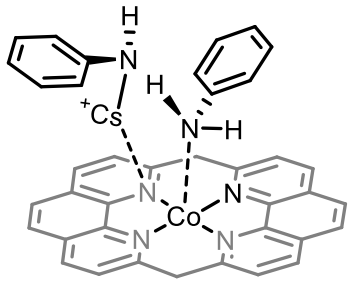
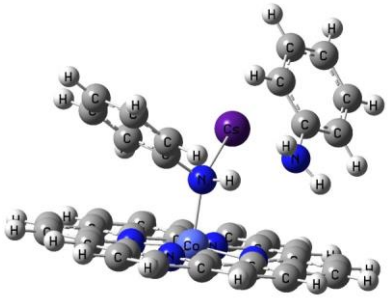
Electronic Energy = -1956.91293610

Internal Energy (E) = -1956.2806831

Enthalpy (H) = -1956.2794061

Gibbs Free Energy (G) = -1956.4534831

Gibbs Free Energy of Solvation = -1956.53316457

St. Pt.	General Structure	Ball & Stick model
I6$^{Hyd2(spill)}$		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047

Frequencies

21.4817	33.1548	37.5246
43.7033	47.4649	49.7621
59.1612	65.0853	75.1878
88.5364	92.9647	96.6811
98.9162	108.5485	115.2970
136.0705	143.0991	168.3507
175.7162	203.5515	219.4539
228.8327	246.7953	251.7288
254.3096	258.7280	275.7885
281.1627	282.5955	315.5857
342.6130	351.2272	354.5080
382.4032	387.0311	402.7603
406.7792	406.9176	410.1711
423.7099	429.5880	441.1361
448.7835	461.7893	468.2209
478.2275	481.2236	486.5736
493.6796	496.3018	501.9359
522.2865	538.4215	539.2928
556.6308	571.4623	585.7081
586.0794	595.3750	598.2573
602.8254	606.2142	626.9769
631.1232	633.0281	677.9675
681.6837	687.2931	687.9392
712.2890	713.0354	715.8215
720.0083	721.5013	741.7975
746.2813	755.2784	766.4781
767.8519	776.0517	791.7818
796.9987	810.2814	820.9921
823.2026	837.7258	845.7619
854.1803	858.1584	860.3441
860.4975	861.8218	864.9033
872.2203	881.6402	887.6316
907.4864	913.6455	920.5858
934.7347	941.3663	949.3013
983.5028	985.9424	989.0292
993.1726	995.4765	1008.6959
1009.3772	1010.3071	1016.1688

H	-5.98116	1.23509	-0.05313	1016.5862	1017.8391	1018.0739
H	-4.60015	3.45511	-0.02958	1026.4657	1027.7648	1042.8703
C	-2.47341	-3.43094	-0.00962	1065.6499	1073.4950	1084.7679
H	-4.60014	-3.45510	-0.02964	1118.3177	1123.8052	1138.3146
H	-5.98117	-1.23506	-0.05312	1145.4151	1145.7754	1158.2144
H	-2.37687	-4.51149	-0.00276	1171.6509	1177.3056	1184.1070
N	-1.38780	1.30028	-0.01186	1186.0634	1186.9467	1191.4529
N	-1.38782	-1.30028	-0.01191	1206.1265	1206.4957	1233.7857
H	0.00022	-0.00008	1.45530	1240.6502	1244.7761	1247.7488
C	-0.00001	3.27742	0.01504	1259.0632	1259.3035	1277.2882
H	-0.00000	4.36099	0.02340	1280.8882	1295.9817	1301.8855
C	-0.00000	-3.27741	0.01489	1304.4375	1329.5091	1331.2102
H	0.00001	-4.36099	0.02318	1364.2514	1364.8538	1366.4541
				1386.6041	1396.2646	1411.1359
				1418.7671	1423.9504	1434.6000
				1453.3126	1459.7405	1463.9713
				1471.5745	1476.6871	1481.5149
				1481.8660	1487.7211	1518.3662
				1521.0887	1524.9542	1530.5759
				1549.0499	1556.7023	1566.7891
				1569.8606	1575.5975	1623.0031
				1634.5942	1650.4487	1655.7574
				1670.5494	1672.3030	1678.8514
				1692.9148	1695.1829	1698.5844
				1703.5428	1707.1605	1715.9607
				3183.9134	3193.8151	3200.9790
				3201.9319	3205.9300	3209.3131
				3213.0732	3217.3374	3217.3983
				3217.6417	3221.1259	3221.7303
				3223.6103	3223.9707	3224.3703
				3226.4241	3231.8094	3232.2541
				3232.3320	3233.4398	3234.0894
				3244.0441	3247.9332	3252.6922
				3458.1419	3570.2029	3677.7904

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.571991

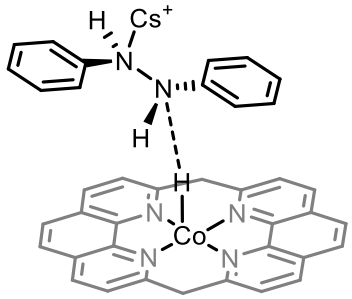
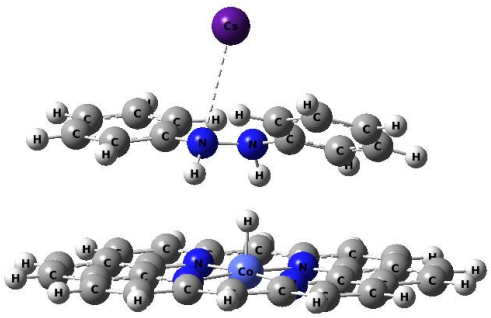
Electronic Energy = -1957.03005497

Internal Energy (E) = -1956.39467097

Enthalpy (H) = -1956.39339397

Gibbs Free Energy (G) =-1956.56427697

Gibbs Free Energy of Solvation = -1956.63011925

St. Pt.	General Structure	Ball & Stick model
I2^{Hyd2}		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962

Frequencies

16.9569	25.4394	26.7676
37.1292	43.3067	48.0280
53.8723	59.6475	69.3911
83.4228	90.7692	97.9678
106.8019	114.6939	138.7374
155.7978	166.0397	168.9702
198.4005	216.2651	223.0832
241.4715	250.7159	259.4537
260.9144	267.5350	280.1315
283.9772	306.7578	310.3568
317.9275	337.3091	341.4832
353.1764	384.9222	405.0945
408.8068	411.5751	419.3972
424.4491	449.0387	459.9257
462.0349	478.8585	484.9398
488.1842	492.1401	495.3822
498.4351	524.5668	529.8682
537.2445	548.6582	558.9875
584.8351	585.8788	596.1246
598.0507	600.2751	624.2247
627.0077	629.1458	644.9346
679.7283	688.1640	689.3049
697.7692	711.7609	712.5082
715.5411	718.2731	722.5859
740.6602	746.2230	751.4726
754.5671	761.5804	766.9901
769.5958	770.9329	773.5602
808.5684	818.8057	819.9496
827.0750	830.4881	832.9065
855.5556	858.4606	861.8210
866.9805	867.6540	869.7141
874.8875	881.4767	900.0704
907.9731	919.6585	923.3653
928.9500	942.7792	950.4764
952.5315	980.3631	981.4182
990.3667	998.1915	1006.1241
1009.9667	1011.3081	1012.8491
1016.4432	1018.4464	1018.9914
1020.3479	1020.8258	1043.4790
1066.5306	1069.1851	1114.0667

H	-4.60014	-3.45510	-0.02964	1118.6748	1123.1820	1136.7728
H	-5.98117	-1.23506	-0.05312	1141.6229	1159.7086	1168.3716
H	-2.37687	-4.51149	-0.00276	1172.9410	1174.0124	1182.5670
N	-1.38780	1.30028	-0.01186	1184.7052	1186.5961	1190.9753
N	-1.38782	-1.30028	-0.01191	1202.3824	1205.1077	1230.6665
H	0.00022	-0.00008	1.45530	1237.1828	1243.4634	1246.8711
C	-0.00001	3.27742	0.01504	1255.9281	1256.1598	1275.1954
H	-0.00000	4.36099	0.02340	1282.3436	1299.3624	1303.0695
C	-0.00000	-3.27741	0.01489	1317.1653	1331.4023	1336.1891
H	0.00001	-4.36099	0.02318	1352.1561	1368.1998	1377.8998
				1384.3808	1396.7328	1415.6026
				1421.4716	1433.2760	1451.2648
				1456.9177	1466.8187	1471.1862
				1473.8639	1478.7900	1480.5364
				1482.2485	1485.2802	1490.1686
				1520.2046	1527.7855	1532.5224
				1538.7919	1552.8269	1561.5010
				1567.4494	1569.3662	1574.9494
				1624.6842	1635.2849	1656.7266
				1677.8248	1681.2301	1683.5015
				1697.8203	1698.2889	1702.0608
				1703.5793	1709.5842	1719.0807
				2212.8249	3196.8910	3201.3579
				3202.3252	3203.1801	3205.7701
				3207.9680	3208.4912	3212.5157
				3214.7384	3220.9662	3221.0628
				3222.7645	3222.9519	3224.2014
				3225.2897	3226.3468	3227.3136
				3230.6549	3234.7430	3235.8702
				3236.4952	3239.6063	3240.2944
				3245.6145	3436.6434	3448.3200

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction= 0.569874

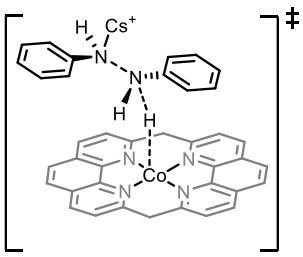
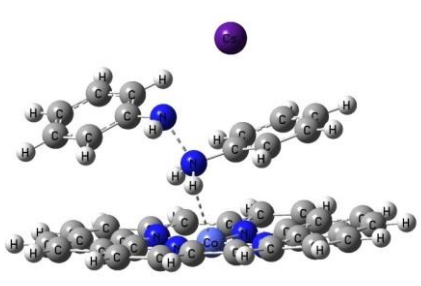
Electronic Energy = -1956.97508279

Internal Energy (E)= -1956.34248379

Enthalpy (H) = -1956.34120679

Gibbs Free Energy (G) = -1956.51221579

Gibbs Free Energy of Solvation = -1956.58926926

St. Pt.	General Structure	Ball & Stick model
TS1^{Hyd2}		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583
H	-1.75333	1.79240	2.17372
C	-2.96423	0.07010	-1.07621
H	-1.56292	1.36600	-2.09154
C	-3.51235	-0.30873	0.15241
H	-3.50543	0.05370	2.27510
H	-3.33006	-0.37886	-1.99522
H	-4.29697	-1.05644	0.19757
C	1.55284	1.51899	-0.26755
C	2.57342	1.03639	-1.10339
C	1.52644	1.11662	1.07431
C	3.53929	0.17265	-0.60458
H	2.59701	1.34604	-2.14455
C	2.50452	0.24790	1.56385
H	0.75747	1.48483	1.74416
C	3.50750	-0.23907	0.73169
H	4.32665	-0.18078	-1.26264
H	2.48615	-0.03088	2.61352
H	4.27156	-0.90311	1.12010
H	0.84940	3.04753	-1.46726
H	-0.31192	3.11093	0.83413
Cs	-0.01646	-1.68112	-0.13529
C	-5.04390	0.68674	-0.04268
C	-3.70087	2.84513	-0.02388
H	-2.37687	4.51148	-0.00260
C	-3.70086	-2.84511	-0.02396
C	-5.04390	-0.68672	-0.04268
C	-1.25756	-2.64674	0.00047
H	-5.98116	1.23509	-0.05313
H	-4.60015	3.45511	-0.02958
C	-2.47341	-3.43094	-0.00962
H	-4.60014	-3.45510	-0.02964
H	-5.98117	-1.23506	-0.05312
H	-2.37687	-4.51149	-0.00276
N	-1.38780	1.30028	-0.01186
N	-1.38782	-1.30028	-0.01191
H	0.00022	-0.00008	1.45530
C	-0.00001	3.27742	0.01504
H	-0.00000	4.36099	0.02340
C	-0.00000	-3.27741	0.01489
H	0.00001	-4.36099	0.02318

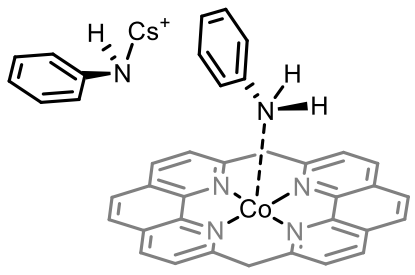
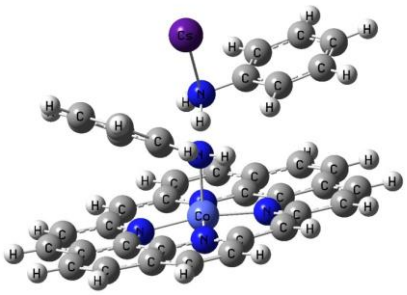
Frequencies

-509.3505	11.3017	23.3004
34.9088	36.6040	46.5672
51.6789	58.8183	67.6799
71.4463	75.6747	97.1493
105.3381	118.4823	127.6636
135.4432	146.0110	153.4559
165.7854	172.0982	183.9593
215.8340	239.8574	246.5932
256.7376	263.5117	263.7118
268.8324	276.2650	304.4251
322.3103	331.8118	343.6950
354.1560	374.9104	389.7278
400.7037	402.1720	408.4925
421.6885	427.3784	437.2777
444.5763	459.0381	463.0917
473.7937	483.4862	485.8507
490.3471	492.4329	507.2652
532.6411	533.6439	550.3685
557.4561	574.9915	582.3223
584.7285	595.1611	595.8421
602.4659	623.8122	625.8044
629.4145	673.1113	683.4643
688.7722	694.1385	707.9108
709.9852	713.0257	720.4845
725.5097	733.6005	740.6914
743.6524	754.3683	764.5701
765.8115	774.2584	797.9505
807.8188	812.9005	819.3415
824.5673	833.8408	851.5824
852.9125	855.2657	860.2971
861.6919	863.6928	868.7975
869.7843	875.8388	903.1265
917.0857	927.2644	934.8260
936.7991	947.1773	970.0491
974.8571	996.3414	1000.1715
1004.1804	1007.6464	1010.5035
1012.6822	1013.5880	1016.7502
1017.0461	1021.3083	1029.5700
1033.2048	1042.0754	1057.7769
1063.6059	1066.5481	1105.9001
1112.8560	1120.8791	1131.5680
1136.4985	1141.1429	1152.4484
1166.7211	1171.6220	1178.8679
1184.1989	1184.6864	1186.1251
1200.7301	1201.0549	1226.6747
1231.5137	1234.4805	1239.7379
1240.0936	1252.4910	1254.3380
1265.3896	1272.6584	1286.0797
1288.6125	1294.9638	1319.6111
1359.8428	1361.8053	1364.8432
1379.5085	1382.1744	1395.3516
1405.3352	1409.3239	1412.7306
1446.1794	1453.7530	1466.8901

	1469.4150	1472.6080	1474.2381
	1477.2618	1482.3739	1509.9011
	1518.0625	1518.9347	1520.6009
	1540.2477	1544.6949	1549.3633
	1564.1645	1570.0278	1604.5935
	1613.6427	1628.8447	1650.4095
	1670.3184	1673.4479	1679.1537
	1684.0085	1685.8065	1691.6641
	1695.8862	1704.1251	1714.1872
	3183.5566	3185.5107	3188.9898
	3191.6285	3195.9906	3197.1309
	3200.4244	3204.9197	3208.9294
	3209.1017	3212.4860	3213.3990
	3213.5846	3220.3552	3223.2821
	3224.4409	3224.5720	3228.0830
	3228.1413	3235.6048	3235.9836
	3240.2547	3248.0005	3252.9995
	3317.6856	3414.8126	3489.8059

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.569071	Electronic Energy = -1956.90709230
Internal Energy (E) = -1956.2753233	Enthalpy (H) = -1956.2740463
Gibbs Free Energy (G) = -1956.4450383	Gibbs Free Energy of Solvation = -1956.53863653

St. Pt.	General Structure	Ball & Stick model
$I3^{Hyd2}$		

Cartesian coordinate

Atoms	X	Y	Z
N	0.55028	2.32408	-0.82740
N	-0.54762	2.68055	-0.05672
C	-1.53113	1.67478	0.03206
C	-2.08469	1.30294	1.26086
C	-1.97825	1.04943	-1.14050
C	-3.07348	0.32093	1.31583

Frequencies

17.1962	18.6349	28.1475
36.5522	40.0763	42.3814
53.7406	56.6904	59.5008
69.6040	87.3412	89.0867
95.3646	101.0910	119.6022
130.4048	143.0340	165.7156
169.1819	203.3706	217.4108
228.0997	246.9479	250.7097
258.7487	273.7988	275.8928
280.6677	285.5568	314.1698

H	-1.75333	1.79240	2.17372	340.3321	347.6390	355.5404
C	-2.96423	0.07010	-1.07621	383.1081	393.3731	403.4975
H	-1.56292	1.36600	-2.09154	407.3101	410.0090	424.1130
C	-3.51235	-0.30873	0.15241	425.3702	426.3678	448.9532
H	-3.50543	0.05370	2.27510	457.8622	465.7580	472.1023
H	-3.33006	-0.37886	-1.99522	483.3859	486.3387	490.8313
H	-4.29697	-1.05644	0.19757	495.2079	499.2837	505.6027
C	1.55284	1.51899	-0.26755	535.3127	538.8377	540.9203
C	2.57342	1.03639	-1.10339	556.7193	569.6514	584.3081
C	1.52644	1.11662	1.07431	585.4520	593.8475	594.5867
C	3.53929	0.17265	-0.60458	597.2455	600.9838	625.3389
H	2.59701	1.34604	-2.14455	630.8593	631.6804	677.5900
C	2.50452	0.24790	1.56385	685.9829	687.3656	712.9658
H	0.75747	1.48483	1.74416	714.7269	716.7791	719.6850
C	3.50750	-0.23907	0.73169	722.5846	743.1109	746.6338
H	4.32665	-0.18078	-1.26264	756.8222	767.2735	772.1103
H	2.48615	-0.03088	2.61352	773.5799	774.6206	796.0773
H	4.27156	-0.90311	1.12010	815.4205	819.5423	826.2166
H	0.84940	3.04753	-1.46726	830.0489	833.6312	851.9921
H	-0.31192	3.11093	0.83413	855.5523	861.1349	863.2341
Cs	-0.01646	-1.68112	-0.13529	864.6695	870.4307	871.2106
C	-5.04390	0.68674	-0.04268	873.7131	882.0170	900.9765
C	-3.70087	2.84513	-0.02388	908.3390	920.7293	926.6193
H	-2.37687	4.51148	-0.00260	938.5794	941.7799	947.7396
C	-3.70086	-2.84511	-0.02396	952.4421	975.2053	981.7360
C	-5.04390	-0.68672	-0.04268	997.2448	999.7719	1006.7290
C	-1.25756	-2.64674	0.00047	1009.3260	1012.4065	1013.3120
H	-5.98116	1.23509	-0.05313	1015.6127	1016.2777	1017.1304
H	-4.60015	3.45511	-0.02958	1019.5655	1021.3148	1042.9309
C	-2.47341	-3.43094	-0.00962	1067.5698	1068.9735	1105.2832
H	-4.60014	-3.45510	-0.02964	1117.7714	1119.6575	1134.7878
H	-5.98117	-1.23506	-0.05312	1144.1354	1158.5814	1168.0292
H	-2.37687	-4.51149	-0.00276	1170.1815	1173.7512	1183.0242
N	-1.38780	1.30028	-0.01186	1184.3690	1185.9908	1186.7402
N	-1.38782	-1.30028	-0.01191	1201.3077	1205.1468	1236.2784
H	0.00022	-0.00008	1.45530	1241.2470	1245.5745	1249.1548
C	-0.00001	3.27742	0.01504	1258.2687	1259.6570	1266.1520
H	-0.00000	4.36099	0.02340	1278.9959	1297.8025	1301.4136
C	-0.00000	-3.27741	0.01489	1303.1028	1312.2751	1330.8945
H	0.00001	-4.36099	0.02318	1360.6345	1362.6905	1376.3141
				1386.6477	1394.1839	1398.0774
				1422.3582	1427.0187	1437.9913
				1457.1296	1458.7243	1459.3948
				1472.6285	1475.9414	1479.1297
				1480.5990	1484.2400	1516.0021
				1518.7577	1524.5551	1530.3989
				1543.2112	1556.1044	1564.5757
				1568.8228	1576.8097	1626.1080
				1633.4631	1656.2218	1658.7824
				1663.6480	1679.6910	1684.2578
				1687.6307	1698.4913	1702.7911
				1705.6326	1707.6026	1716.8104
				3174.5363	3178.0879	3191.6974
				3196.3939	3203.9592	3204.2580
				3208.2318	3208.5673	3210.5381

3210.7977	3213.8919	3215.0030
3220.3197	3223.1744	3223.9173
3224.4521	3226.1011	3227.0629
3228.3837	3231.9292	3234.3960
3236.1893	3236.7283	3237.3924
3415.9850	3472.5241	3611.0719

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.571352

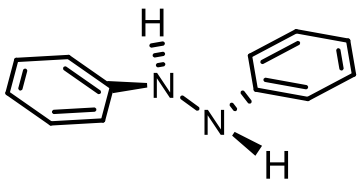
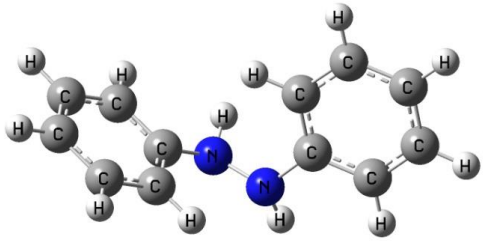
Electronic Energy = -1957.02713211

Internal Energy (E) = -1956.39230011

Enthalpy (H) = -1956.39102311

Gibbs Free Energy (G) = -1956.56500811

Gibbs Free Energy of Solvation = -1956.63531432

St. Pt.	General Structure	Ball & Stick model
Hydroazobenzene		

Cartesian coordinate

Atoms	X	Y	Z
C	-1.59132	-0.55569	-0.33936
C	-2.52583	0.01320	-1.21175
C	-3.62311	0.69949	-0.70773
C	-3.80531	0.83130	0.66686
C	-2.86991	0.26676	1.52963
C	-1.76563	-0.42235	1.03972
H	-2.39021	-0.09261	-2.28537
H	-4.33978	1.13443	-1.39750
H	-4.66217	1.36834	1.05868
H	-2.99515	0.36634	2.60360
H	-1.03067	-0.85462	1.70814
N	-0.51656	-1.28507	-0.88411
H	-0.25577	-0.96723	-1.81517
N	0.57640	-1.50826	-0.05795
H	0.88139	-2.47146	-0.09771
C	1.62013	-0.56940	-0.04146
C	1.41369	0.75931	-0.42515
C	2.88666	-0.96753	0.40461
C	2.46743	1.66716	-0.36071
H	0.43200	1.08677	-0.75014

Frequencies

31.6743	42.8056	59.0835
180.0005	190.8358	273.8449
301.2901	348.5481	417.4308
420.4240	491.9594	518.3637
528.6575	541.7592	586.2277
627.0738	629.8272	664.8776
710.4348	712.5571	742.8324
772.4518	778.0717	847.6298
854.5930	862.3977	874.7736
908.2723	917.4813	983.7082
989.1672	1006.1803	1009.5242
1012.2350	1013.4468	1068.1104
1073.6758	1113.6753	1128.7800
1175.9481	1182.3122	1195.4195
1203.2230	1214.8859	1285.2695
1331.1326	1347.9046	1353.8997
1368.2967	1376.6143	1472.7577
1490.1658	1540.9569	1544.5855
1560.6968	1564.6729	1685.6010
1687.4993	1703.5932	1708.9396
3186.2398	3190.0473	3201.5423
3203.1731	3213.0750	3216.8439
3225.8220	3230.1418	3230.8239

C	3.92626	-0.05085	0.46366	3249.2533	3506.3378	3614.8208
H	3.04766	-1.99995	0.70430			
C	3.72640	1.27442	0.07975			
H	2.29337	2.69669	-0.65803			
H	4.90254	-0.37674	0.80875			
H	4.54117	1.98841	0.12634			
C	3.82628	1.39527	-0.09170			
C	5.04592	-0.71999	-0.18079			
C	3.68573	-2.85612	-0.15703			
H	2.32963	-4.51250	-0.19077			
C	3.72116	2.82537	-0.09574			
C	5.04215	0.64935	-0.16783			
C	1.27913	2.64979	0.02889			
H	5.97926	-1.26824	-0.25207			
H	4.57397	-3.47685	-0.23081			
C	2.50038	3.42118	-0.03734			
H	4.62414	3.42615	-0.14688			
H	5.97941	1.19435	-0.22462			
H	2.41296	4.50196	-0.04125			
N	1.39837	-1.30919	0.06494			
N	1.39857	1.30012	0.04294			
H	0.19989	0.13900	1.59991			
C	-0.04820	-3.26690	-0.06233			
H	-0.03262	-4.33522	-0.25561			
C	0.02703	3.28554	0.04759			
H	0.03107	4.36759	0.00562			
H	-1.39197	-1.36276	1.51537			

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure= 1 atm

Zero-point correction = 0.217559

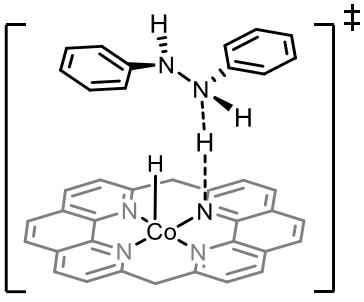
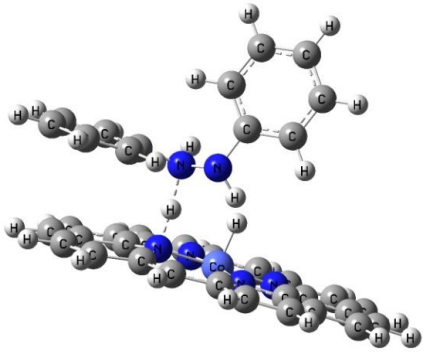
Electronic Energy = -573.740563624

Internal Energy (E) = -573.507559624

Enthalpy (H)= -573.506441624

Gibbs Free Energy (G) =-573.571301624

Gibbs Free Energy of Solvation=-573.579751928

St. Pt.	General Structure	Ball & Stick model
TS1$^{\text{Hyd2(MLC)}}$		

Cartesian coordinate

Frequencies

Atoms	X	Y	Z
C	-1.59132	-0.55569	-0.33936
C	-2.52583	0.01320	-1.21175
C	-3.62311	0.69949	-0.70773
C	-3.80531	0.83130	0.66686
C	-2.86991	0.26676	1.52963
C	-1.76563	-0.42235	1.03972
H	-2.39021	-0.09261	-2.28537
H	-4.33978	1.13443	-1.39750
H	-4.66217	1.36834	1.05868
H	-2.99515	0.36634	2.60360
H	-1.03067	-0.85462	1.70814
N	-0.51656	-1.28507	-0.88411
H	-0.25577	-0.96723	-1.81517
N	0.57640	-1.50826	-0.05795
H	0.88139	-2.47146	-0.09771
C	1.62013	-0.56940	-0.04146
C	1.41369	0.75931	-0.42515
C	2.88666	-0.96753	0.40461
C	2.46743	1.66716	-0.36071
H	0.43200	1.08677	-0.75014
C	3.92626	-0.05085	0.46366
H	3.04766	-1.99995	0.70430
C	3.72640	1.27442	0.07975
H	2.29337	2.69669	-0.65803
H	4.90254	-0.37674	0.80875
H	4.54117	1.98841	0.12634
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889
H	5.97926	-1.26824	-0.25207
H	4.57397	-3.47685	-0.23081
C	2.50038	3.42118	-0.03734
H	4.62414	3.42615	-0.14688
H	5.97941	1.19435	-0.22462
H	2.41296	4.50196	-0.04125
N	1.39837	-1.30919	0.06494
N	1.39857	1.30012	0.04294
H	0.19989	0.13900	1.59991
C	-0.04820	-3.26690	-0.06233
H	-0.03262	-4.33522	-0.25561
C	0.02703	3.28554	0.04759
H	0.03107	4.36759	0.00562
H	-1.39197	-1.36276	1.51537

-744.8852	11.8960	21.9109
29.5133	37.0112	51.4242
52.6416	60.0822	66.3070
81.1780	82.7442	112.8138
125.5632	143.5098	161.1357
180.6343	199.2285	212.7984
225.5173	240.4088	246.9579
254.6187	256.4449	265.2306
281.6696	288.4699	307.6257
316.6561	334.2803	338.7242
348.8341	382.4749	396.4891
405.4175	408.0786	410.0429
415.2007	446.8716	452.5855
456.4416	472.3715	481.1130
483.5493	489.9509	491.2577
502.1338	512.2641	526.2411
537.0996	555.6408	565.7456
579.8164	584.2946	591.1939
593.9119	599.3002	605.8515
623.3655	624.0830	632.6021
648.1026	674.7345	684.7605
685.5180	697.7472	702.7766
709.6310	710.8918	716.5076
718.9371	739.9382	745.3404
751.3500	765.0394	765.6150
777.6964	779.0815	781.9065
786.4268	811.4555	816.8582
821.1661	830.2837	832.0377
844.1879	844.7969	848.6232
855.9069	857.0509	866.0841
875.3760	880.3289	884.8426
891.9344	897.7921	916.4284
919.2825	932.4438	932.9071
952.8505	981.2416	987.9815
992.5516	997.4568	1005.0455
1007.2981	1014.5138	1018.3734
1020.8227	1021.8484	1022.0884
1024.3470	1029.0341	1036.0199
1041.5781	1063.8674	1079.5002
1111.0031	1114.9259	1127.6107
1134.4084	1143.9693	1157.0649
1170.9484	1174.5579	1181.6467
1182.0570	1183.5488	1193.3121
1194.3061	1196.2042	1220.5334
1225.4695	1241.8239	1245.7606
1247.9979	1253.6435	1256.6965
1258.1784	1271.6836	1282.4853
1301.1652	1312.5882	1329.1784
1335.2204	1354.6912	1357.7903
1367.3734	1379.1632	1392.8609
1409.0954	1417.9089	1422.4072
1443.4617	1448.2993	1450.0733
1458.7173	1463.9120	1469.5267
1478.5981	1480.1447	1485.0203
1501.8189	1510.6320	1527.9677

	1531.2481	1536.2858	1546.9928
	1562.5756	1568.6953	1574.0611
	1575.8597	1603.2441	1629.2466
	1629.8849	1649.3532	1667.8653
	1683.2868	1695.1055	1697.4574
	1697.8154	1702.1920	1703.8414
	1706.8085	1714.7576	1722.1244
	2133.4595	3179.4346	3192.5536
	3207.5750	3210.6050	3211.2750
	3212.5935	3215.2993	3219.1937
	3220.0821	3221.3791	3222.8547
	3224.2249	3224.8552	3227.8621
	3228.4111	3229.3013	3234.9288
	3239.2669	3239.6832	3241.4288
	3242.4336	3246.7274	3246.8926
	3247.8787	3407.9653	3566.2699

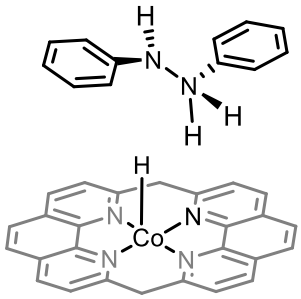
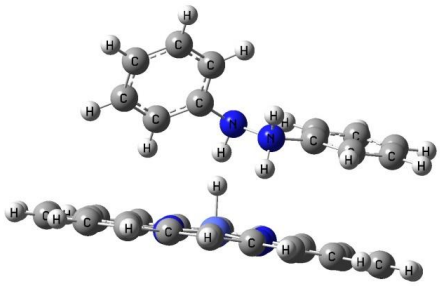
Statistical Thermodynamic Analysis

Temperature = 353.15 K Pressure = 1 atm

Zero-point correction = 0.577333 Electronic Energy = -1937.62461250

Internal Energy (E) = -1937.0018905 Enthalpy (H) = -1937.0007715

Gibbs Free Energy (G) = -1937.1294625 Gibbs Free Energy of Solvation = -1937.18501043

St. Pt.	General Structure	Ball & Stick model
$I2^{Hyd2(MLC)}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-1.59132	-0.55569	-0.33936
C	-2.52583	0.01320	-1.21175
C	-3.62311	0.69949	-0.70773
C	-3.80531	0.83130	0.66686
C	-2.86991	0.26676	1.52963
C	-1.76563	-0.42235	1.03972
H	-2.39021	-0.09261	-2.28537
H	-4.33978	1.13443	-1.39750

Frequencies

13.8590	21.6987	29.8109
43.7489	51.2559	52.9671
54.4181	66.1216	73.5237
100.0022	111.8898	126.4151
141.0195	164.0268	168.5883
174.3953	185.7569	210.0110
221.6353	242.6403	249.1870
260.0494	260.6001	265.5966
276.5906	284.2906	306.8324
334.3540	340.5225	345.2681
352.4735	384.5463	406.0712
408.7349	411.7528	412.0980

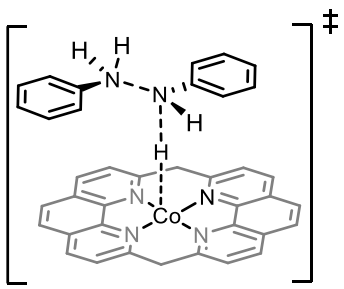
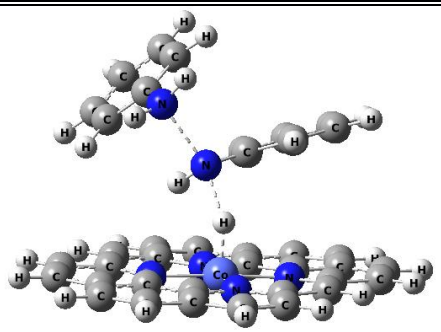
H	-4.66217	1.36834	1.05868
H	-2.99515	0.36634	2.60360
H	-1.03067	-0.85462	1.70814
N	-0.51656	-1.28507	-0.88411
H	-0.25577	-0.96723	-1.81517
N	0.57640	-1.50826	-0.05795
H	0.88139	-2.47146	-0.09771
C	1.62013	-0.56940	-0.04146
C	1.41369	0.75931	-0.42515
C	2.88666	-0.96753	0.40461
C	2.46743	1.66716	-0.36071
H	0.43200	1.08677	-0.75014
C	3.92626	-0.05085	0.46366
H	3.04766	-1.99995	0.70430
C	3.72640	1.27442	0.07975
H	2.29337	2.69669	-0.65803
H	4.90254	-0.37674	0.80875
H	4.54117	1.98841	0.12634
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889
H	5.97926	-1.26824	-0.25207
H	4.57397	-3.47685	-0.23081
C	2.50038	3.42118	-0.03734
H	4.62414	3.42615	-0.14688
H	5.97941	1.19435	-0.22462
H	2.41296	4.50196	-0.04125
N	1.39837	-1.30919	0.06494
N	1.39857	1.30012	0.04294
H	0.19989	0.13900	1.59991
C	-0.04820	-3.26690	-0.06233
H	-0.03262	-4.33522	-0.25561
C	0.02703	3.28554	0.04759
H	0.03107	4.36759	0.00562
H	-1.39197	-1.36276	1.51537

424.4612	448.8902	450.3445
457.4569	460.7631	462.7252
478.0721	485.3086	486.9264
491.7483	496.4871	538.0944
538.6575	541.1601	559.1472
584.3429	586.4228	594.2237
595.4533	599.9621	620.8046
626.7461	627.8044	634.7766
669.3397	679.1563	688.5484
689.7333	695.9964	711.9680
715.3392	720.5725	724.5417
741.3807	746.6094	752.4526
758.5174	766.9519	770.3578
776.3131	777.7222	798.6500
815.9081	819.7943	823.4842
831.7275	837.7028	853.8413
855.8877	859.5682	861.7193
863.8003	869.4410	871.5946
876.0318	885.6000	889.1272
906.8245	919.4596	935.4049
941.9849	943.8943	952.4742
976.3470	992.6945	999.9192
1000.8722	1009.9472	1012.7800
1014.6718	1018.0942	1018.7266
1020.9429	1022.8299	1026.1217
1030.8176	1038.1859	1044.7297
1064.1628	1070.7059	1094.2018
1120.1932	1124.1887	1134.8997
1136.9034	1144.3050	1160.6501
1170.9635	1175.7344	1184.3281
1186.1010	1189.0500	1189.2915
1193.8013	1208.9439	1219.7218
1236.1211	1243.6319	1245.4956
1248.8739	1256.6617	1259.6527
1269.5910	1275.0380	1296.7983
1302.3846	1316.4626	1330.6371
1338.0585	1359.3442	1366.9219
1371.3468	1379.7891	1394.8276
1419.0913	1420.2671	1423.3410
1433.2388	1451.1087	1458.1572
1464.4183	1470.3051	1475.8165
1479.1964	1482.2937	1486.5779
1504.2688	1517.3412	1523.1595
1530.4814	1547.1382	1551.8148
1565.2113	1567.0639	1570.9207
1574.3565	1619.0529	1626.3758
1635.8293	1656.9772	1679.7065
1689.2942	1696.0447	1697.3257
1699.0933	1702.3447	1708.4213
1709.8851	1719.1066	2080.0312
3176.2483	3189.9796	3198.9804
3202.2314	3210.7064	3211.0449
3212.7904	3216.0270	3218.7192
3219.6730	3226.5884	3227.4556
3227.9574	3228.3947	3231.7680

	3235.4189	3235.5952	3237.7010
	3239.3072	3240.0382	3241.1471
	3244.4618	3244.5604	3252.5999
	3265.4405	3426.3812	3439.9461

Statistical Thermodynamic Analysis

Temperature = 353.15 K
Pressure = 1 atm
Zero-point correction = 0.582679
Electronic Energy = -1937.63840114
Internal Energy (E) = -1937.00980714
Enthalpy (H)= -1937.00868914
Gibbs Free Energy (G) = -1937.13818814
Gibbs Free Energy of Solvation=-1937.1969452

St. Point	General Structure	Ball & Stick model
$TS2^{Hyd2(MLC)}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-1.59132	-0.55569	-0.33936
C	-2.52583	0.01320	-1.21175
C	-3.62311	0.69949	-0.70773
C	-3.80531	0.83130	0.66686
C	-2.86991	0.26676	1.52963
C	-1.76563	-0.42235	1.03972
H	-2.39021	-0.09261	-2.28537
H	-4.33978	1.13443	-1.39750
H	-4.66217	1.36834	1.05868
H	-2.99515	0.36634	2.60360
H	-1.03067	-0.85462	1.70814
N	-0.51656	-1.28507	-0.88411
H	-0.25577	-0.96723	-1.81517
N	0.57640	-1.50826	-0.05795
H	0.88139	-2.47146	-0.09771
C	1.62013	-0.56940	-0.04146
C	1.41369	0.75931	-0.42515
C	2.88666	-0.96753	0.40461
C	2.46743	1.66716	-0.36071
H	0.43200	1.08677	-0.75014
C	3.92626	-0.05085	0.46366

Frequencies

-499.0177	16.7566	27.2179
35.3179	38.0863	55.6009
59.3574	69.6039	71.9292
79.7597	95.2402	112.7508
123.4325	134.2896	138.4214
163.0025	166.2698	178.7245
218.2390	242.2081	249.8588
255.7511	259.8201	262.2089
271.1953	282.4510	308.5209
312.7484	338.5479	340.9584
352.9684	377.7556	382.4435
405.7619	407.7913	410.1227
416.9960	430.5540	447.6063
452.3514	462.0510	465.3520
477.5259	485.7550	486.6900
492.3731	494.3883	519.3630
521.3696	534.0071	536.7446
556.4665	559.3537	584.3102
586.4664	594.4209	597.3468
599.0122	625.2058	626.4752
627.2099	677.9859	679.8313
688.0898	689.9285	702.9933
708.4435	713.9684	716.2347
722.1583	734.7514	746.1621
749.0459	759.4791	766.5835

H	3.04766	-1.99995	0.70430	774.5399	782.3931	786.7271
C	3.72640	1.27442	0.07975	800.1582	819.2162	822.1445
H	2.29337	2.69669	-0.65803	827.4037	832.8841	835.8140
H	4.90254	-0.37674	0.80875	837.4674	853.6895	859.0153
H	4.54117	1.98841	0.12634	862.0862	863.0783	867.6310
C	3.82628	1.39527	-0.09170	872.6377	877.3378	883.2262
C	5.04592	-0.71999	-0.18079	884.9979	907.9968	919.0497
C	3.68573	-2.85612	-0.15703	919.7800	944.7476	949.3593
H	2.32963	-4.51250	-0.19077	952.8668	979.8238	980.9633
C	3.72116	2.82537	-0.09574	987.8194	997.5817	1012.4907
C	5.04215	0.64935	-0.16783	1014.4711	1015.2118	1016.0578
C	1.27913	2.64979	0.02889	1016.7967	1018.0681	1020.2887
H	5.97926	-1.26824	-0.25207	1023.0753	1032.7711	1036.2123
H	4.57397	-3.47685	-0.23081	1039.5019	1063.4144	1068.0037
C	2.50038	3.42118	-0.03734	1074.2940	1118.9223	1121.3860
H	4.62414	3.42615	-0.14688	1137.3576	1139.9886	1143.7026
H	5.97941	1.19435	-0.22462	1158.2325	1166.2732	1174.5080
H	2.41296	4.50196	-0.04125	1182.6602	1183.7234	1186.5415
N	1.39837	-1.30919	0.06494	1187.5297	1189.5615	1202.2855
N	1.39857	1.30012	0.04294	1210.8405	1225.8012	1234.8147
H	0.19989	0.13900	1.59991	1240.8478	1244.2434	1246.3797
C	-0.04820	-3.26690	-0.06233	1258.7543	1259.2004	1273.9147
H	-0.03262	-4.33522	-0.25561	1276.5084	1298.7602	1302.5137
C	0.02703	3.28554	0.04759	1305.0847	1330.7982	1365.7932
H	0.03107	4.36759	0.00562	1370.1924	1378.4209	1389.6678
H	-1.39197	-1.36276	1.51537	1396.6695	1400.5973	1416.0344
				1421.9060	1434.4658	1453.1879
				1458.7024	1460.2516	1469.9636
				1473.8361	1476.5253	1481.5337
				1487.3813	1514.0108	1517.1048
				1521.9447	1526.9651	1533.5060
				1550.8547	1553.8818	1567.5054
				1577.7994	1618.8597	1630.8772
				1644.3708	1651.8953	1655.5532
				1673.7971	1677.7063	1682.4976
				1691.4119	1694.6886	1700.1512
				1703.9423	1713.8858	1784.6739
				3201.4474	3204.8395	3205.9525
				3206.0831	3208.2428	3208.3620
				3214.6865	3215.3558	3216.2461
				3219.8510	3220.8820	3224.2427
				3224.5952	3225.2340	3226.6275
				3228.6344	3228.8720	3235.8991
				3236.3506	3238.7425	3241.0996
				3242.5522	3250.1753	3250.4326
				3419.6617	3528.8584	3638.4703

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction = 0.578882

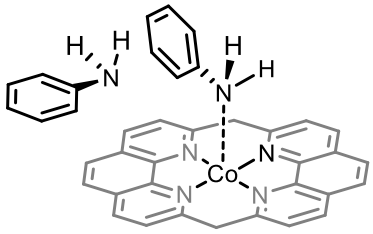
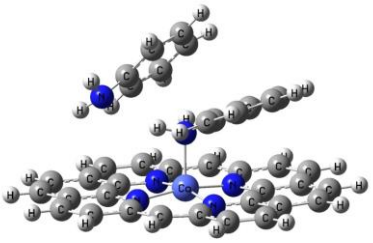
Electronic Energy = -1937.60190442

Internal Energy (E) = -1936.97723642

Enthalpy (H) = -1936.97611742

Gibbs Free Energy (G) = -1937.10448342

Gibbs Free Energy of Solvation = -1937.16577563

St. Point	General Structure	Ball & Stick model
$I3^{Hyd2(MLC)}$		

Cartesian coordinate

Atoms	X	Y	Z
C	-1.59132	-0.55569	-0.33936
C	-2.52583	0.01320	-1.21175
C	-3.62311	0.69949	-0.70773
C	-3.80531	0.83130	0.66686
C	-2.86991	0.26676	1.52963
C	-1.76563	-0.42235	1.03972
H	-2.39021	-0.09261	-2.28537
H	-4.33978	1.13443	-1.39750
H	-4.66217	1.36834	1.05868
H	-2.99515	0.36634	2.60360
H	-1.03067	-0.85462	1.70814
N	-0.51656	-1.28507	-0.88411
H	-0.25577	-0.96723	-1.81517
N	0.57640	-1.50826	-0.05795
H	0.88139	-2.47146	-0.09771
C	1.62013	-0.56940	-0.04146
C	1.41369	0.75931	-0.42515
C	2.88666	-0.96753	0.40461
C	2.46743	1.66716	-0.36071
H	0.43200	1.08677	-0.75014
C	3.92626	-0.05085	0.46366
H	3.04766	-1.99995	0.70430
C	3.72640	1.27442	0.07975
H	2.29337	2.69669	-0.65803
H	4.90254	-0.37674	0.80875
H	4.54117	1.98841	0.12634
C	3.82628	1.39527	-0.09170
C	5.04592	-0.71999	-0.18079
C	3.68573	-2.85612	-0.15703
H	2.32963	-4.51250	-0.19077
C	3.72116	2.82537	-0.09574
C	5.04215	0.64935	-0.16783
C	1.27913	2.64979	0.02889
H	5.97926	-1.26824	-0.25207
H	4.57397	-3.47685	-0.23081

Frequencies

21.6720	28.9476	35.8805
46.6524	51.0832	58.0098
66.0687	78.4247	80.0125
95.2993	98.5182	111.8891
123.6543	131.9762	141.2532
168.4556	187.3811	216.2542
235.3380	246.1770	248.4653
251.9935	260.4543	274.7439
278.1839	279.8357	304.7882
337.6773	344.5121	354.3692
375.9024	384.6293	404.2545
407.6354	408.4136	410.3721
419.7919	427.3925	429.7070
446.6891	450.3281	456.6793
467.0897	484.9694	486.2634
491.9355	495.9645	502.1902
518.4109	538.1201	542.2998
555.7432	559.6140	584.6123
585.4786	587.7357	591.3843
594.8722	599.5481	625.1303
628.8408	633.4053	676.7086
685.0408	686.7552	709.9991
713.2571	714.6612	714.9493
719.5612	744.9590	746.0716
748.2388	758.6131	766.5259
768.6006	779.4674	784.3398
785.3636	805.0178	818.7972
822.9962	828.1963	837.1146
844.4454	845.1127	848.0867
858.7398	862.5417	864.5467
866.2837	876.8477	880.4820
889.5640	907.5709	913.6188
920.7650	940.4380	941.7233
949.0996	984.5353	985.9927
989.1106	998.2786	1008.3411
1011.8445	1017.4444	1018.5319
1018.8267	1019.7187	1021.4500
1022.1600	1024.3525	1042.7436
1069.6484	1070.3953	1092.5771
1114.7646	1120.5732	1133.9523

C	2.50038	3.42118	-0.03734	1145.6837	1145.9618	1159.2448
H	4.62414	3.42615	-0.14688	1162.0100	1166.7293	1176.9530
H	5.97941	1.19435	-0.22462	1186.4482	1187.6986	1189.0217
H	2.41296	4.50196	-0.04125	1190.0789	1204.6197	1208.4582
N	1.39837	-1.30919	0.06494	1212.3860	1237.6956	1243.5347
N	1.39857	1.30012	0.04294	1247.8436	1252.5445	1262.4168
H	0.19989	0.13900	1.59991	1262.9951	1272.5244	1283.0779
C	-0.04820	-3.26690	-0.06233	1302.8969	1307.3636	1312.4372
H	-0.03262	-4.33522	-0.25561	1334.1441	1366.2655	1367.6831
C	0.02703	3.28554	0.04759	1369.1380	1376.0564	1387.7791
H	0.03107	4.36759	0.00562	1397.7775	1424.1717	1428.5452
H	-1.39197	-1.36276	1.51537	1439.3485	1440.3943	1458.5141
				1462.1300	1466.8942	1469.6219
				1477.7058	1483.3913	1491.6503
				1514.7394	1525.6547	1525.9227
				1527.7906	1555.6377	1557.3186
				1560.9276	1573.2087	1579.4566
				1626.0758	1630.4440	1649.3515
				1656.7228	1658.3479	1676.2093
				1685.7289	1696.3910	1698.9404
				1699.6473	1701.0872	1701.6634
				1706.9745	1716.5410	3193.0906
				3197.0748	3202.0645	3207.6847
				3209.9774	3212.1739	3213.4617
				3214.2748	3218.4171	3219.0888
				3220.7797	3224.1321	3224.7731
				3226.5435	3228.5344	3229.4488
				3230.4842	3230.5691	3234.1112
				3234.2871	3235.0157	3237.3278
				3246.7792	3252.4821	3391.9422
				3474.2474	3557.6600	3663.9941

Statistical Thermodynamic Analysis

Temperature = 353.15 K

Pressure = 1 atm

Zero-point correction = 0.584716

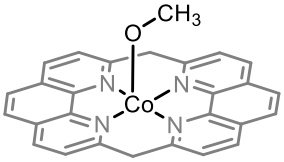
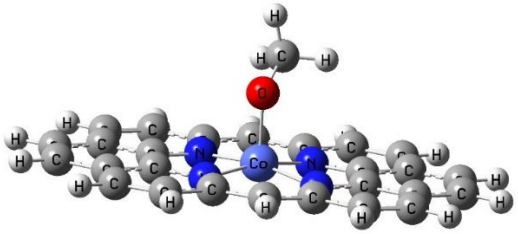
Electronic Energy = -1937.73824487

Internal Energy (E) = -1937.10706087

Enthalpy (H) = -1937.10594287

Gibbs Free Energy (G) = -1937.23516487

Gibbs Free Energy of Solvation = -1937.28902612

St. Pt.	General Structure	Ball & Stick model
I1$_{CH3OH}$		

Cartesian co-ordinate			
Atoms	**X**	**Y**	**Z**
C	-2.49778	-3.45631	-0.09848
C	-3.72237	-2.86539	-0.11593
C	-3.83664	-1.43820	-0.15175
C	-2.62722	-0.73807	-0.17719
C	-1.28003	-2.67652	-0.12042
C	-5.05323	-0.70242	-0.16116
C	-2.62250	0.68522	-0.19644
C	-3.82583	1.39622	-0.20439
C	-5.04873	0.67083	-0.18892
C	-3.70039	2.82202	-0.22899
H	-4.59841	3.43372	-0.23733
C	-2.47140	3.40509	-0.24027
C	-1.26080	2.61595	-0.22332
H	-5.99266	-1.24692	-0.14618
H	-2.40497	-4.53643	-0.05929
H	-4.62494	-3.47004	-0.09615
H	-5.98384	1.22267	-0.19758
H	-2.37048	4.48502	-0.25638
N	-1.40392	-1.33352	-0.18907
N	-1.39273	1.27185	-0.21036
Co	-0.01373	-0.03781	-0.01274
C	2.59667	-0.75936	-0.19681
C	1.23212	-2.68659	-0.12162
C	2.60296	0.66290	-0.22985
C	3.80048	-1.46979	-0.17818
C	2.44450	-3.47614	-0.10651
C	3.81154	1.36428	-0.24625
C	5.02214	-0.74435	-0.20117
C	3.67380	-2.89629	-0.13406
H	2.34269	-4.55541	-0.06551
C	3.69631	2.79218	-0.27285
C	5.02813	0.62949	-0.23495
C	1.25375	2.60464	-0.24543
H	5.95742	-1.29603	-0.19034
H	4.57116	-3.50873	-0.11862
C	2.47203	3.38359	-0.27506
H	4.59870	3.39723	-0.28845
H	5.96764	1.17362	-0.25171
H	2.37931	4.46429	-0.29061
N	1.36674	-1.34313	-0.18729
N	1.37507	1.25737	-0.23693
O	-0.09841	-0.15142	1.80107
C	0.37477	0.94790	2.51034
H	0.09002	0.80374	3.56236
H	1.47266	1.05190	2.47291
H	-0.06697	1.90390	2.18170
C	-0.02551	-3.31128	-0.08246
H	-0.02980	-4.39372	-0.03182

Frequencies		
47.8438	64.0153	82.2672
95.4314	108.8488	129.5337
138.3192	172.5164	194.5546
216.6979	233.7781	243.5490
253.1668	255.0248	257.3945
276.1539	280.2864	295.6052
314.6121	340.3204	349.4642
358.7948	384.8516	405.0038
410.2213	414.2232	449.2187
462.0311	470.6794	479.1165
483.3616	486.1039	495.8549
497.2721	540.6988	557.9145
584.4349	585.9897	595.4556
596.7656	600.6123	611.6386
627.2734	680.6373	686.6930
690.1149	712.7212	716.8891
721.0734	743.0372	746.4514
752.0594	759.4296	766.3444
768.0288	813.9401	820.3002
825.6547	828.6685	856.3243
861.8597	865.5186	868.9308
870.3216	878.2250	909.0743
922.8211	943.0199	949.5246
969.9573	970.6712	1013.0610
1015.8446	1016.5568	1017.5469
1018.0577	1045.3844	1122.0346
1135.9577	1142.8987	1156.5655
1161.0028	1169.5072	1173.7318
1182.7194	1186.0992	1187.6116
1191.7908	1235.9227	1241.5766
1245.2540	1248.6102	1258.1864
1258.7005	1279.3727	1301.4211
1305.2174	1330.7082	1388.7196
1398.8759	1421.7167	1428.7896
1435.9775	1455.5035	1459.8449
1467.5818	1469.2683	1477.3789
1483.2799	1485.6092	1486.6446
1486.7742	1491.9707	1520.9459
1522.6399	1537.8101	1572.1258
1573.6332	1577.9825	1629.1156
1639.2856	1664.6884	1684.5754
1704.4277	1705.8857	1714.9183
1724.6847	2986.7978	3043.5072
3070.2284	3200.0003	3200.0955
3214.3853	3214.8157	3215.6354
3215.9969	3216.4963	3216.6239
3223.5371	3224.8900	3231.5977
3232.6628	3232.8691	3233.8259

C	0.00124	3.24209	-0.22119
H	0.00625	4.32566	-0.22609

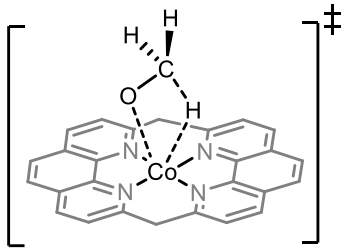
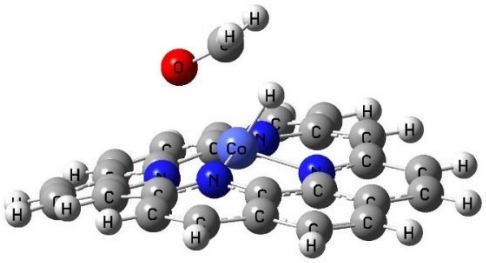
Statistical Thermodynamic Analysis

Temperature = 403.15 K — Pressure = 1 atm

Zero-point correction = 0.384489 — Electronic Energy = -1477.97812357

Internal Energy (E) = -1477.55203957 — Enthalpy (H) = -1477.55076357

Gibbs Free Energy (G)= -1477.67066857 — Gibbs Free Energy of Solvation = -1478.09081533

St. Pt.	General Structure	Ball & Stick model
$TS1_{CH3OH}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.32373	-3.42218	-0.54530
C	-3.54670	-2.85228	-0.71284
C	-3.70223	-1.43630	-0.59209
C	-2.52966	-0.71963	-0.33489
C	-1.14997	-2.62417	-0.27438
C	-4.93586	-0.73238	-0.69772
C	-2.58783	0.69030	-0.13762
C	-3.79802	1.37383	-0.28570
C	-4.98189	0.62981	-0.55924
C	-3.72552	2.79707	-0.16454
H	-4.63756	3.38363	-0.23731
C	-2.52119	3.41098	-0.01149
C	-1.29864	2.64792	0.07929
H	-5.84240	-1.29582	-0.89809
H	-2.19984	-4.49799	-0.61040
H	-4.41822	-3.46682	-0.92221
H	-5.92289	1.16265	-0.65804
H	-2.44694	4.49283	0.01804
N	-1.29562	-1.28545	-0.24531
N	-1.40242	1.30555	0.14538
Co	0.03358	0.03366	0.41991
C	2.63968	-0.65685	-0.10401
C	1.33198	-2.60901	0.04761

Frequencies

-428.2156	46.5474	62.6802
64.8823	96.3888	99.5144
126.1851	134.9340	153.2219
179.9826	205.7392	220.1403
245.3568	249.5581	255.1968
263.5398	266.1041	291.9414
323.1519	330.5082	335.4378
376.1399	381.2453	396.0158
402.0033	417.4554	445.7332
455.5745	458.7726	462.5249
470.1953	487.4914	489.5810
493.0085	528.4040	544.0704
556.8404	582.6428	586.2363
591.0521	595.1497	598.3740
618.5078	625.0149	674.3816
683.5350	684.1627	710.9637
713.0771	720.9077	729.5092
738.6022	744.0375	751.8368
757.5982	766.3772	807.0778
809.8495	817.6959	821.2979
848.4939	855.5725	858.2385
861.3512	864.4892	871.5222
910.1888	922.2831	934.0455
945.2002	947.0298	963.3585
967.7304	1006.8009	1007.7884
1008.9040	1009.9674	1012.3664
1038.9332	1117.4421	1135.6330
1140.6651	1154.7637	1167.1519

C	2.58828	0.75237	-0.27164	1168.3965	1179.3700	1181.6310
C	3.85118	-1.33718	-0.25668	1231.0012	1236.8324	1241.2914
C	2.56237	-3.37188	-0.03317	1242.8951	1245.8238	1252.1554
C	3.75828	1.47904	-0.50482	1256.3574	1257.0990	1274.7542
C	5.03275	-0.58912	-0.51094	1297.5228	1300.7601	1327.4504
C	3.77085	-2.76584	-0.15865	1384.8326	1397.3642	1413.1342
H	2.48301	-4.45389	-0.02202	1417.2441	1423.8572	1447.5303
C	3.59781	2.89936	-0.59748	1452.2826	1469.7114	1473.9337
C	4.98964	0.77839	-0.62361	1479.5031	1481.6863	1484.3098
C	1.19043	2.66418	-0.18544	1486.7217	1489.1788	1521.7111
H	5.97419	-1.11939	-0.61955	1538.2743	1568.9983	1575.7215
H	4.68063	-3.35611	-0.22745	1579.9998	1592.3706	1624.2480
C	2.37358	3.46215	-0.43116	1639.8092	1662.5970	1689.3966
H	4.46875	3.52107	-0.78670	1697.6202	1706.4556	1713.2936
H	5.89630	1.34398	-0.81614	1720.7469	1748.1341	2991.9703
H	2.24710	4.53856	-0.47523	3069.0133	3199.3457	3199.4840
N	1.44728	-1.26413	0.16513	3202.2918	3202.8314	3203.6435
N	1.34450	1.31721	-0.18350	3205.4698	3216.0902	3216.2848
O	-0.82424	-0.80145	2.30643	3223.7971	3224.9709	3226.6159
C	-0.04545	0.03490	2.80919	3227.8365	3230.0988	3231.0179
H	-0.41890	1.01227	3.16196			
H	0.93076	-0.27863	3.21800			
H	0.64233	0.71386	1.61091			
C	0.09497	-3.25396	-0.06640			
H	0.10971	-4.33588	-0.12137			
C	-0.04564	3.29229	0.02747			
H	-0.05196	4.37514	0.00208			

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.377353

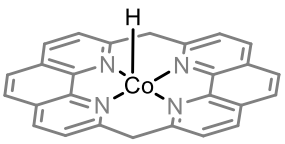
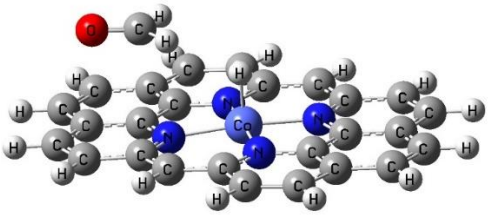
Electronic Energy = -1477.90219699

Internal Energy (E) = -1477.48313999

Enthalpy (H) = -1477.48186299

Gibbs Free Energy (G) = -1477.60243499

Gibbs Free Energy of Solvation = -1478.02484776

St. Pt.	General Structure	Ball & Stick model
$I3_{CH3OH}$		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

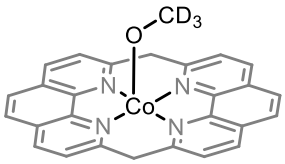
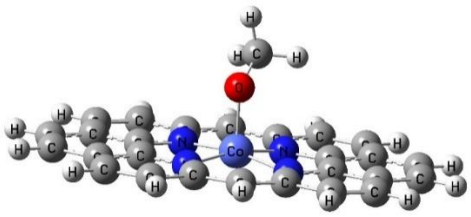
39.8148	50.6518	59.1826
70.4382	98.1882	111.0570
116.9087	140.4088	154.0518
161.0753	173.0031	216.5580

C	-2.55968	-3.08187	-0.59628
C	-3.73526	-2.39888	-0.61488
C	-3.74606	-0.97015	-0.50823
C	-2.49289	-0.36570	-0.39390
C	-1.29066	-2.40370	-0.46021
C	-4.90423	-0.14417	-0.51164
C	-2.38255	1.04769	-0.27343
C	-3.52822	1.84737	-0.27376
C	-4.79881	1.22050	-0.39860
C	-3.29661	3.25492	-0.14157
H	-4.14525	3.93347	-0.13475
C	-2.03019	3.73689	-0.02331
C	-0.88026	2.85915	-0.02471
H	-5.87941	-0.61268	-0.60311
H	-2.54853	-4.16423	-0.66462
H	-4.67842	-2.93093	-0.70079
H	-5.68991	1.84104	-0.40097
H	-1.85150	4.80201	0.07965
N	-1.31207	-1.05281	-0.37101
N	-1.11216	1.53282	-0.15719
Co	0.16403	0.12236	-0.10593
C	2.71893	-0.79204	-0.12477
C	1.21327	-2.60737	-0.31443
C	2.82945	0.62292	-0.01683
C	3.86451	-1.59165	-0.12540
C	2.36345	-3.48535	-0.31884
C	4.08496	1.22652	0.08774
C	5.13680	-0.96421	-0.02364
C	3.63129	-3.00162	-0.23012
H	2.18288	-4.55234	-0.39558
C	4.07368	2.65544	0.19736
C	5.24364	0.40133	0.07958
C	1.62426	2.65611	0.09147
H	6.02780	-1.58490	-0.02813
H	4.47975	-3.68040	-0.23595
C	2.89667	3.33673	0.19976
H	5.01706	3.18825	0.28124
H	6.22004	0.87011	0.15813
H	2.88452	4.41805	0.28660
N	1.44818	-1.27788	-0.22183
N	1.65017	1.30820	-0.02323
O	-2.91189	-2.17662	2.48509
C	-1.93353	-1.47611	2.49409
H	-2.00104	-0.36955	2.51568
H	-0.90744	-1.89405	2.46784
H	0.10284	0.03344	1.27360
C	-0.08808	-3.13351	-0.41266
H	-0.17238	-4.21162	-0.48228
C	0.42002	3.38282	0.10021
H	0.50286	4.45896	0.19774

242.5969	248.1655	257.3115
258.7696	263.1638	284.1412
302.5174	312.0598	335.7914
340.1040	351.3689	384.3055
405.3442	407.4793	410.8672
449.2526	461.3802	462.9278
478.4085	487.3078	487.8316
493.8049	496.1752	538.4476
559.5572	583.9113	586.7868
596.3152	598.9560	599.8880
627.2279	680.0424	687.6906
689.0513	712.2788	716.4519
720.4865	737.0819	741.4498
750.0466	750.7672	755.0080
758.7122	766.1937	772.5860
817.2788	822.2097	828.8142
831.6784	853.1670	862.1559
865.3904	869.4405	870.3628
876.6653	908.4651	920.9036
945.0334	952.8002	976.3605
979.2426	1009.7680	1010.9145
1012.6503	1013.0086	1013.1416
1043.6670	1117.7216	1138.5932
1145.1360	1158.5150	1170.7595
1171.4882	1182.8717	1184.7950
1207.7329	1234.4436	1239.5606
1243.6997	1246.7858	1259.3928
1260.2172	1278.0780	1280.3050
1300.4502	1303.9215	1330.0108
1384.5721	1395.8967	1418.0100
1424.9514	1428.7309	1452.7350
1459.9909	1467.3057	1478.3173
1480.5418	1482.5742	1484.0491
1486.1769	1519.2595	1534.1531
1551.3091	1571.7692	1573.6451
1578.6483	1627.8320	1636.1153
1658.7706	1684.3823	1699.6828
1707.1863	1712.3641	1720.4987
1889.6886	2138.6430	2967.0479
3042.0742	3200.6770	3202.8027
3203.2144	3205.3473	3210.8228
3215.6443	3223.1417	3223.5764
3225.8071	3227.4971	3229.3100
3231.3269	3231.6550	3233.2827

Statistical Thermodynamic Analysis

Temperature = 403.15 K	Pressure = 1 atm
Zero-point correction = 0.379087	Electronic Energy = -1477.95831218
Internal Energy (E) = -1477.53615318	Enthalpy (H) = -1477.53487618
Gibbs Free Energy (G) = -1477.65980118	Gibbs Free Energy of Solvation = -1478.08123757

St. Pt.	General Structure	Ball & Stick model
$I1_{CD3OD}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.49772	3.45629	-0.09828
C	3.72232	2.86538	-0.11575
C	3.83659	1.43821	-0.15172
C	2.62717	0.73807	-0.17731
C	1.27999	2.67650	-0.12043
C	5.05319	0.70243	-0.16109
C	2.62249	-0.68522	-0.19654
C	3.82581	-1.39621	-0.20446
C	5.04871	-0.67082	-0.18891
C	3.70037	-2.82202	-0.22908
H	4.59838	-3.43371	-0.23744
C	2.47138	-3.40510	-0.24034
C	1.26078	-2.61595	-0.22335
H	5.99262	1.24694	-0.14603
H	2.40490	4.53640	-0.05890
H	4.62488	3.47004	-0.09584
H	5.98382	-1.22265	-0.19756
H	2.37047	-4.48503	-0.25644
N	1.40386	1.33352	-0.18932
N	1.39273	-1.27186	-0.21045
Co	0.01374	0.03771	-0.01289
C	-2.59670	0.75934	-0.19670
C	-1.23214	2.68655	-0.12169
C	-2.60302	-0.66292	-0.22967
C	-3.80051	1.46977	-0.17814
C	-2.44454	3.47611	-0.10670
C	-3.81159	-1.36430	-0.24610
C	-5.02217	0.74433	-0.20111
C	-3.67384	2.89627	-0.13419

Frequencies

47.6996	63.0705	74.5665
93.1005	103.7537	129.2899
130.6778	170.2326	184.7294
196.8599	216.7227	229.2987
242.1587	254.1476	257.3864
272.9698	279.2026	283.3611
306.2084	340.2618	349.0215
357.8710	384.7328	404.8070
410.2052	412.2452	449.2100
461.9880	470.5683	478.0702
482.0795	486.0892	495.8377
497.2525	540.6992	557.8774
584.4280	585.3919	587.4109
595.4846	597.2872	600.6538
627.2007	680.6346	686.6855
689.9337	712.7193	716.8196
721.0584	743.0214	746.4182
752.0577	759.4207	766.3387
768.0179	813.9367	820.2974
825.6386	828.6643	856.3219
861.8568	865.4841	868.9101
870.3166	878.2197	908.9827
921.4895	922.8190	942.9959
947.5243	951.3608	969.9560
970.6729	1013.0414	1015.8379
1016.5589	1017.5502	1018.0563
1045.3731	1056.9218	1075.5889
1091.3453	1122.0385	1136.0374
1142.9624	1161.0341	1169.4150
1173.7557	1182.6632	1186.0931
1199.6577	1235.9321	1241.5781
1245.2639	1248.6102	1258.1903
1258.7050	1279.3957	1301.4534

H	-2.34271	4.55539	-0.06586	1305.2442	1330.7430	1388.7936
C	-3.69635	-2.79221	-0.27271	1398.9145	1421.7319	1428.8172
C	-5.02818	-0.62951	-0.23483	1436.0610	1455.5194	1459.8681
C	-1.25380	-2.60466	-0.24528	1467.9380	1477.4137	1484.0643
H	-5.95745	1.29601	-0.19031	1485.3296	1486.6791	1486.9914
H	-4.57119	3.50873	-0.11884	1521.7788	1537.5791	1572.0626
C	-2.47207	-3.38361	-0.27490	1573.6080	1577.9776	1629.1145
H	-4.59875	-3.39726	-0.28832	1639.2871	1664.6901	1684.5718
H	-5.96770	-1.17365	-0.25159	1704.4281	1705.8879	1714.9147
H	-2.37934	-4.46432	-0.29046	1724.6773	2140.7206	2255.2773
N	-1.36676	1.34309	-0.18724	2273.8974	3200.0007	3200.0970
N	-1.37514	-1.25739	-0.23673	3214.3824	3214.8110	3215.6381
O	0.09888	0.15163	1.80089	3215.9907	3216.4972	3216.6226
C	-0.37439	-0.94752	2.51039	3223.5359	3224.8970	3231.5982
H	0.06711	-1.90363	2.18179	3232.6672	3232.8718	3233.8212
C	0.02546	3.31127	-0.08251			
H	0.02975	4.39370	-0.03186			
C	-0.00127	-3.24209	-0.22107			
H	-0.00627	-4.32567	-0.22597			
H	-1.47230	-1.05130	2.47313			
H	-0.08945	-0.80326	3.56234			

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure=1 atm

Zero-point correction = 0.374671

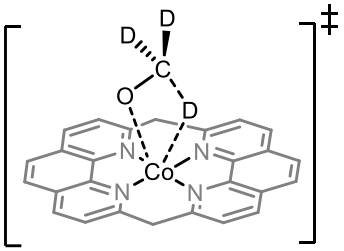
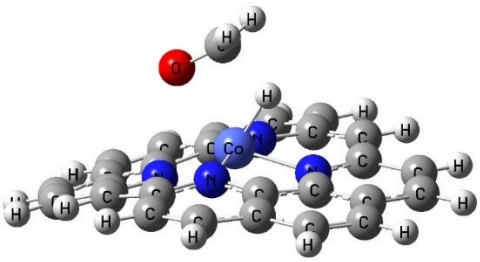
Electronic Energy = -1477.97812360

Internal Energy (E) = -1477.5612336

Enthalpy (H) = -1477.5599566

Gibbs Free Energy (G) = -1477.6812716

Gibbs Free Energy of Solvation = -1478.10141818

St. Pt.	General Structure	Ball & Stick model
TS1$_{CD3OD}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.32343	-3.42232	-0.54489
C	-3.54635	-2.85241	-0.71281
C	-3.70182	-1.43639	-0.59252
C	-2.52925	-0.71970	-0.33537
C	-1.14969	-2.62427	-0.27411

Frequencies

-403.7652	46.4203	59.9185
63.0826	93.0211	99.1604
121.1746	126.5097	152.8622
178.3722	205.6959	218.8336
243.6852	249.2653	255.0355
262.3348	265.8420	291.3102
314.3534	324.6154	332.6246
361.7189	378.6742	386.1735
399.5429	408.0579	410.6259

C	-4.93543	-0.73247	-0.69841	444.9719	457.8059	458.1410
C	-2.58744	0.69027	-0.13826	463.3234	471.3058	486.4710
C	-3.79762	1.37377	-0.28654	489.6864	494.2161	497.6071
C	-4.98146	0.62973	-0.56014	538.8740	555.9885	582.0607
C	-3.72518	2.79701	-0.16531	586.2331	590.8926	595.8149
H	-4.63723	3.38354	-0.23828	598.1292	623.9557	673.5513
C	-2.52093	3.41096	-0.01187	677.7121	683.4306	684.6861
C	-1.29838	2.64794	0.07918	710.9723	713.0257	720.7994
H	-5.84196	-1.29594	-0.89876	729.1554	738.5301	743.9510
H	-2.19960	-4.49817	-0.60956	751.7871	757.3515	766.2217
H	-4.41788	-3.46697	-0.92208	807.0767	809.9003	817.6588
H	-5.92245	1.16257	-0.65909	821.1897	848.5208	855.6779
H	-2.44672	4.49281	0.01779	857.9481	861.3229	864.4555
N	-1.29525	-1.28554	-0.24557	871.5075	910.2230	922.5402
N	-1.40210	1.30555	0.14491	933.9423	937.5143	948.0915
Co	0.03377	0.03359	0.42022	963.3641	967.7128	975.3802
C	2.63990	-0.65693	-0.10364	1006.8165	1007.7293	1008.8906
C	1.33224	-2.60908	0.04816	1009.9314	1012.2628	1038.9414
C	2.58849	0.75228	-0.27137	1103.9103	1117.3337	1135.4873
C	3.85136	-1.33728	-0.25655	1140.6611	1154.8362	1167.2177
C	2.56261	-3.37197	-0.03277	1168.4881	1179.2868	1180.5191
C	3.75847	1.47891	-0.50480	1184.0746	1231.5578	1237.0266
C	5.03288	-0.58926	-0.51116	1242.9663	1246.0353	1256.2259
C	3.77107	-2.76594	-0.15846	1257.0012	1274.7877	1297.3132
H	2.48323	-4.45398	-0.02162	1300.7476	1327.4791	1384.7393
C	3.59803	2.89924	-0.59735	1397.4600	1413.1121	1417.4403
C	4.98979	0.77824	-0.62386	1423.8714	1447.5347	1452.2682
C	1.19071	2.66412	-0.18492	1470.5301	1474.3385	1479.5507
H	5.97428	-1.11957	-0.61998	1483.4806	1484.3077	1486.7114
H	4.68084	-3.35620	-0.22741	1521.6425	1538.5297	1569.0171
C	2.37385	3.46206	-0.43072	1575.6673	1579.6253	1607.8277
H	4.46896	3.52093	-0.78672	1624.2174	1639.7616	1662.6365
H	5.89641	1.34381	-0.81662	1689.3701	1697.6182	1706.4378
H	2.24740	4.53848	-0.47471	1713.4204	1720.9042	2169.2332
N	1.44757	-1.26421	0.16587	2290.0849	3199.3483	3199.4902
N	1.34475	1.31716	-0.18296	3202.3242	3202.7872	3203.6124
O	-0.82782	-0.80004	2.30530	3205.4327	3216.1101	3216.2808
C	-0.04953	0.03588	2.80947	3223.7851	3224.9754	3226.6068
H	0.64324	0.71234	1.61167	3227.8361	3230.0851	3231.0210
C	0.09523	-3.25404	-0.06582			
H	0.10997	-4.33598	-0.12064			
C	-0.04536	3.29229	0.02789			
H	-0.05163	4.37514	0.00256			
H	0.92529	-0.27818	3.22114			
H	-0.42279	1.01416	3.15986			

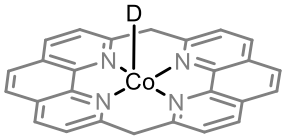
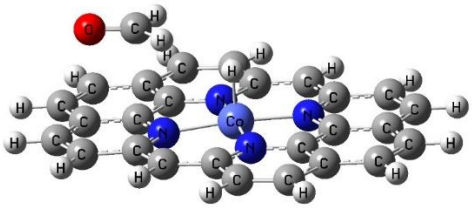
Statistical Thermodynamic Analysis

Temperature = 403.15 K Pressure = 1 atm

Zero-point correction = 0.368899 Electronic Energy = -1477.90219709

Internal Energy (E) = -1477.49076409 Enthalpy (H) = -1477.48948709

Gibbs Free Energy (G) = -1477.61165309 Gibbs Free Energy of Solvation =-1478.03405812

St. Pt.	General Structure	Ball & Stick model
$I3_{CD3OD}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.55979	-3.08172	-0.59684
C	-3.73530	-2.39864	-0.61537
C	-3.74608	-0.96991	-0.50835
C	-2.49291	-0.36551	-0.39390
C	-1.29072	-2.40365	-0.46050
C	-4.90421	-0.14390	-0.51157
C	-2.38241	1.04786	-0.27320
C	-3.52808	1.84755	-0.27338
C	-4.79870	1.22076	-0.39828
C	-3.29646	3.25510	-0.14108
H	-4.14511	3.93363	-0.13410
C	-2.03003	3.73704	-0.02297
C	-0.88009	2.85929	-0.02460
H	-5.87942	-0.61233	-0.60311
H	-2.54869	-4.16406	-0.66543
H	-4.67850	-2.93059	-0.70149
H	-5.68977	1.84133	-0.40053
H	-1.85130	4.80215	0.08002
N	-1.31216	-1.05277	-0.37124
N	-1.11196	1.53298	-0.15699
Co	0.16380	0.12202	-0.10583
C	2.71901	-0.79202	-0.12452
C	1.21327	-2.60730	-0.31431
C	2.82944	0.62294	-0.01671
C	3.86455	-1.59168	-0.12515
C	2.36341	-3.48532	-0.31868
C	4.08497	1.22652	0.08767
C	5.13684	-0.96422	-0.02350
C	3.63127	-3.00162	-0.22987
H	2.18283	-4.55231	-0.39550
C	4.07375	2.65546	0.19693
C	5.24365	0.40132	0.07956
C	1.62431	2.65608	0.09124
H	6.02785	-1.58490	-0.02797
H	4.47970	-3.68045	-0.23566
C	2.89674	3.33672	0.19923
H	5.01714	3.18831	0.28060
H	6.22005	0.87013	0.15800

Frequencies

39.1317	50.1730	58.6440
69.4475	97.0602	98.8183
113.0724	139.9237	142.2881
160.7899	167.3450	216.0004
226.7988	241.6544	247.9751
257.0178	258.6837	262.6103
284.1404	302.5799	334.1795
339.3422	348.1657	384.3018
402.1257	405.2557	410.5513
449.2502	455.0038	461.5296
476.3895	486.8497	487.8233
493.2384	495.6160	538.4100
541.8210	547.2422	564.9951
585.2466	586.8127	596.4232
599.8856	604.6623	627.2242
680.0420	687.7466	689.7214
712.2803	716.7670	721.5496
741.4119	744.5225	750.1551
753.8468	766.1591	768.3297
816.9092	822.1145	827.6276
831.6642	853.1626	862.1509
865.3079	869.3701	870.3532
876.6594	908.4535	920.8963
945.0251	952.6573	968.4144
976.3531	979.2468	1009.1262
1009.9678	1010.9317	1012.6495
1013.0188	1013.1661	1043.6641
1117.7149	1128.3207	1138.5984
1145.1445	1158.5198	1170.7732
1171.5030	1182.8747	1184.7961
1234.4453	1239.5651	1243.7033
1246.7797	1259.3930	1260.2077
1278.2482	1300.4032	1303.9095
1330.0064	1384.5552	1395.8768
1418.0081	1424.9495	1428.7356
1452.7319	1459.9797	1467.3042
1478.3147	1480.5496	1482.5523
1484.0329	1485.6446	1517.9680
1528.8640	1534.9516	1571.7797
1573.5821	1578.6427	1627.8309
1636.0976	1658.7759	1684.3871
1699.6851	1707.1799	1712.3884

H	2.88457	4.41807	0.28574	1720.4909	1831.0351	2175.3561
N	1.44830	-1.27782	-0.22152	2270.1754	3200.6772	3202.7953
N	1.65009	1.30813	-0.02319	3203.2094	3205.3561	3210.7915
O	-2.91182	-2.17739	2.48439	3215.6690	3223.1391	3223.5819
C	-1.93370	-1.47655	2.49417	3225.7990	3227.5006	3229.3220
H	0.10209	0.03331	1.27368	3231.3123	3231.6469	3233.2891
C	-0.08811	-3.13339	-0.41284			
H	-0.17236	-4.21149	-0.48259			
C	0.42019	3.38294	0.10005			
H	0.50312	4.45909	0.19743			
H	-0.90743	-1.89411	2.46831			
H	-2.00164	-0.37002	2.51601			

Statistical Thermodynamic Analysis

Temperature = 403.15 K

Pressure = 1 atm

Zero-point correction = 0.370611

Electronic Energy = -1477.95831200

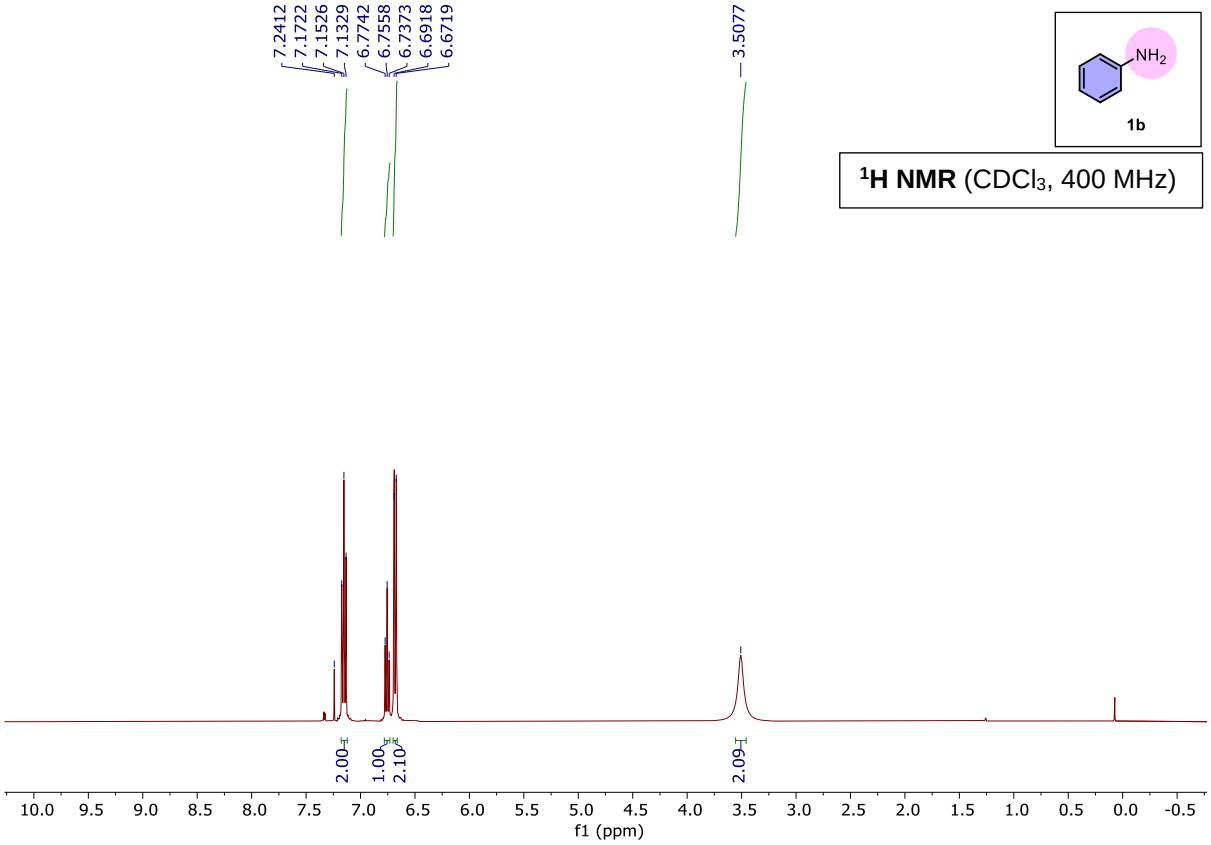
Internal Energy (E) = -1477.543836

Enthalpy (H) = -1477.542559

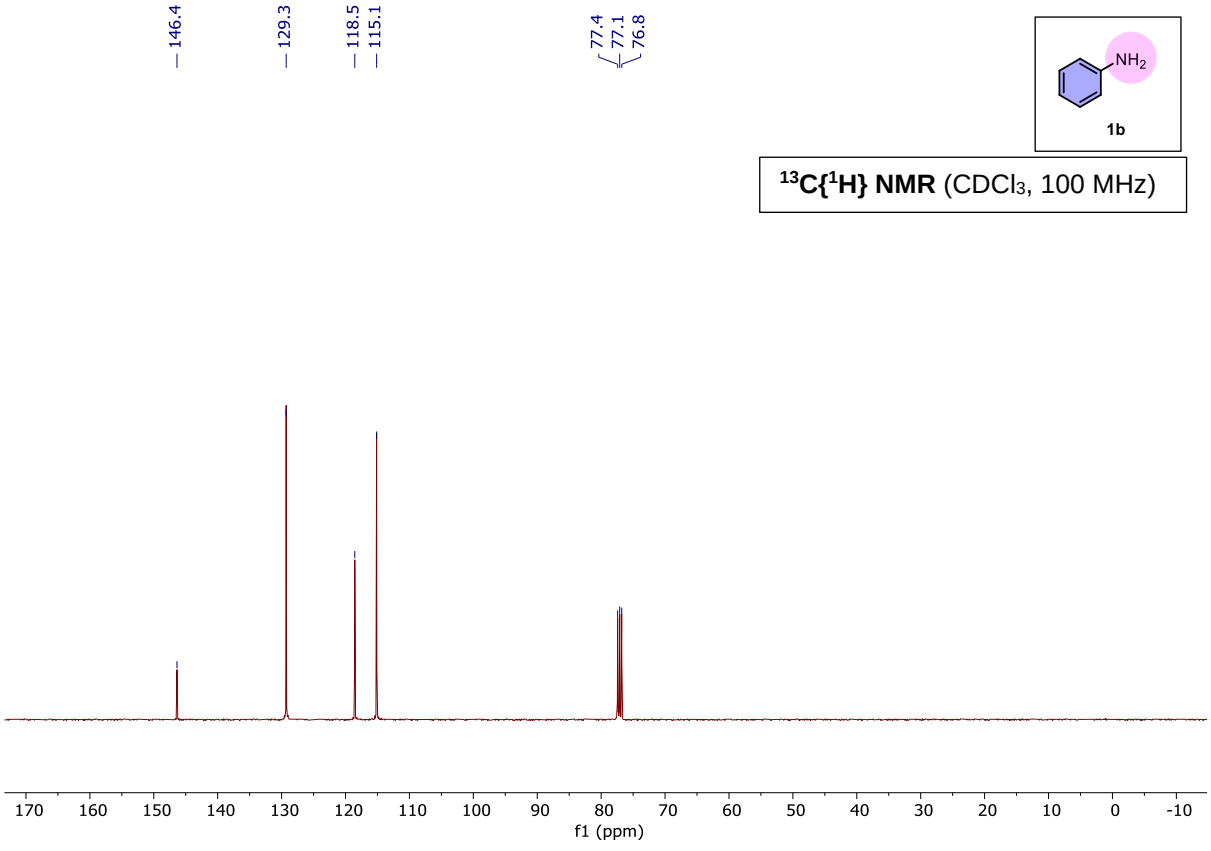
Gibbs Free Energy (G) = -1477.669198

Gibbs Free Energy of Solvation = -1478.0906332

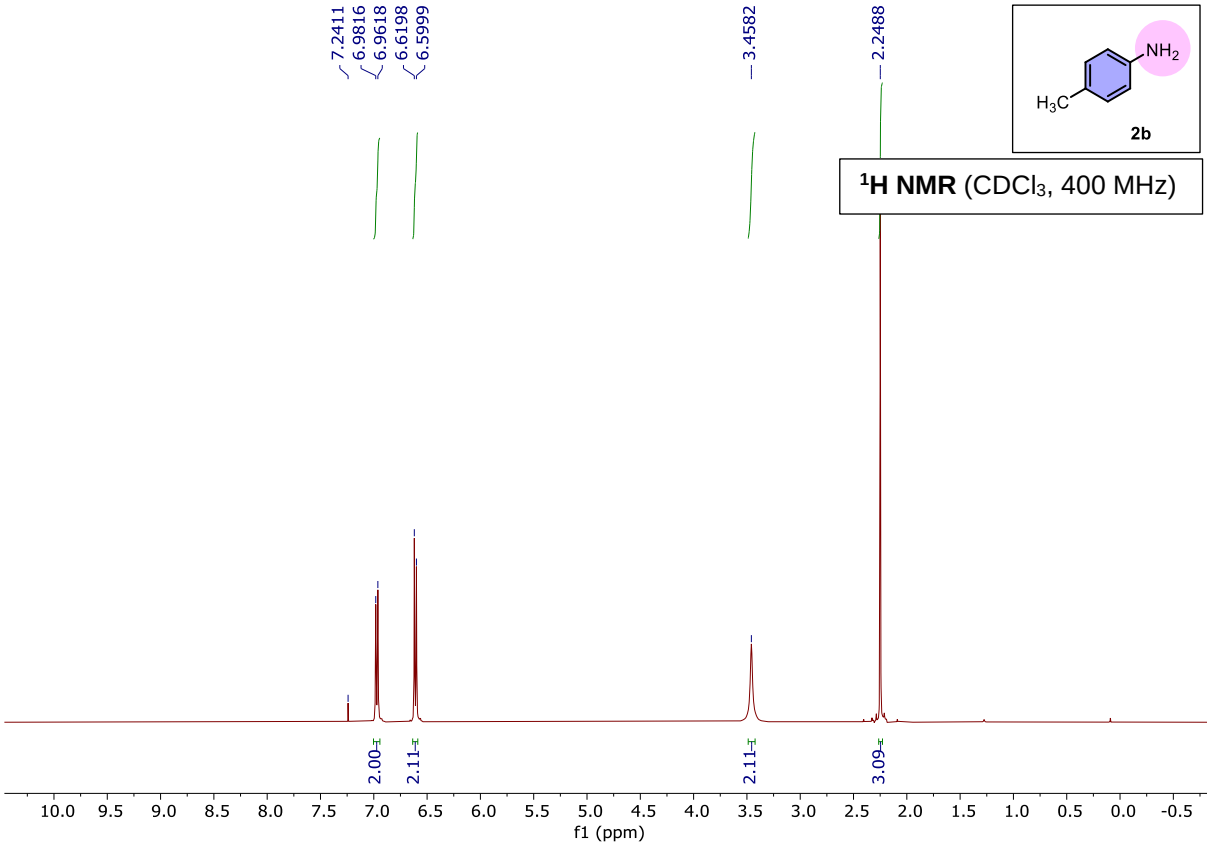
12. Copies of ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of the amines:



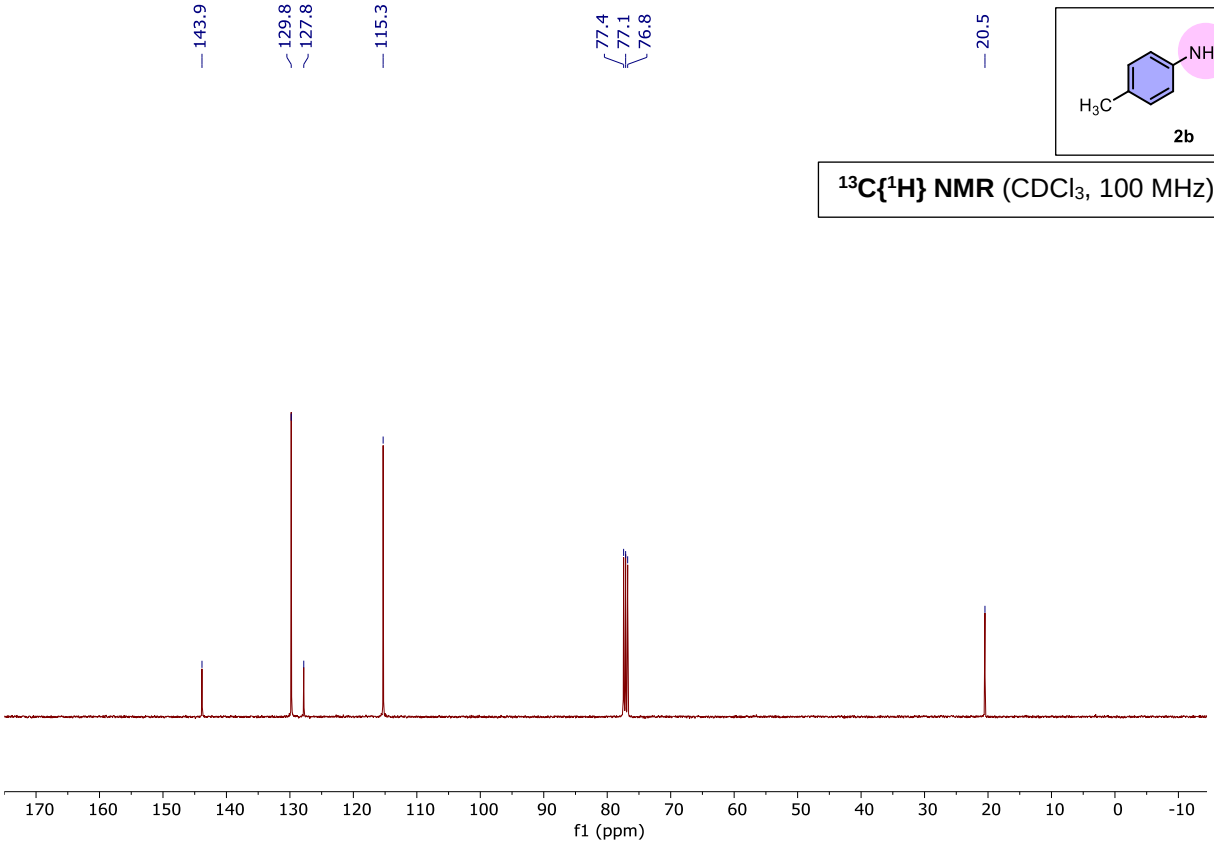
^{1}H NMR ($CDCl_3$, 400 MHz)



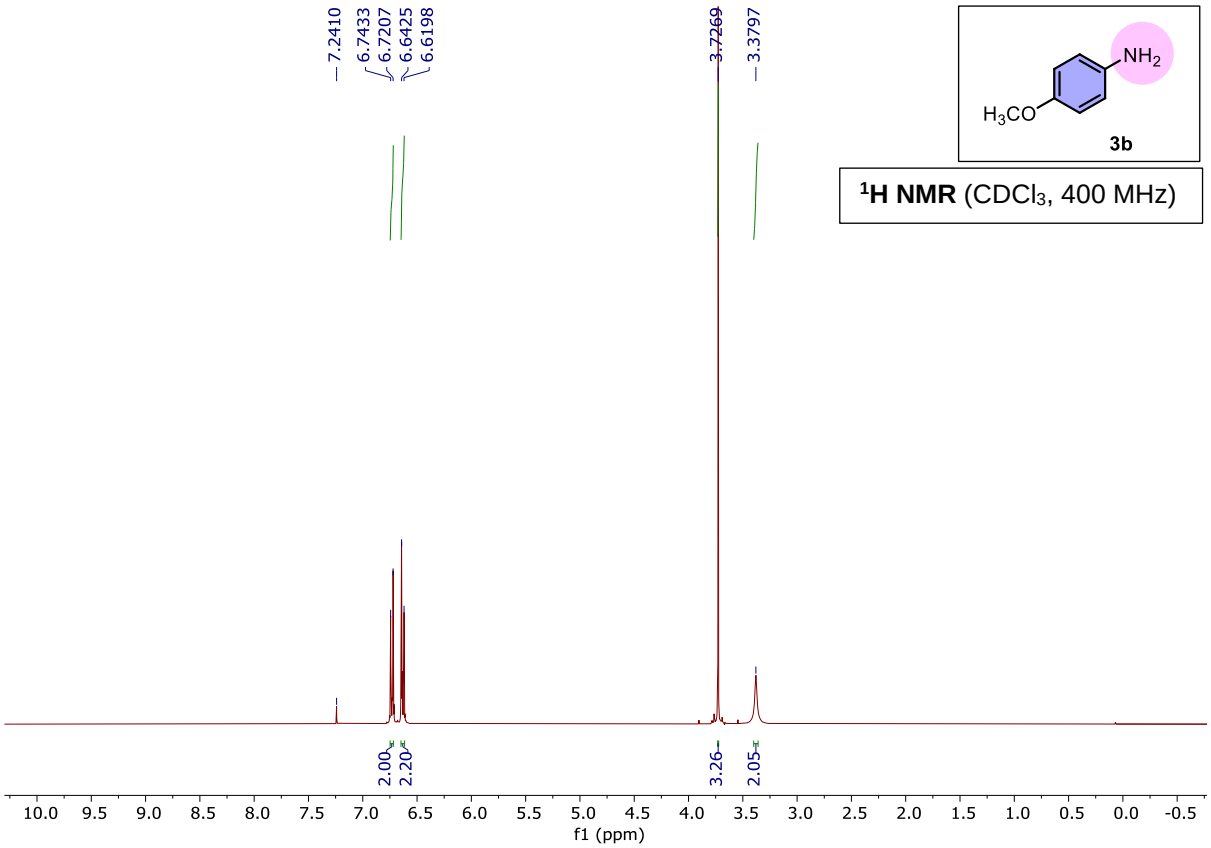
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz)

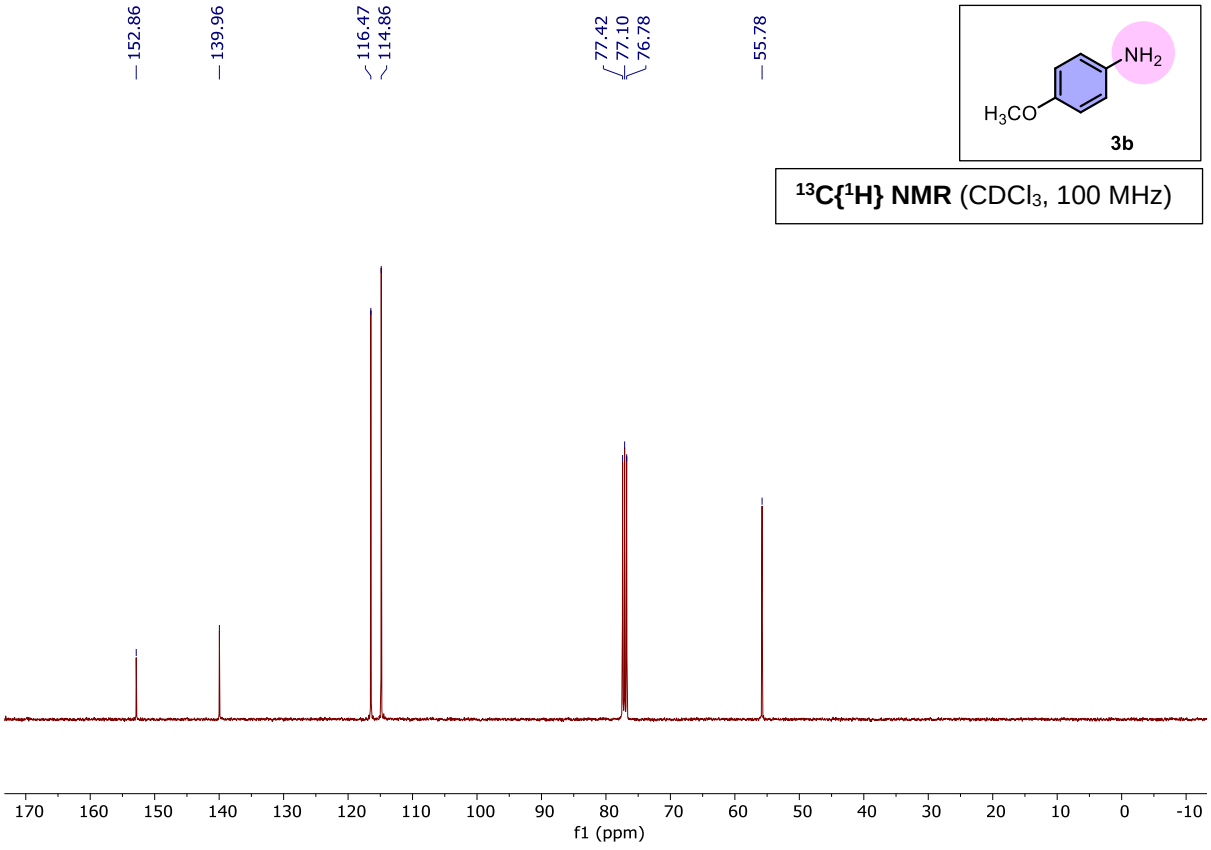


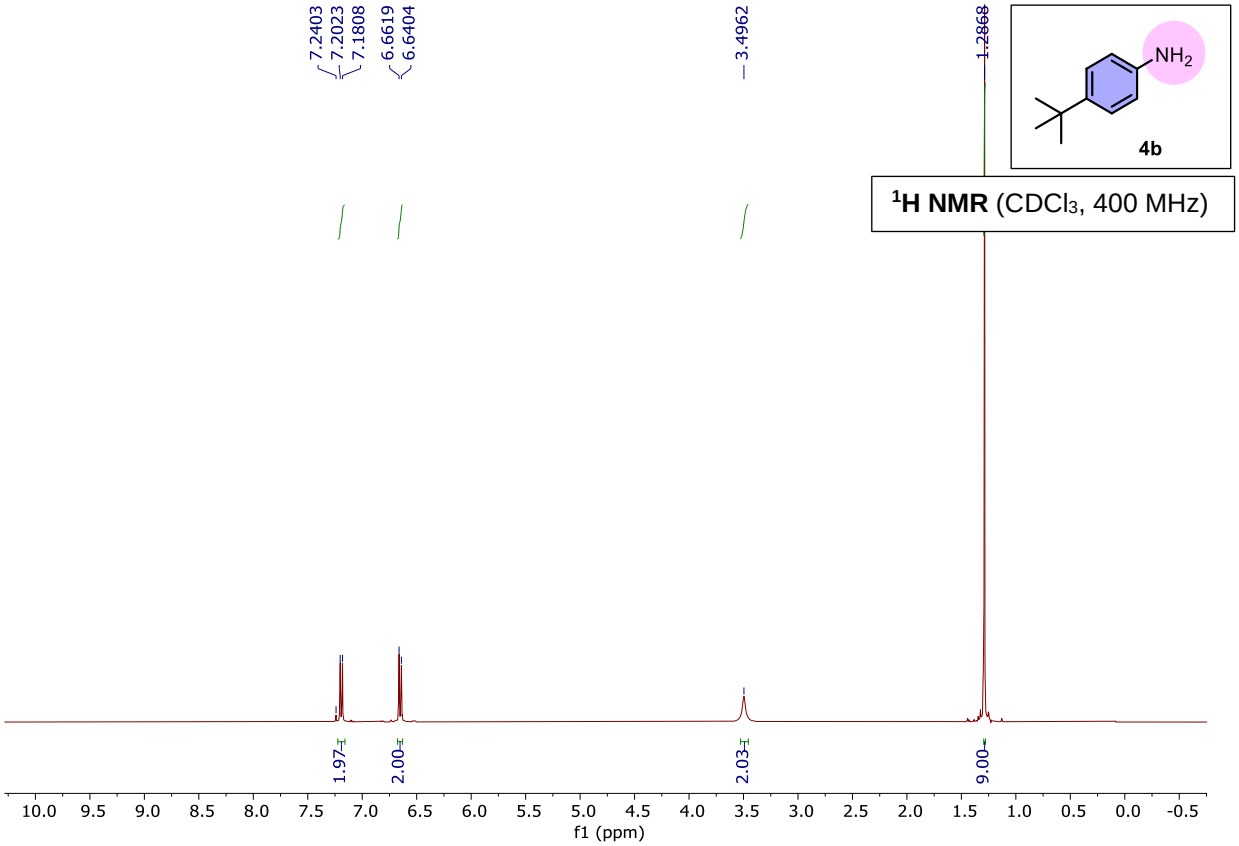
^{1}H NMR ($CDCl_3$, 400 MHz)



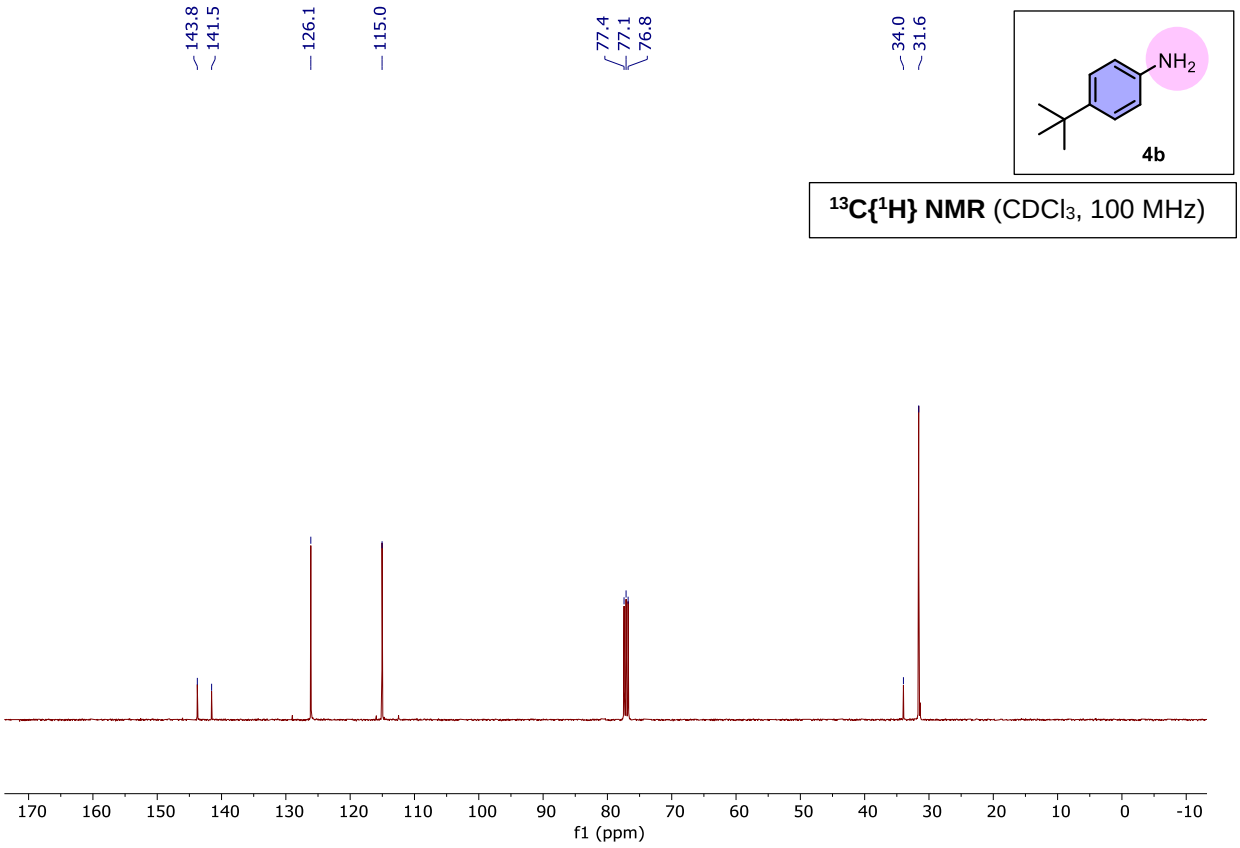
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)


7.2410
6.7433
6.7207
6.6425
6.6198
3.7269
3.3797
2.00
2.20
3.26
2.05
f1 (ppm)
NH2
H3CO
3b
1H NMR (CDCl3, 400 MHz)

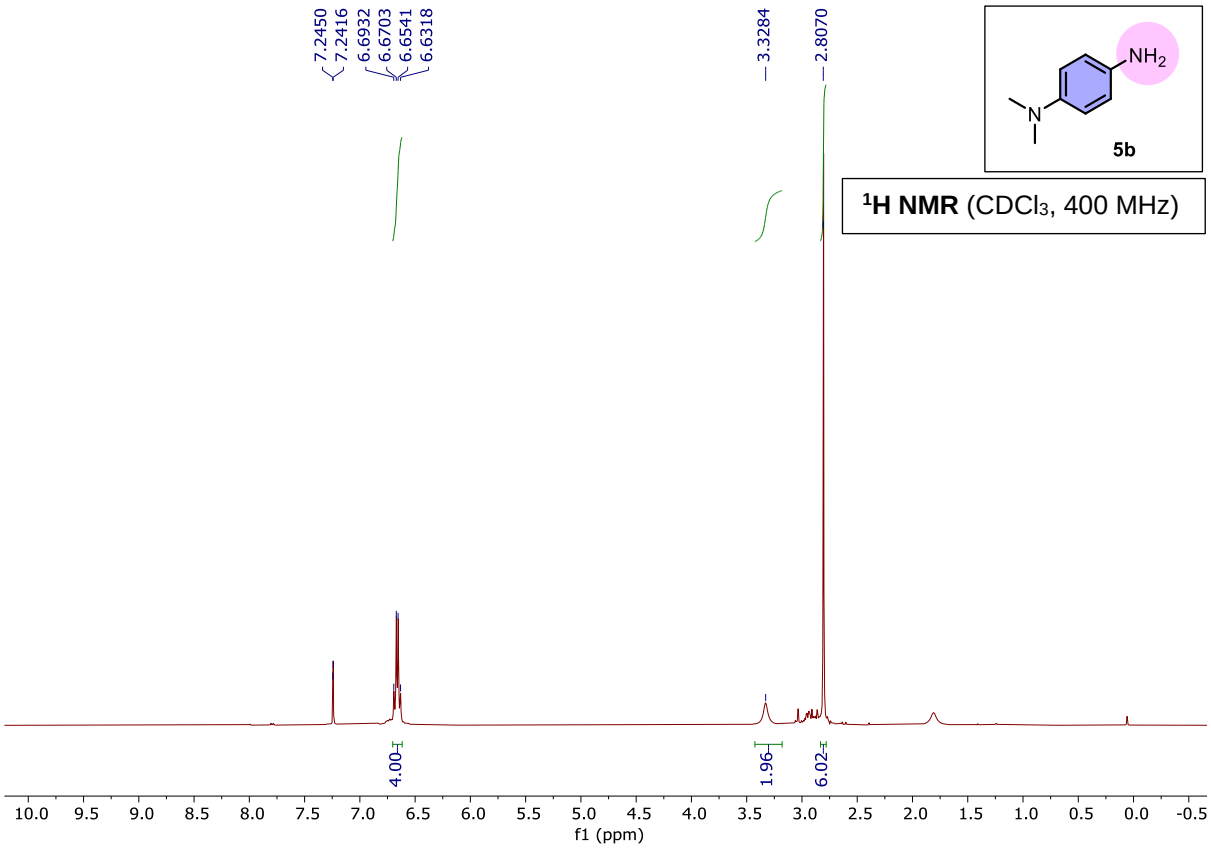

152.86
139.96
116.47
114.86
77.42
77.10
76.78
55.78
f1 (ppm)
NH2
H3CO
3b
13C{1H} NMR (CDCl3, 100 MHz)



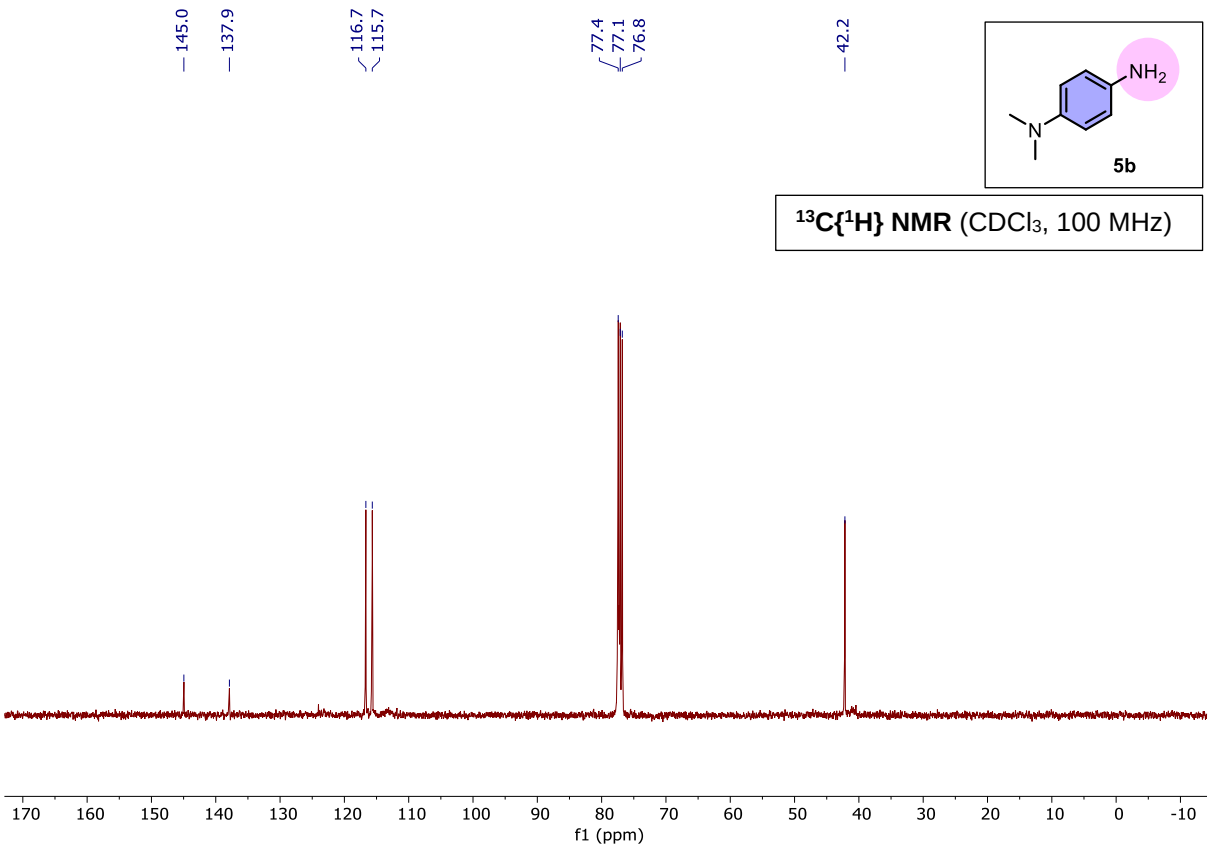
^{1}H NMR ($CDCl_3$, 400 MHz)



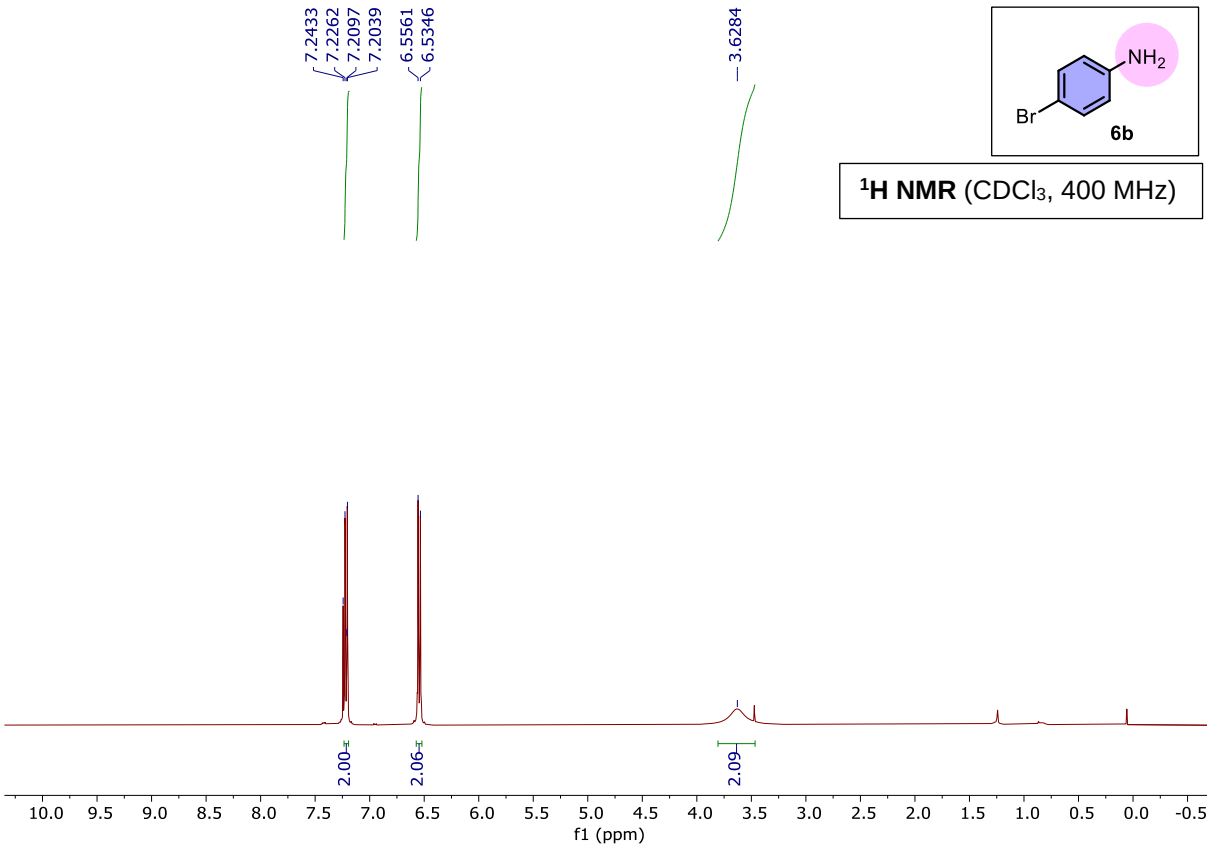
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



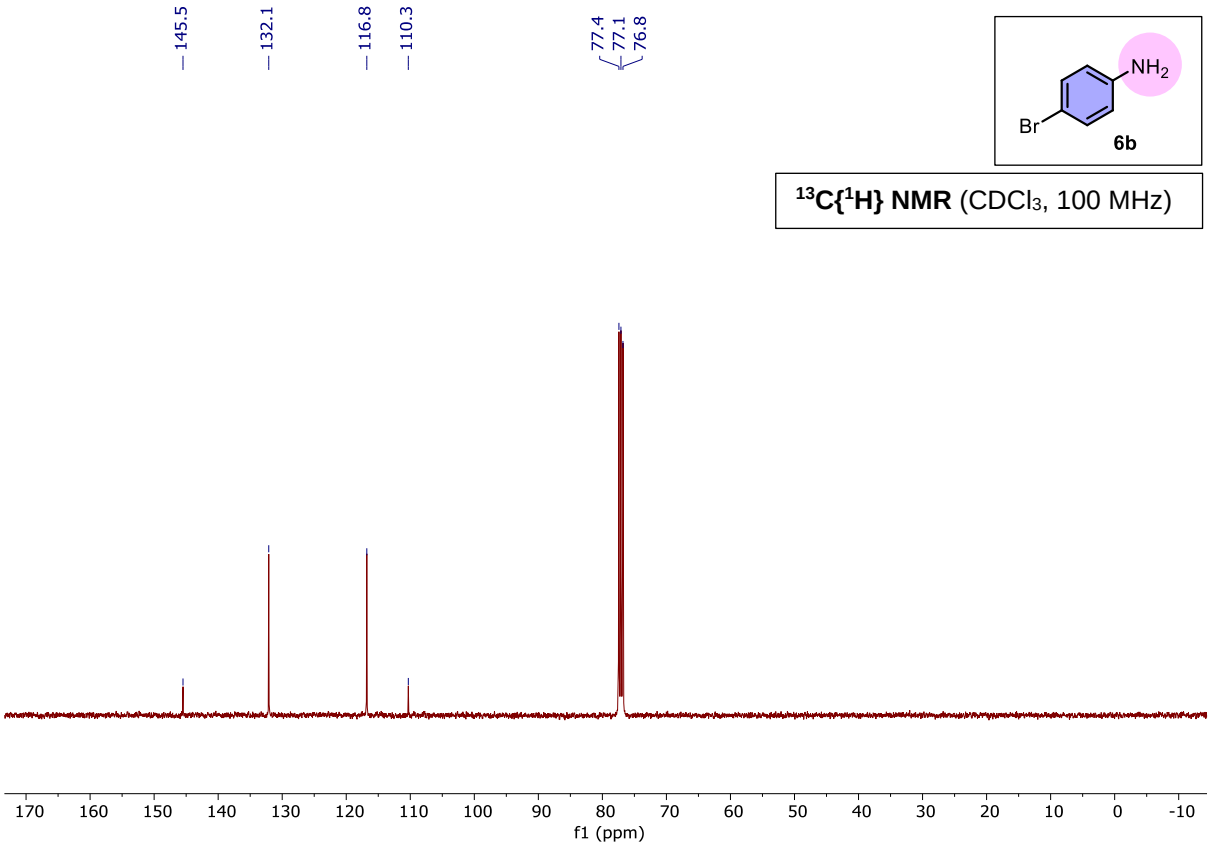
^{1}H NMR ($CDCl_3$, 400 MHz)



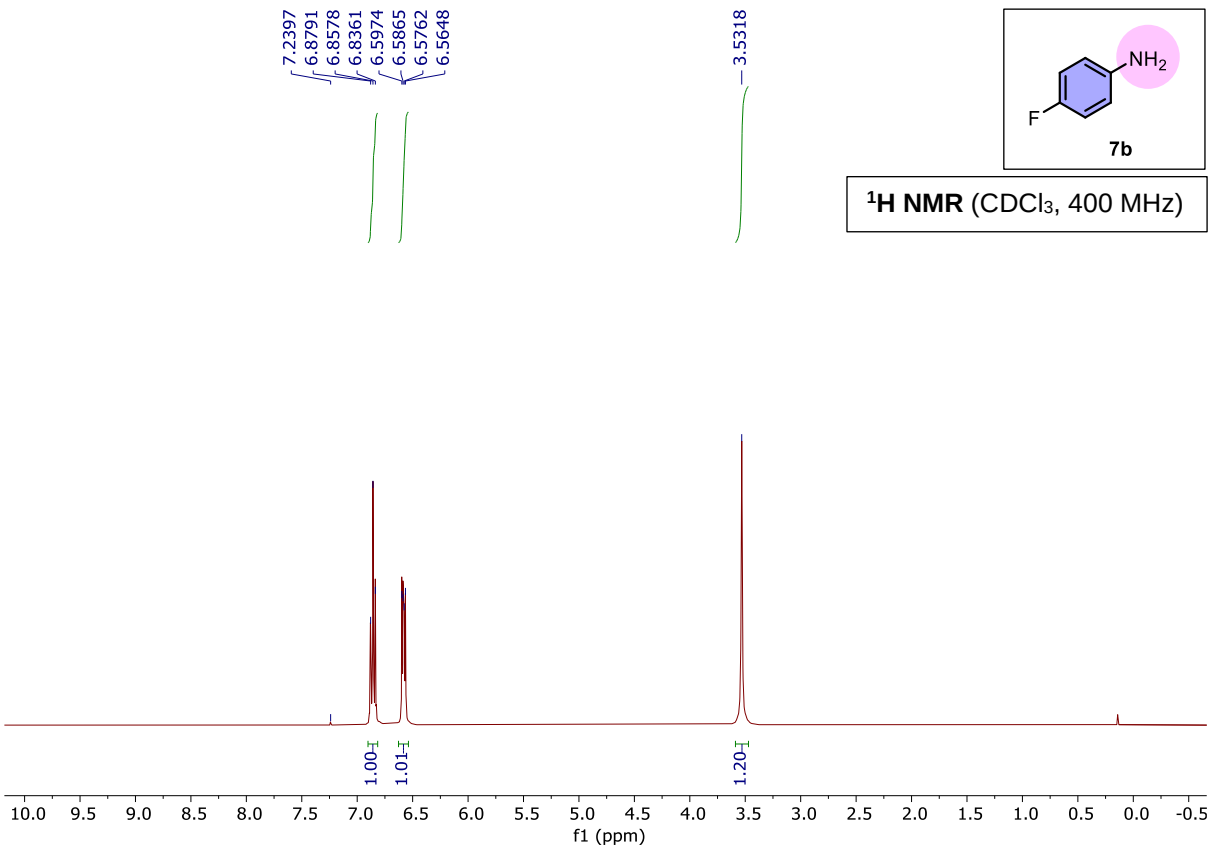
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

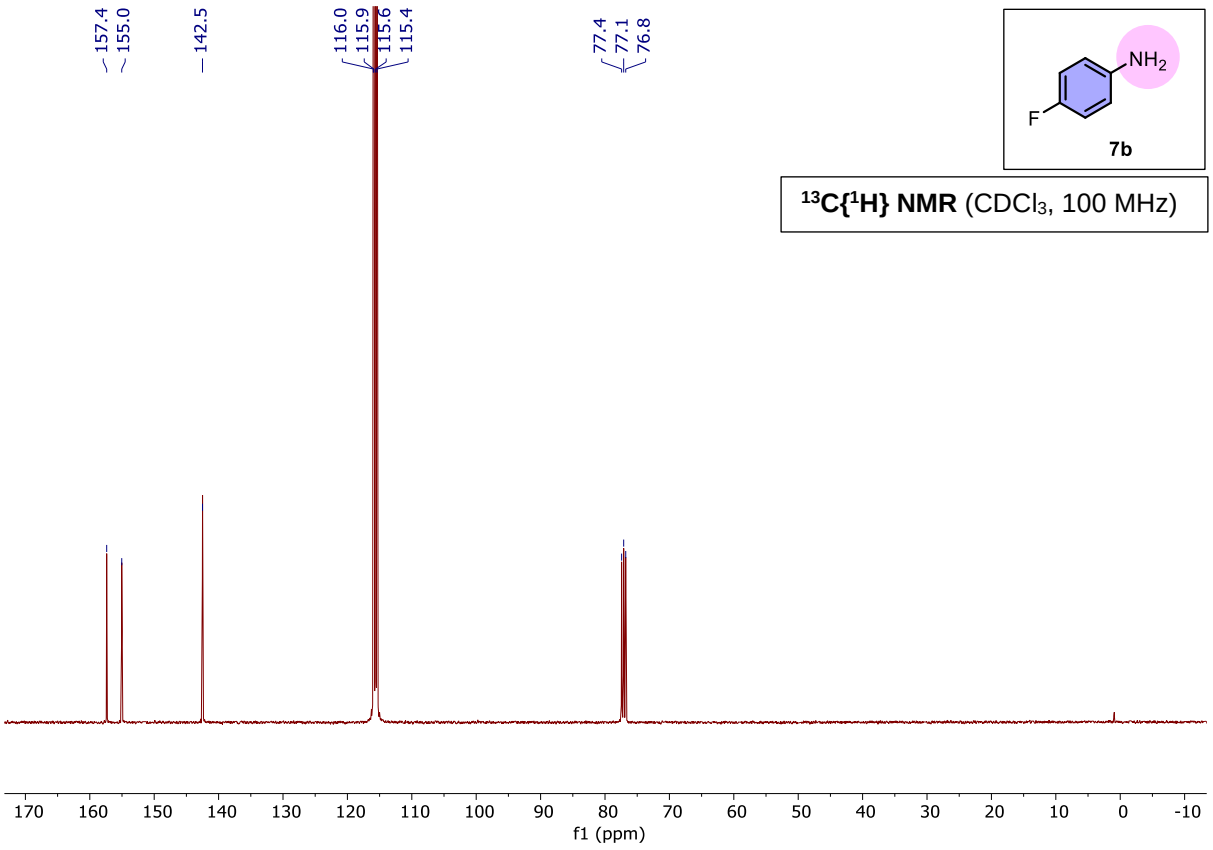


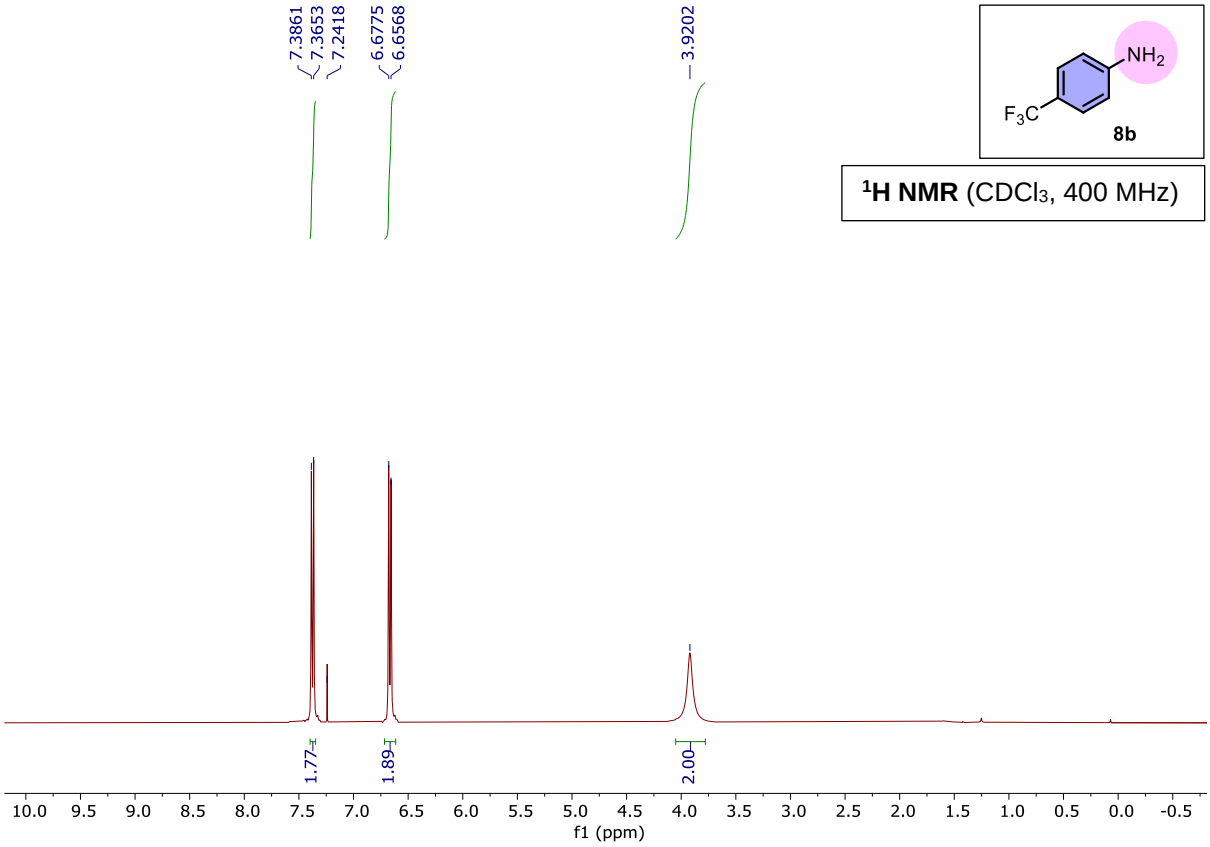
^{1}H NMR ($CDCl_3$, 400 MHz)

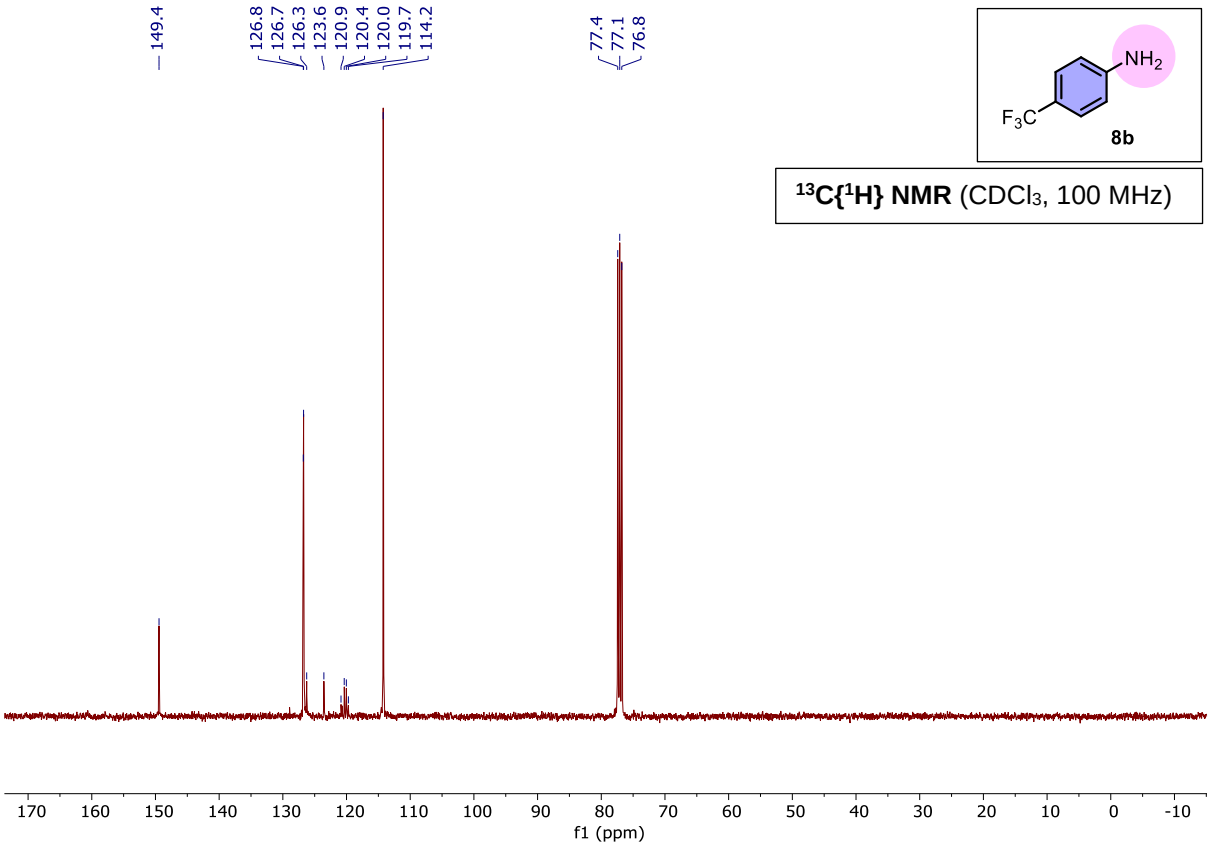


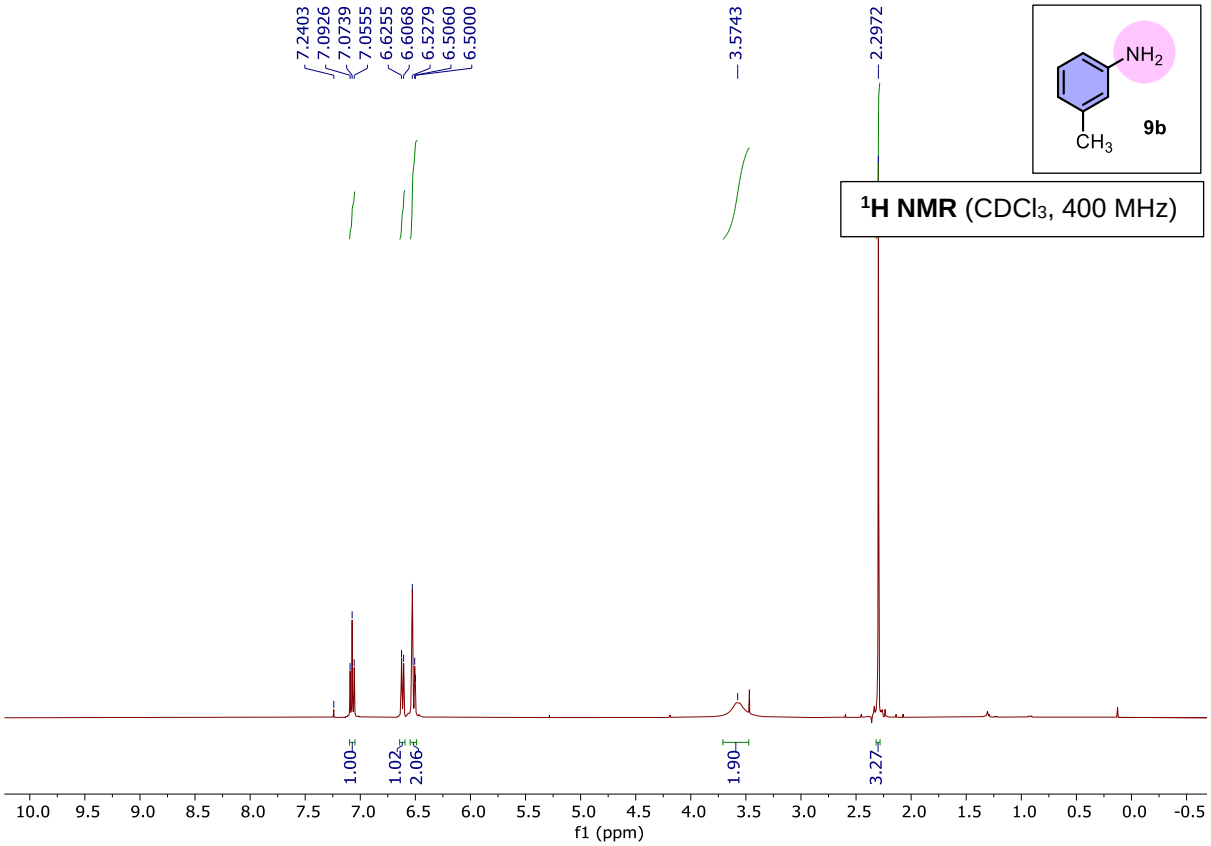
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)


7.2397
6.8791
6.8578
6.8361
6.5974
6.5865
6.5762
6.5648
3.5318
NH2
F
7b
1H NMR (CDCl3, 400 MHz)
1.00
1.01
1.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

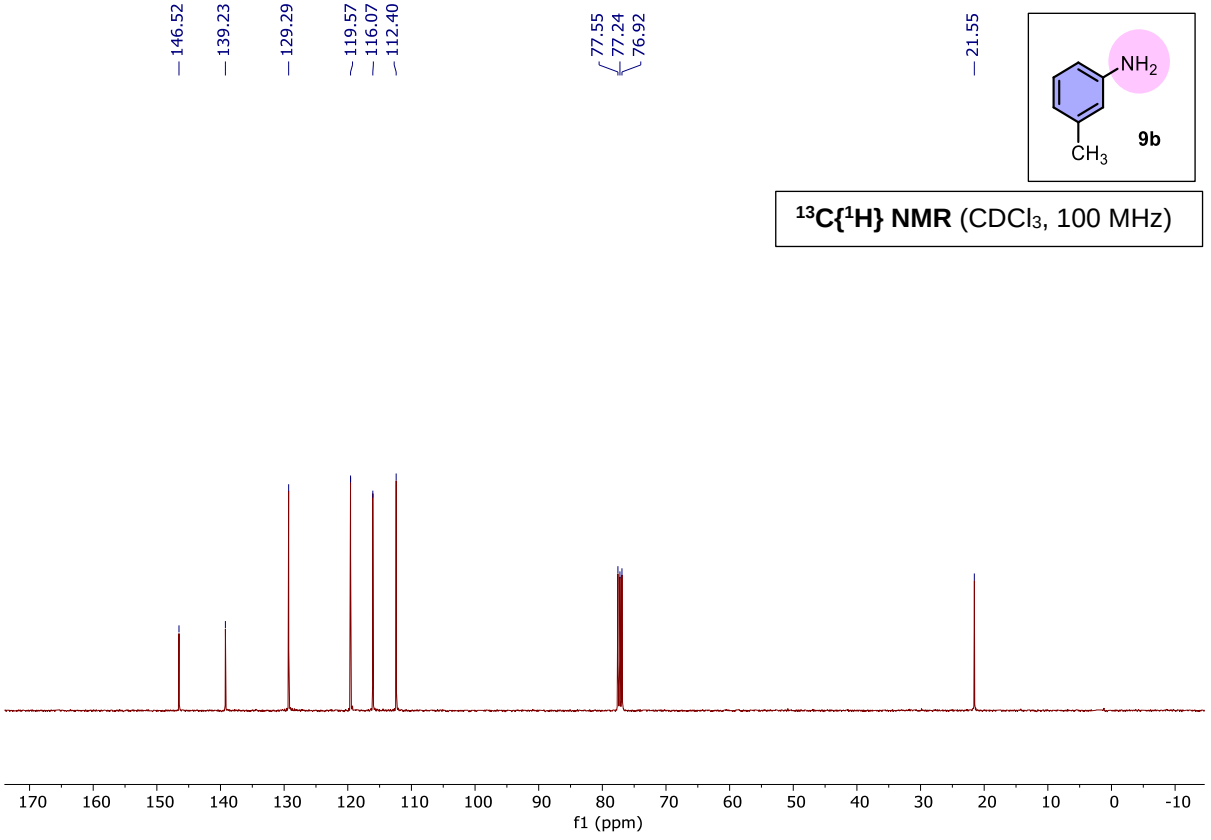

157.4
155.0
142.5
116.0
115.9
115.6
115.4
77.4
77.1
76.8
NH2
F
7b
13C{1H} NMR (CDCl3, 100 MHz)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.3861
7.3653
7.2418
6.6775
6.6568
3.9202
NH2
F3C
8b
1H NMR (CDCl3, 400 MHz)
1.77
1.89
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

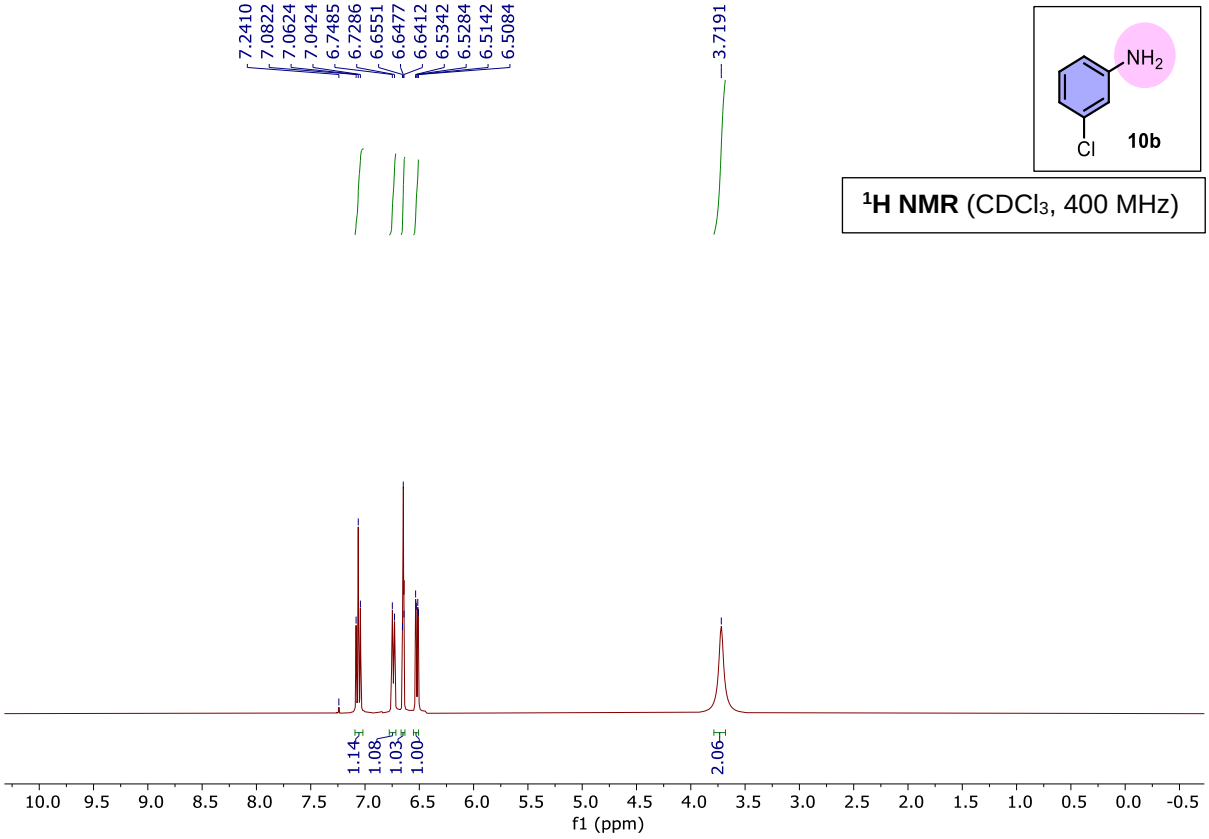

149.4
126.8
126.7
126.3
123.6
120.9
120.4
120.0
119.7
114.2
77.4
77.1
76.8
NH2
F3C
8b
13C{1H} NMR (CDCl3, 100 MHz)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



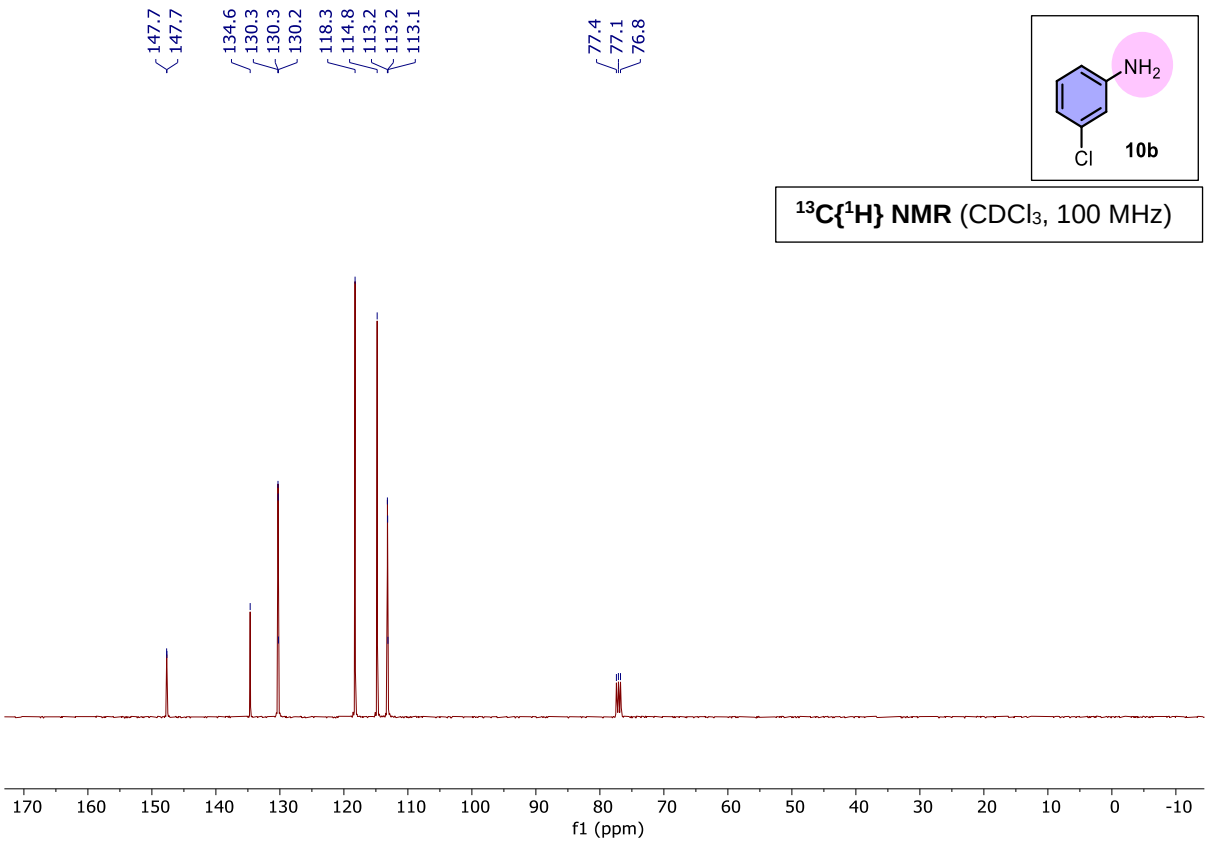
^{1}H NMR ($CDCl_3$, 400 MHz)



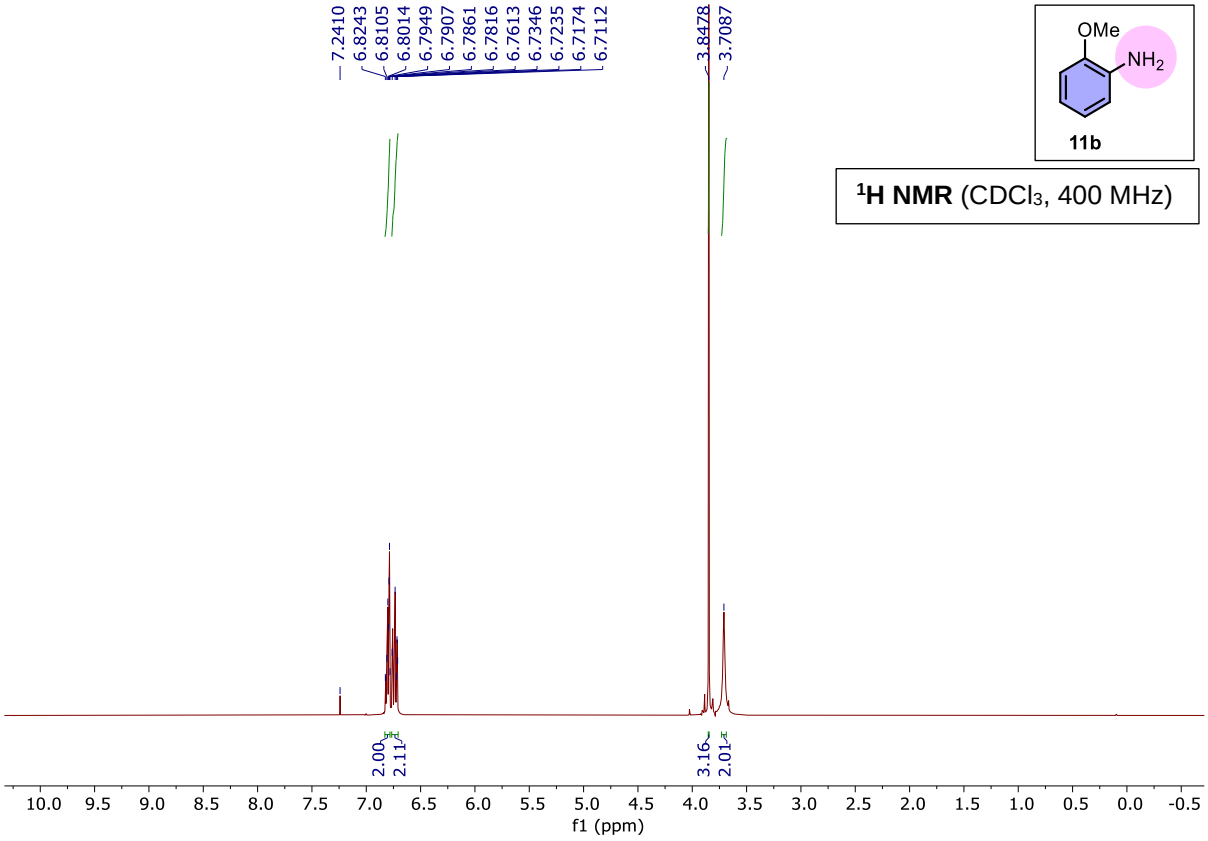
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



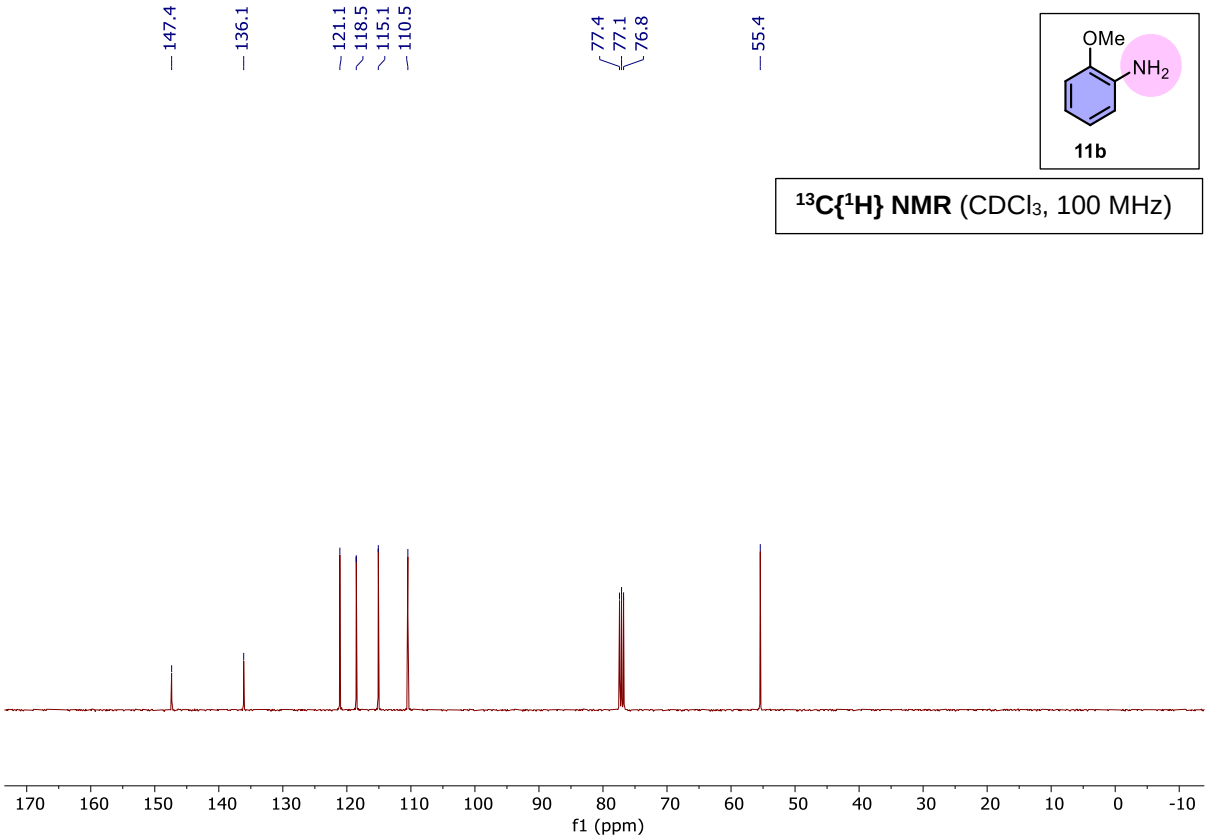
^{1}H NMR ($CDCl_3$, 400 MHz)



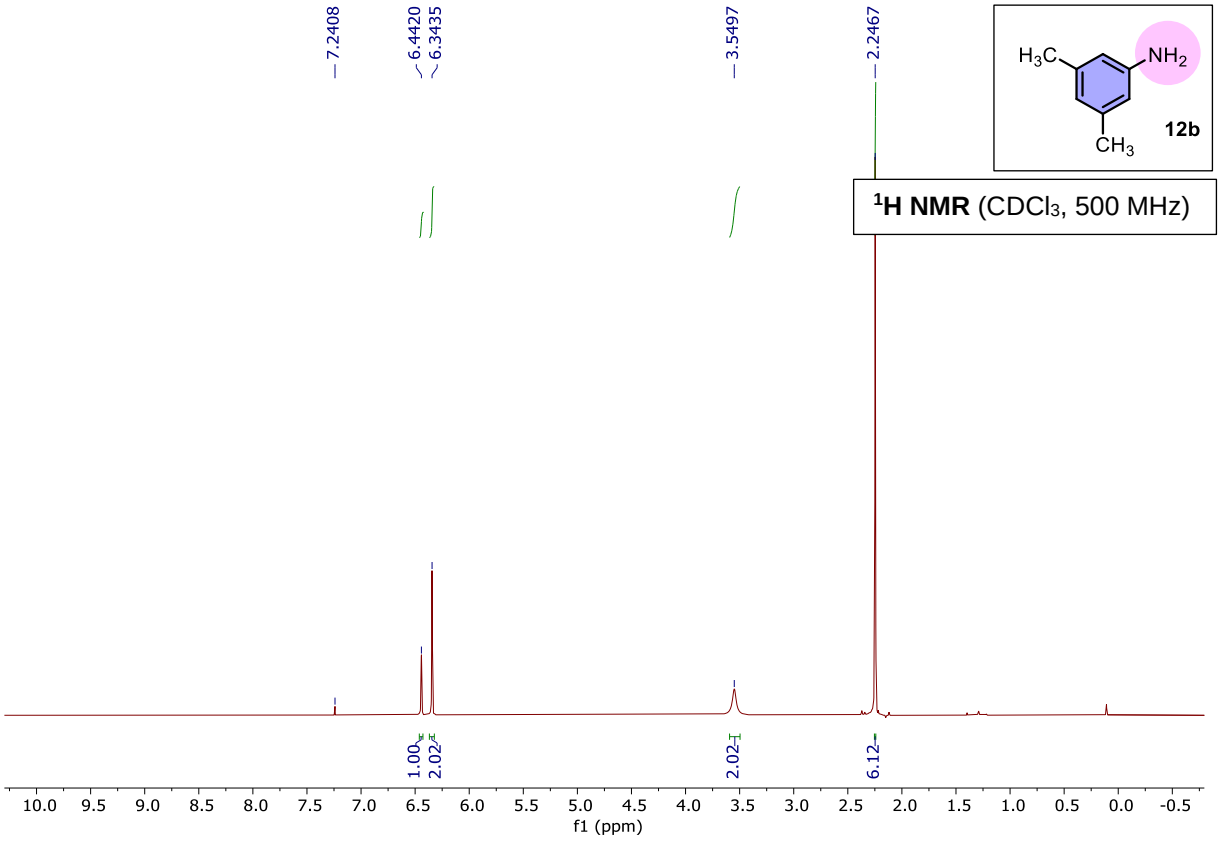
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



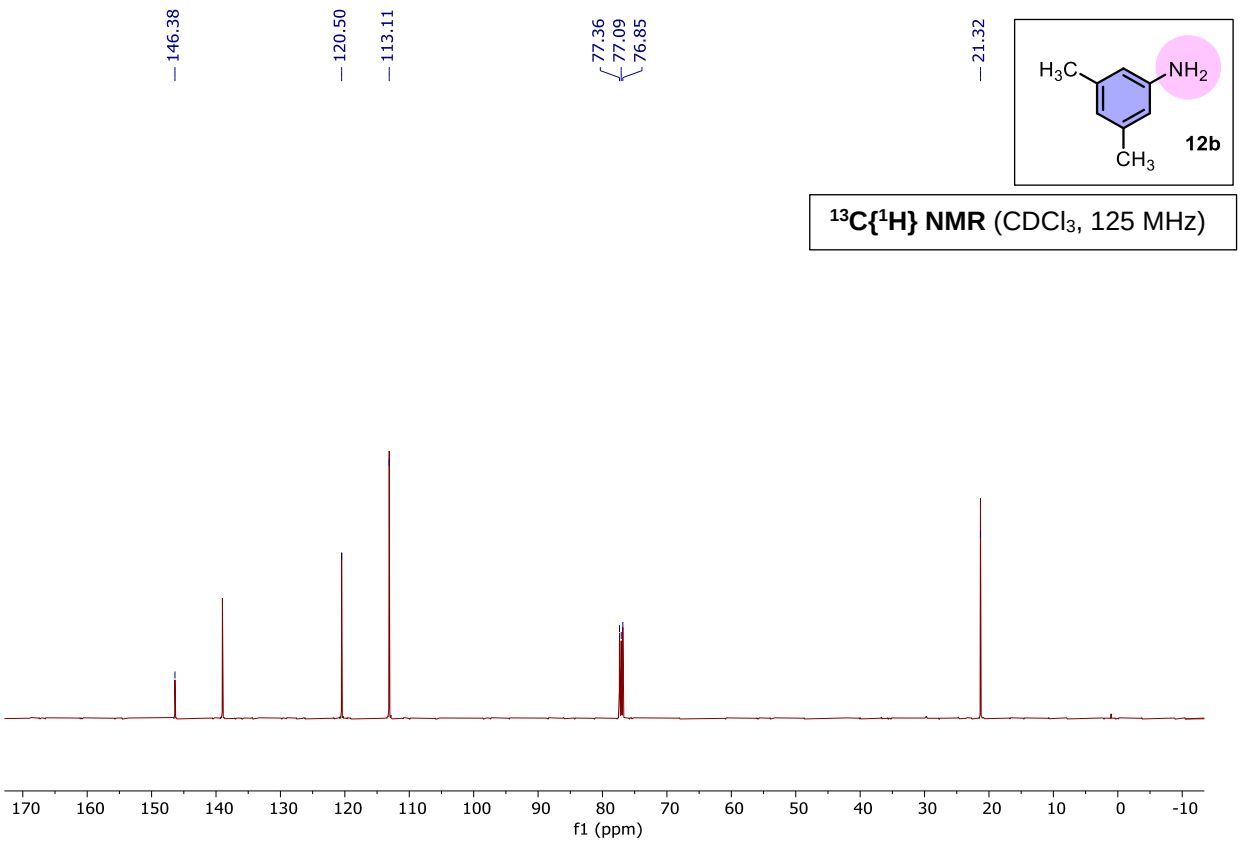
^{1}H NMR ($CDCl_3$, 400 MHz)



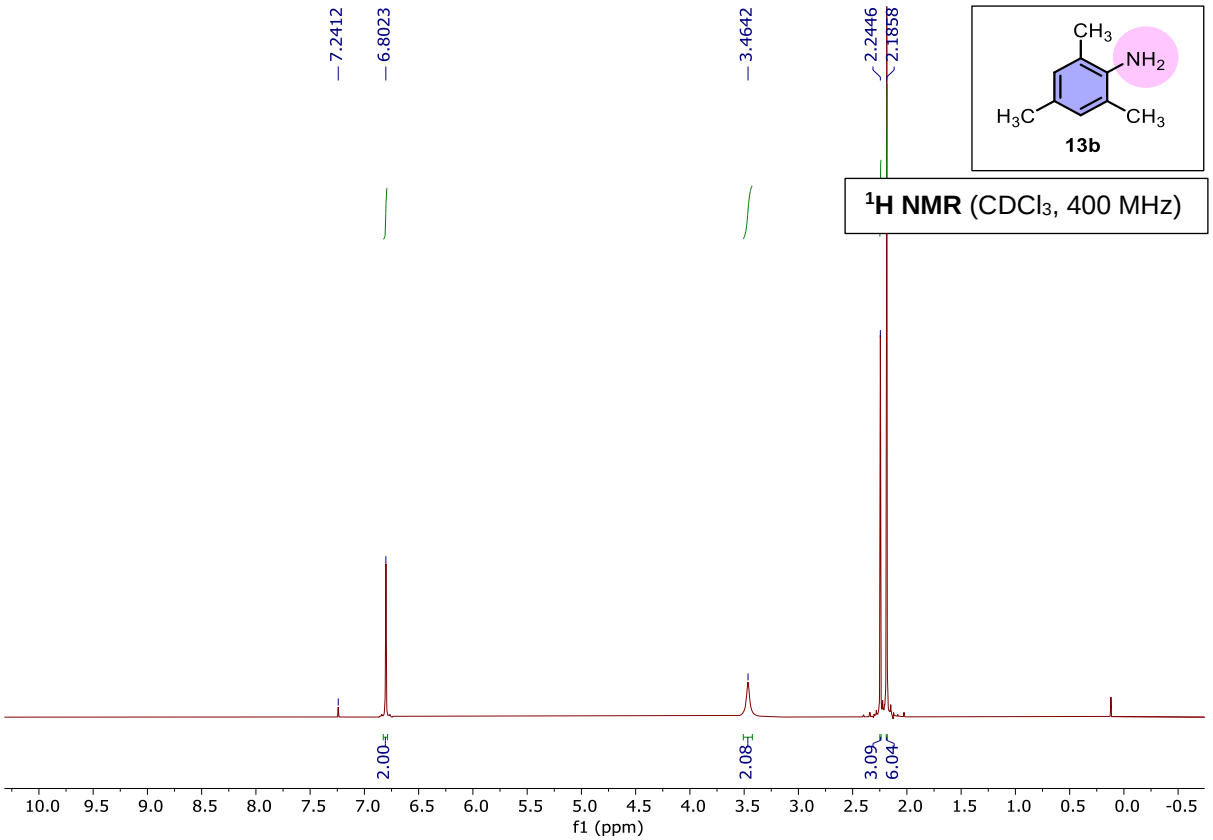
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

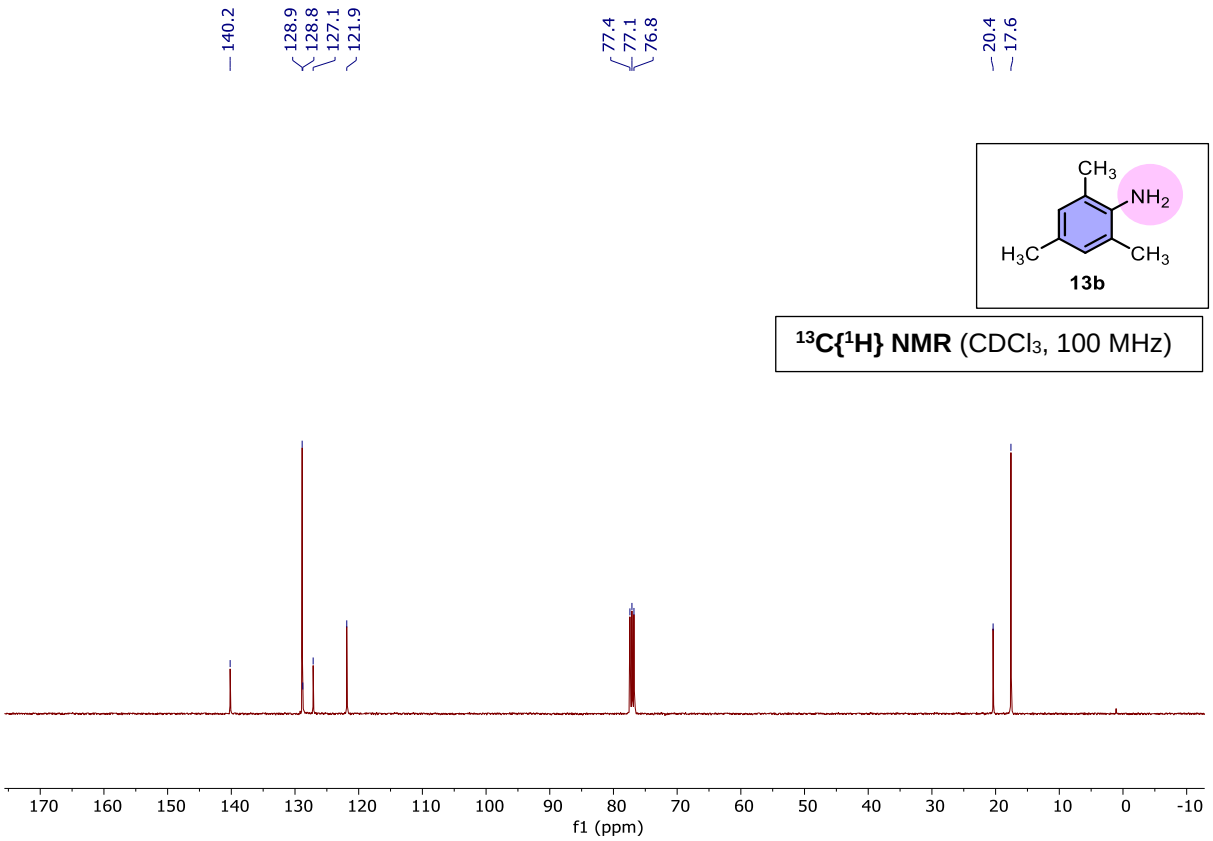


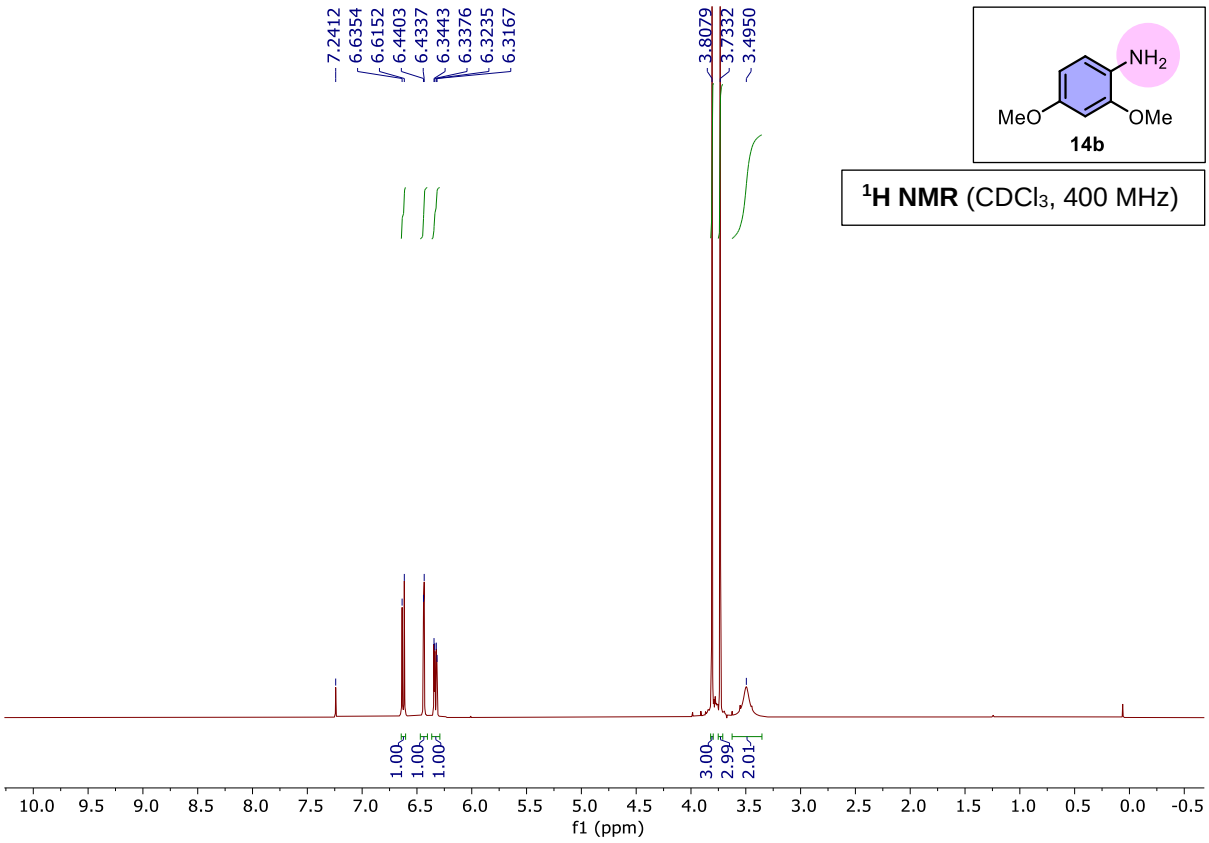
^{1}H NMR ($CDCl_3$, 500 MHz)



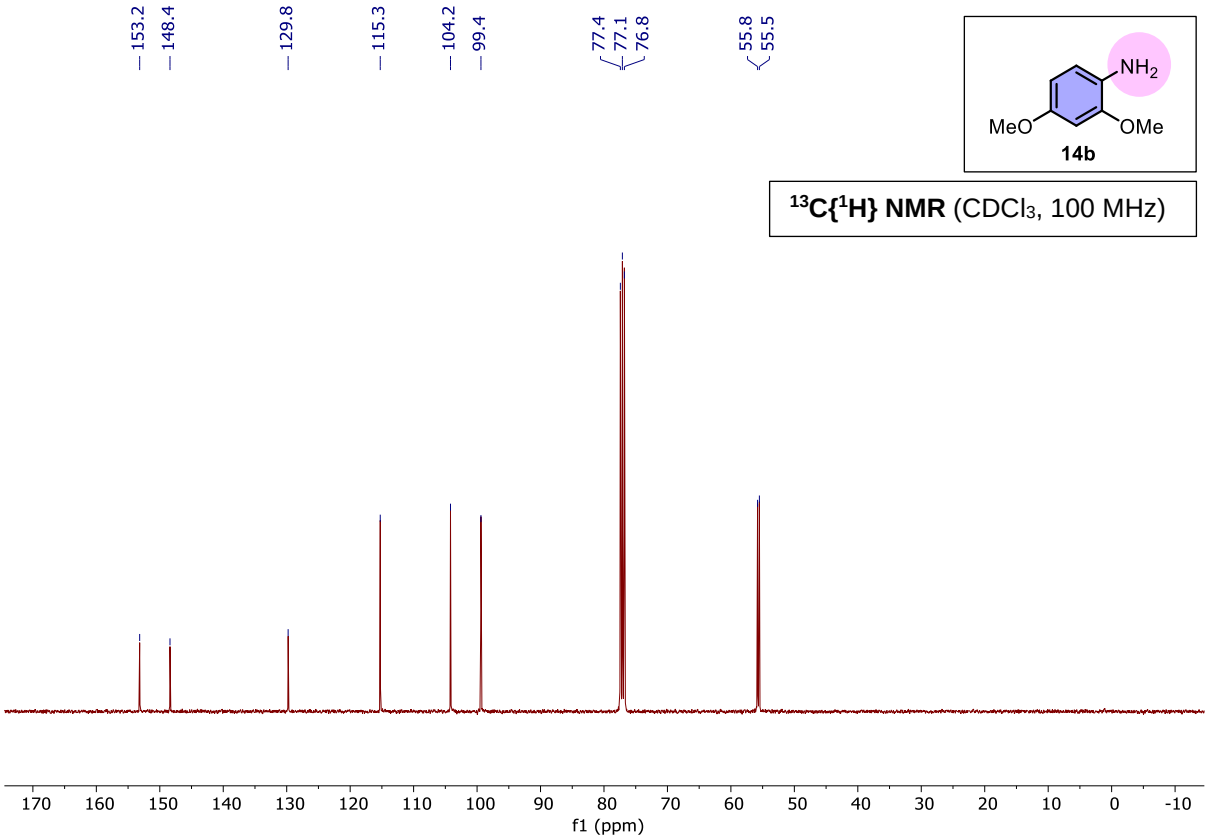
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)


7.2412
6.8023
3.4642
2.2446
2.1858
2.00
2.08
3.09
6.04
f1 (ppm)
13b
^{1}H NMR (CDCl$_3$, 400 MHz)

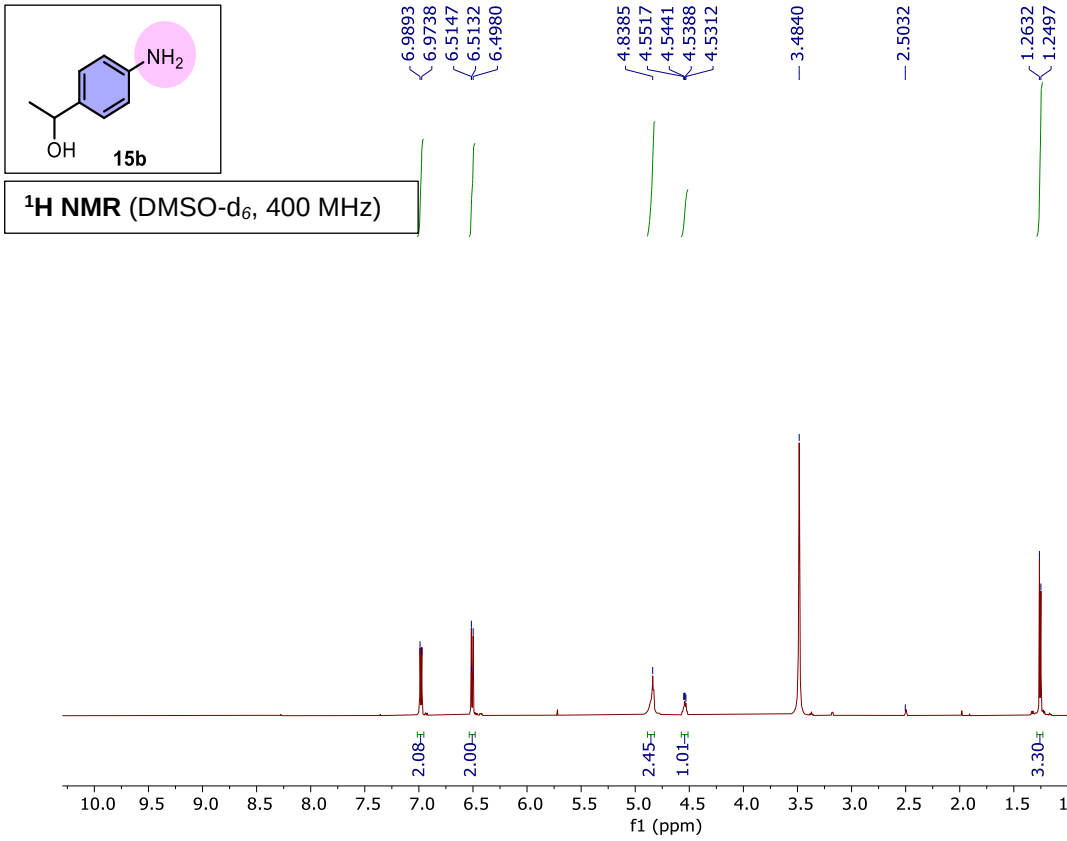

140.2
128.9
128.8
127.1
121.9
77.4
77.1
76.8
20.4
17.6
f1 (ppm)
13b
^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz)



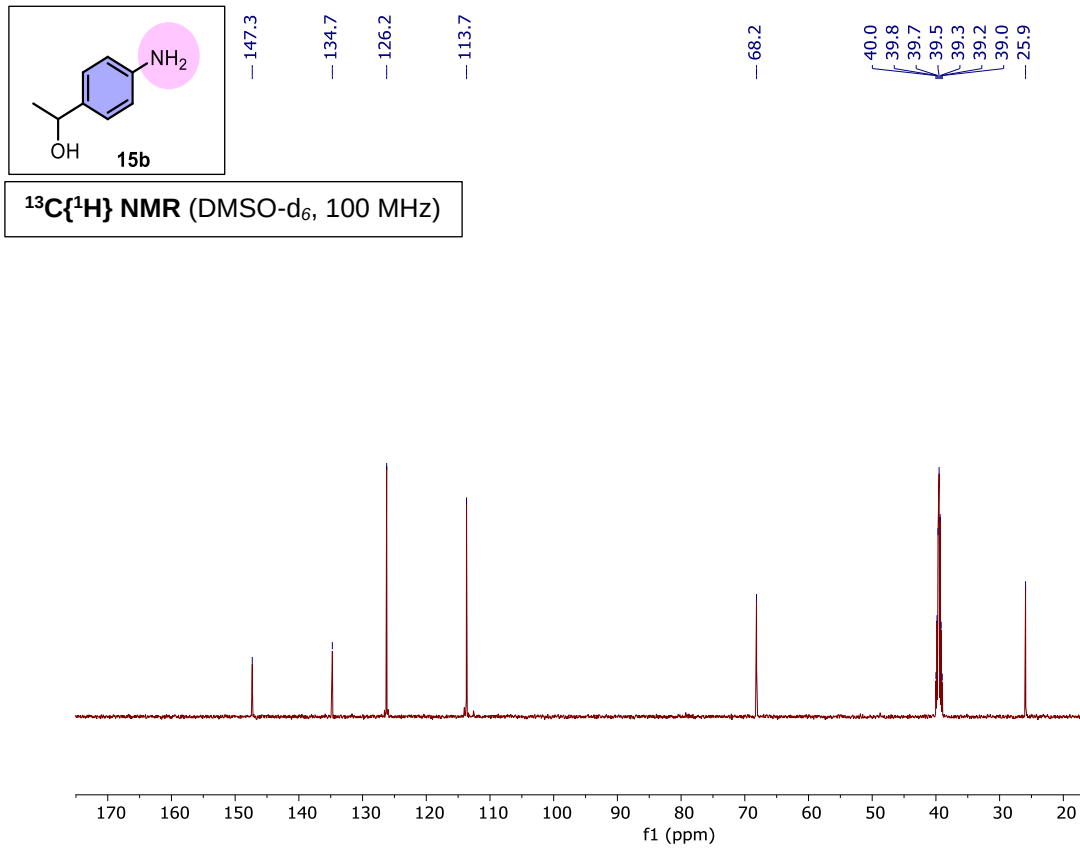
^{1}H NMR ($CDCl_3$, 400 MHz)



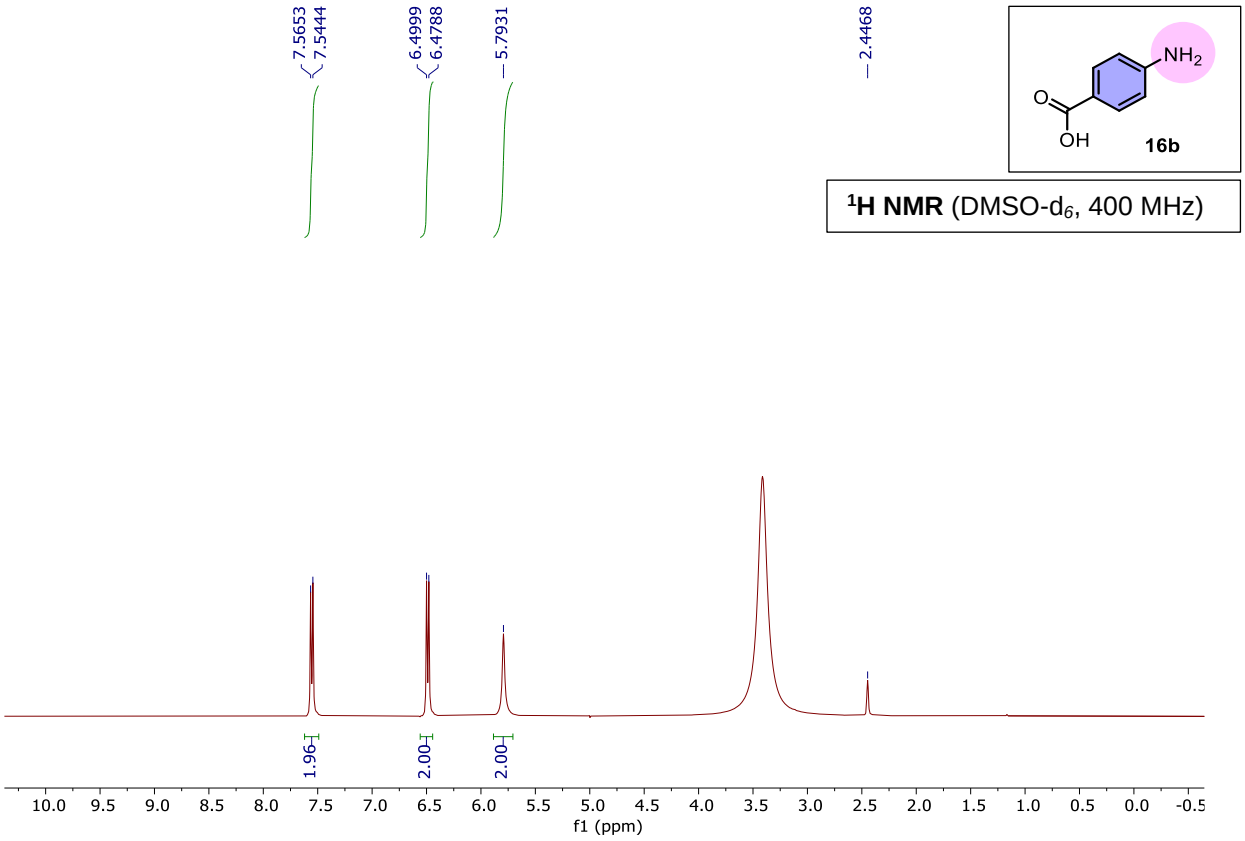
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



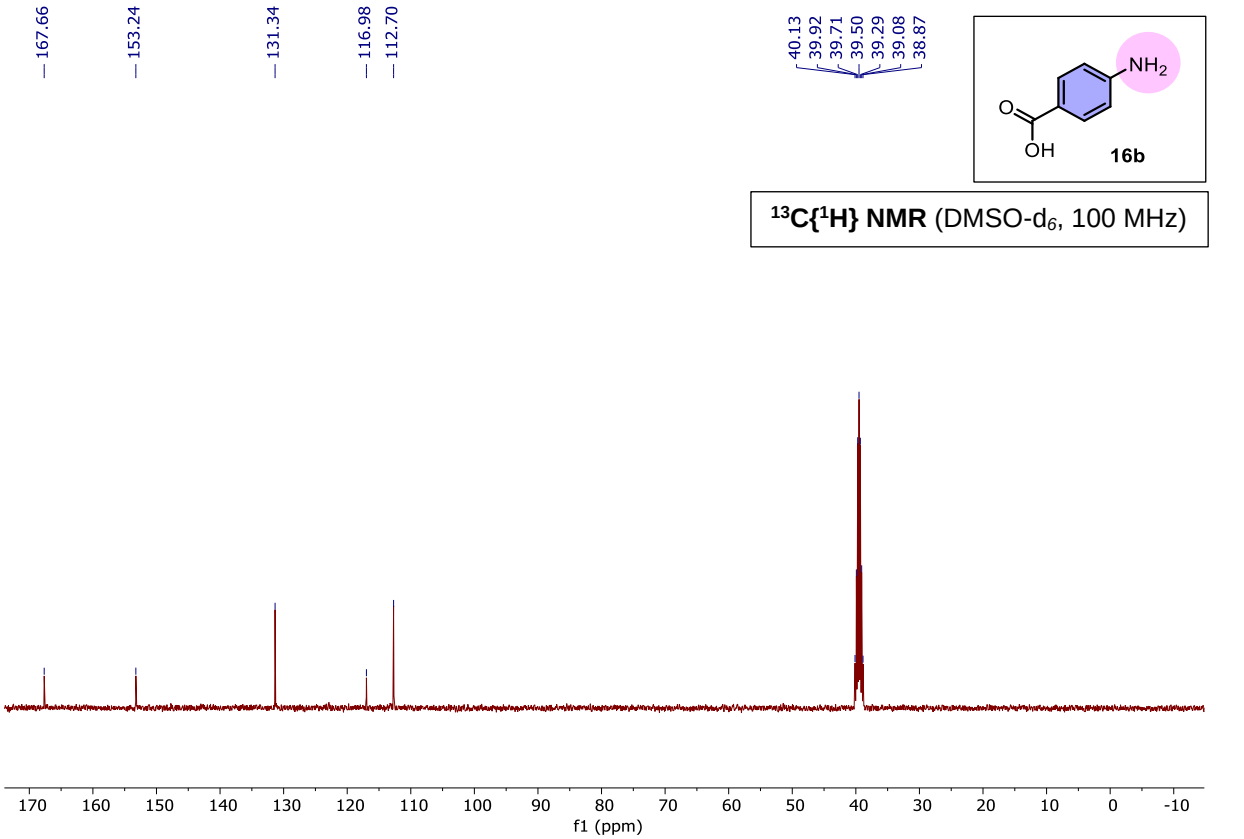
^{1}H NMR (DMSO-d$_6$, 400 MHz)



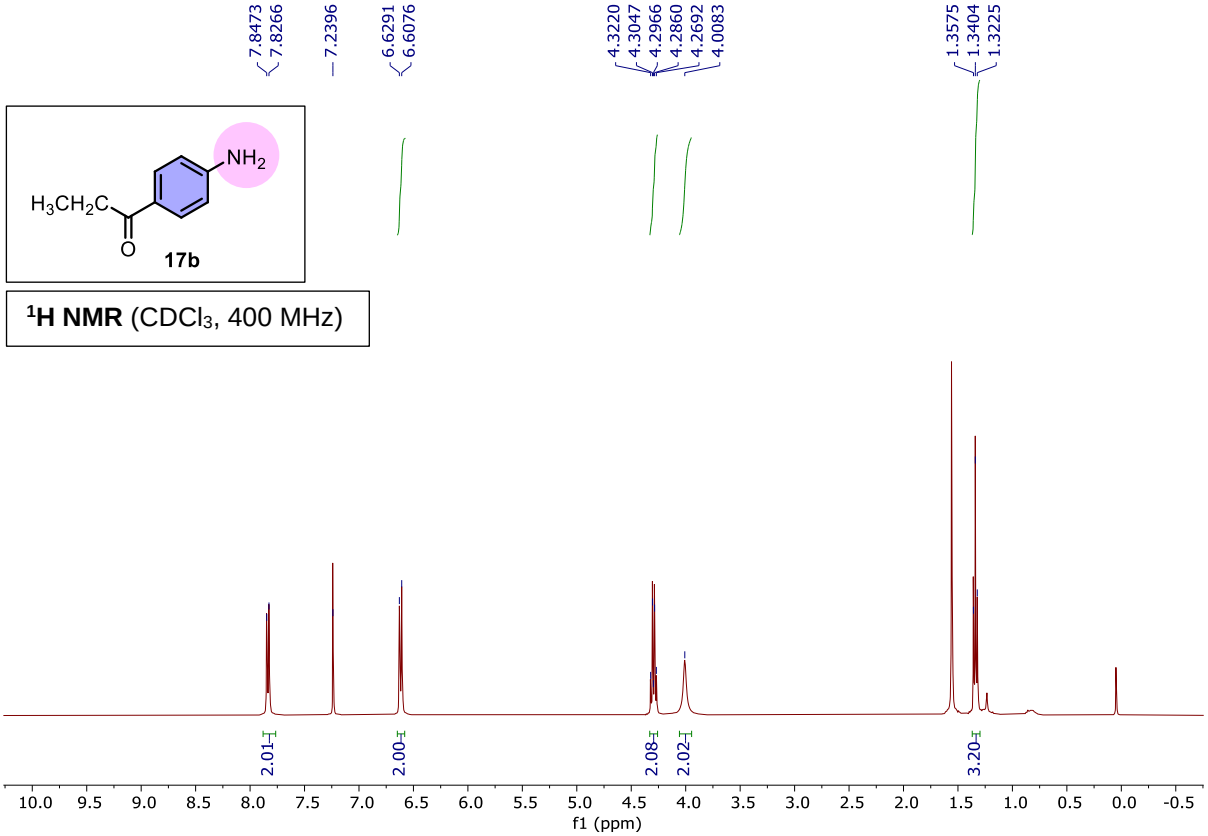
^{13}C{^{1}H} NMR (DMSO-d$_6$, 100 MHz)



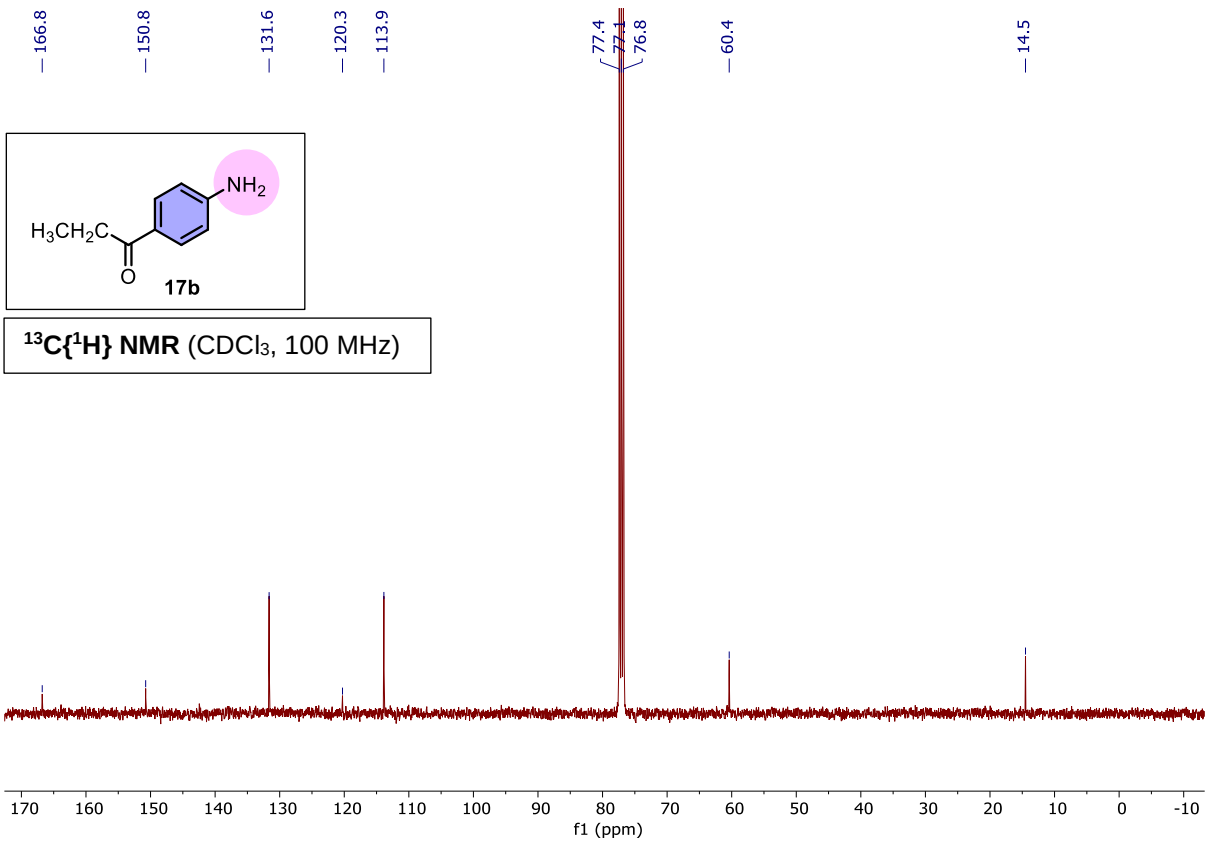
^{1}H NMR (DMSO-d$_6$, 400 MHz)



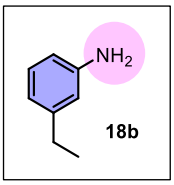
^{13}C{^{1}H} NMR (DMSO-d$_6$, 100 MHz)



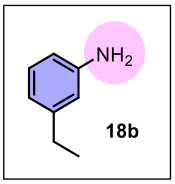
^{1}H NMR ($CDCl_3$, 400 MHz)



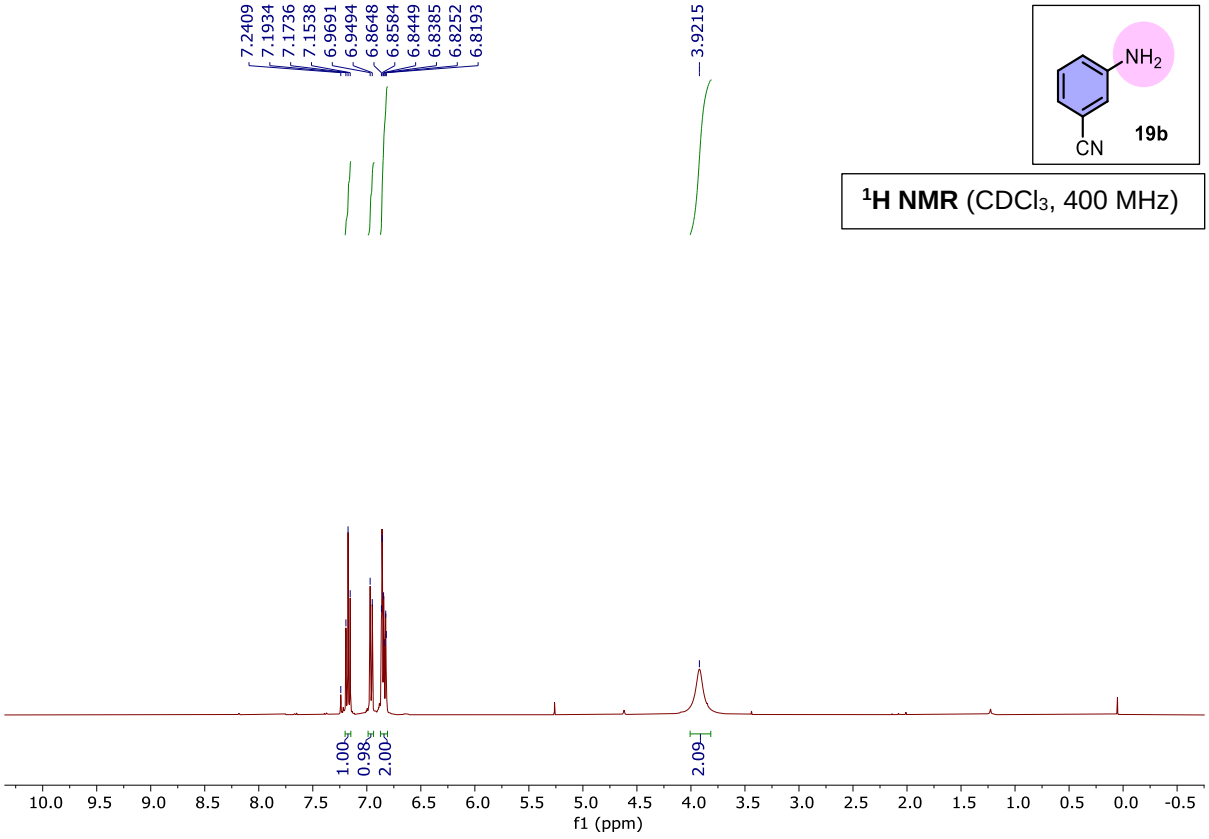
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



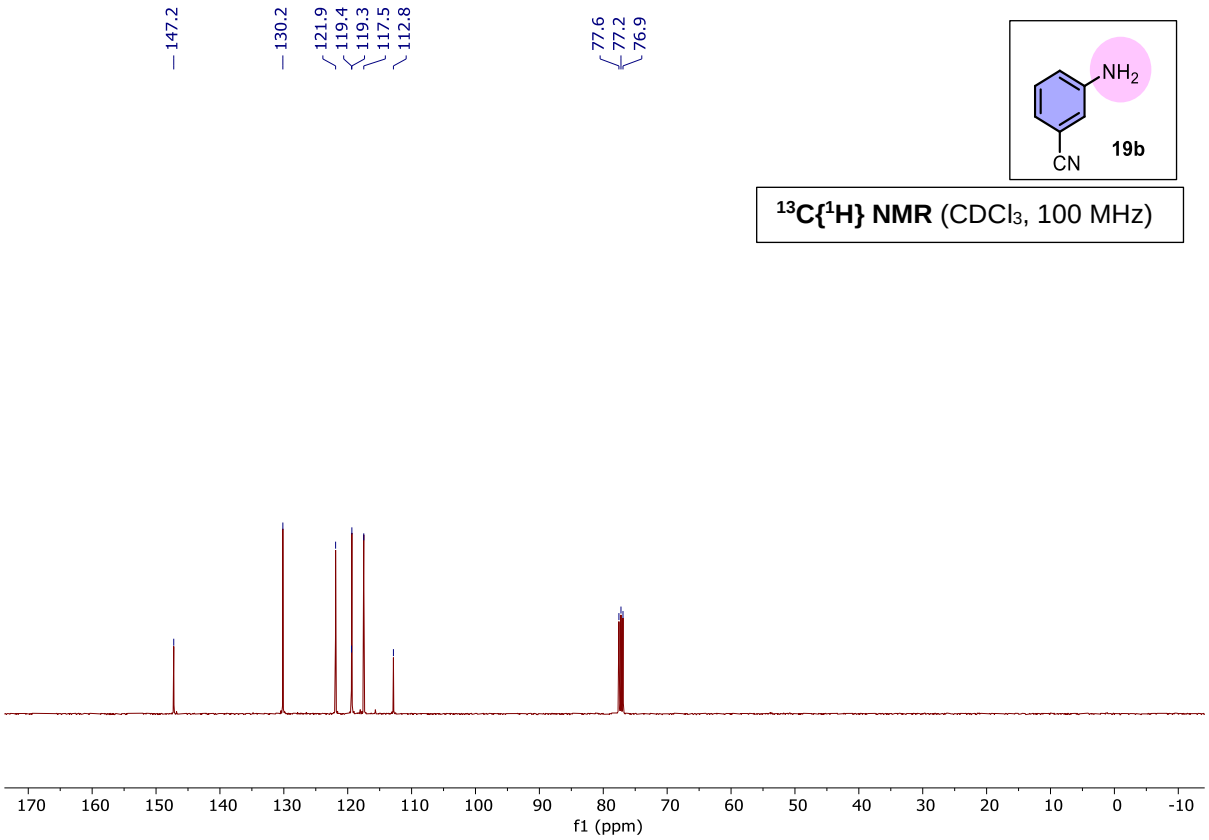
^{1}H NMR ($CDCl_3$, 400 MHz)



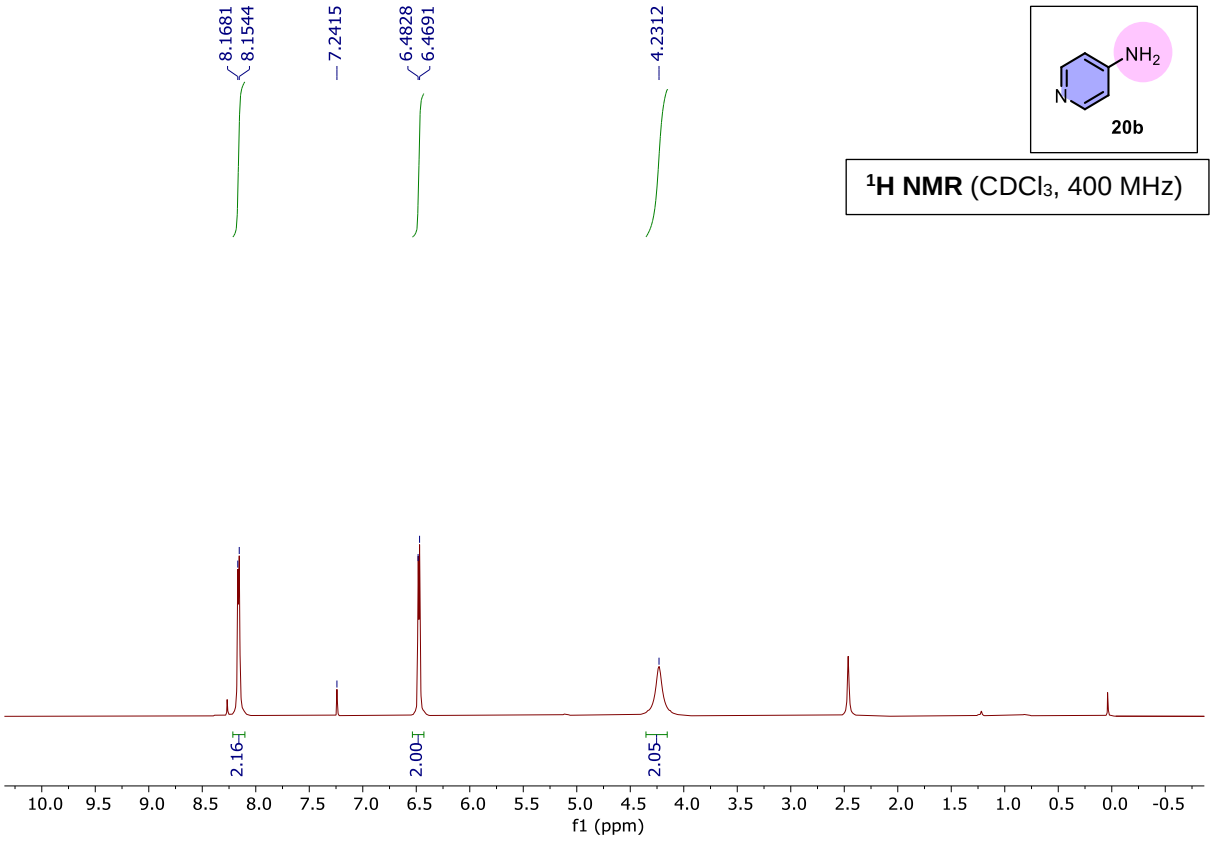
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz)

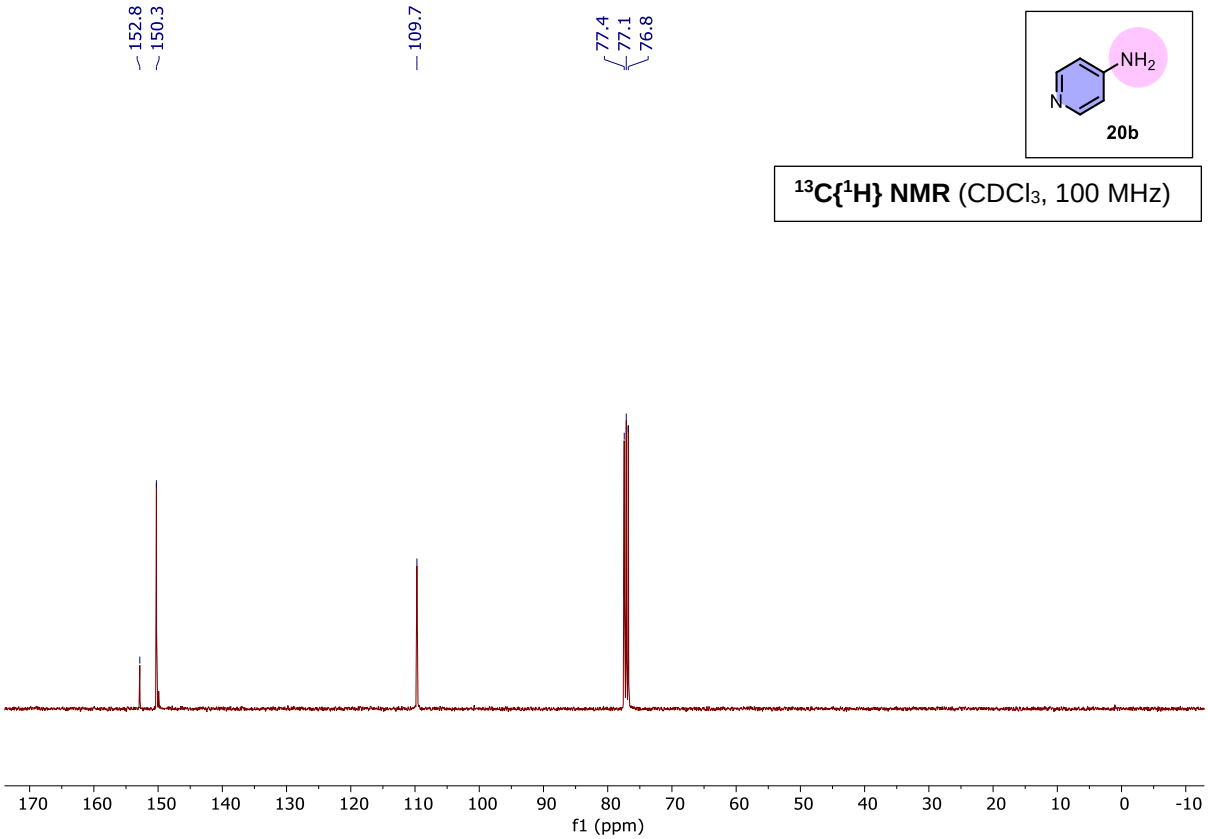


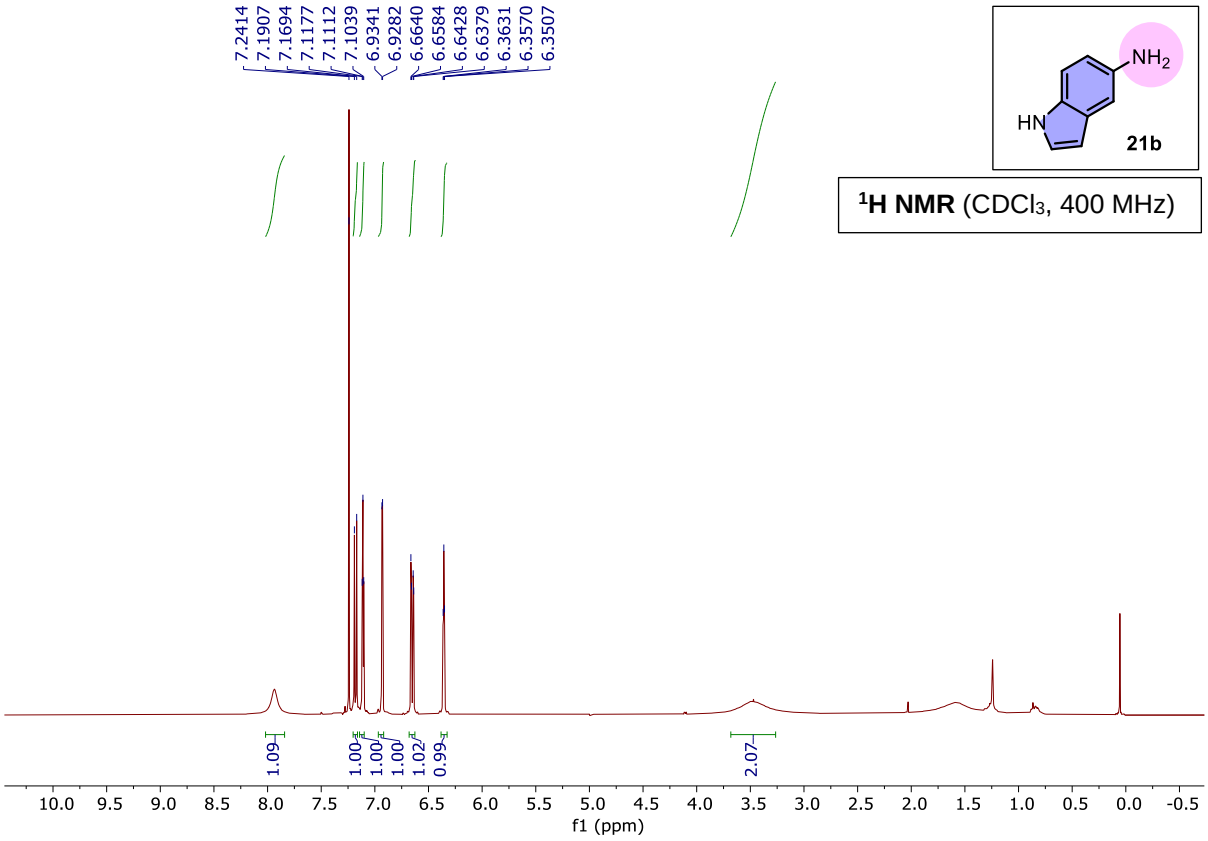
^{1}H NMR ($CDCl_3$, 400 MHz)



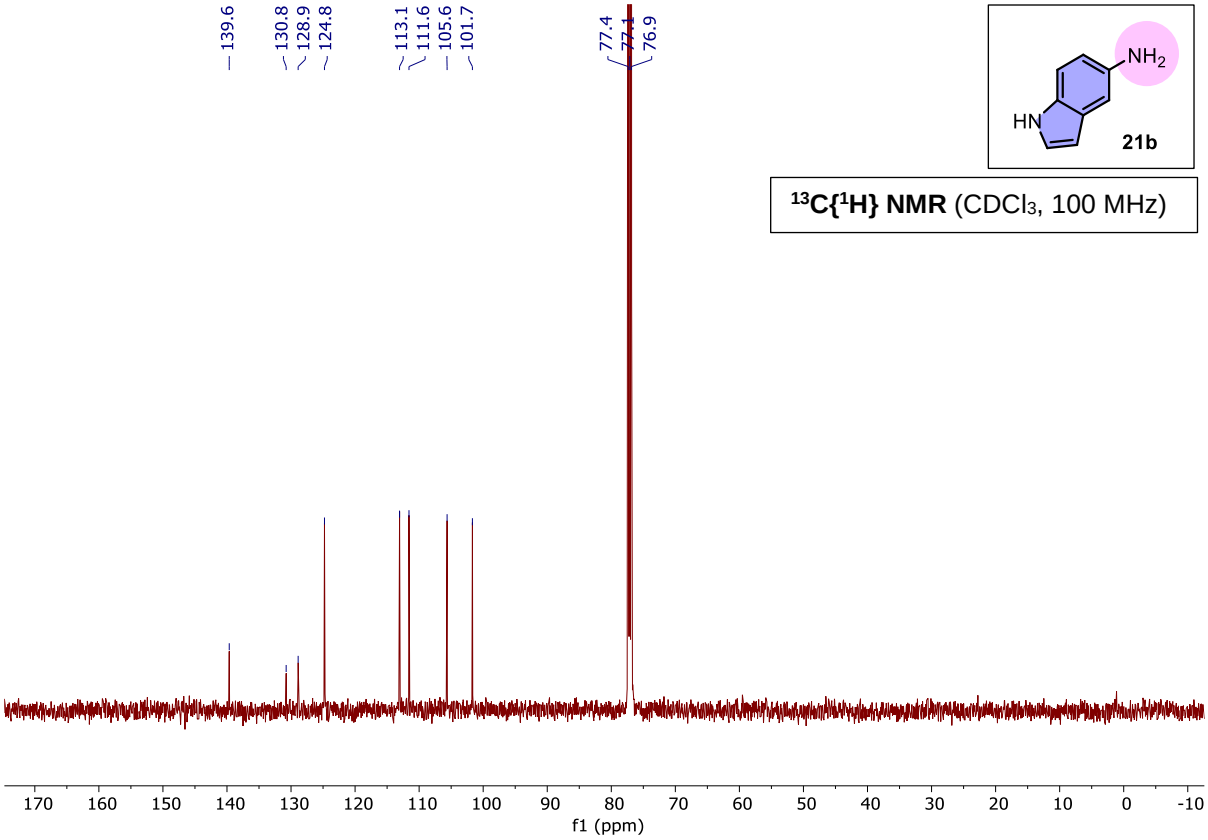
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)


8.1681
8.1544
7.2415
6.4828
6.4691
4.2312
NH2
N
20b
1H NMR (CDCl3, 400 MHz)
2.16
2.00
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

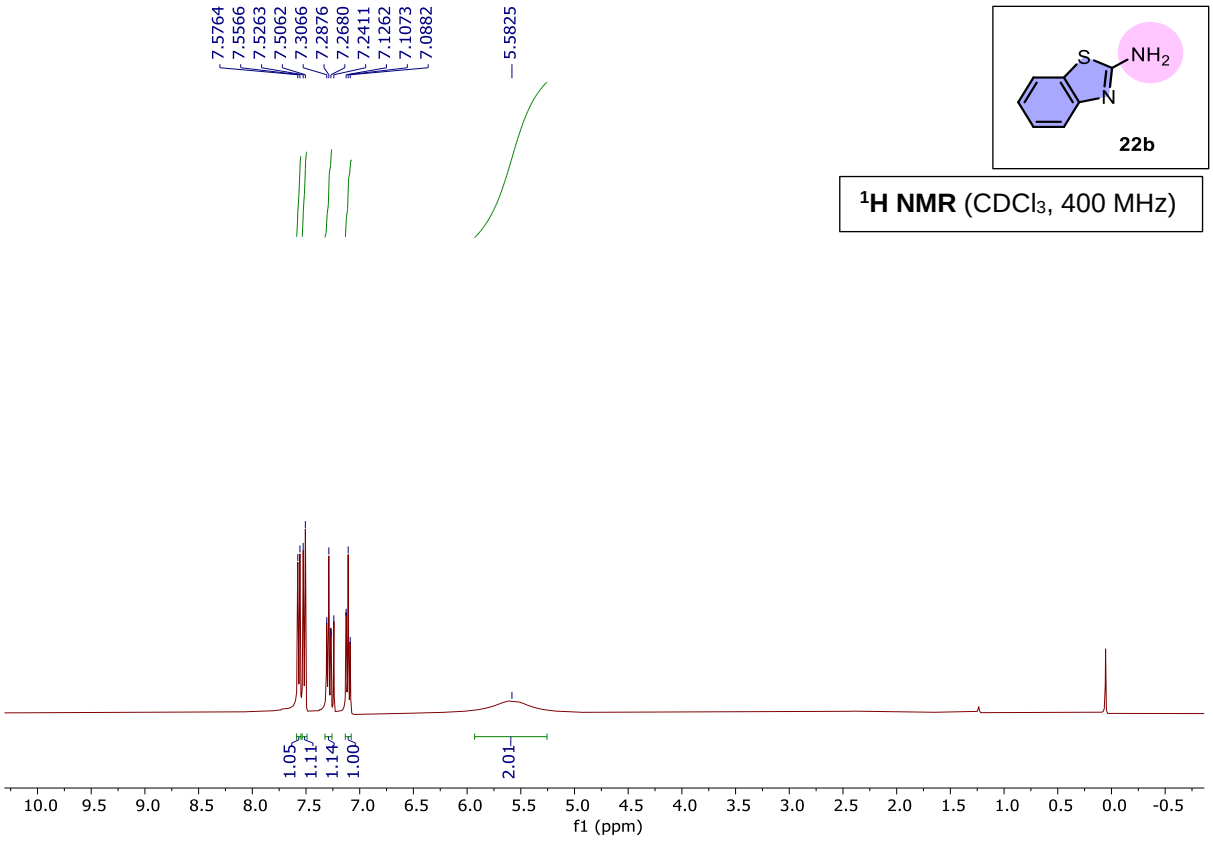

152.8
150.3
109.7
77.4
77.1
76.8
NH2
N
20b
13C{1H} NMR (CDCl3, 100 MHz)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



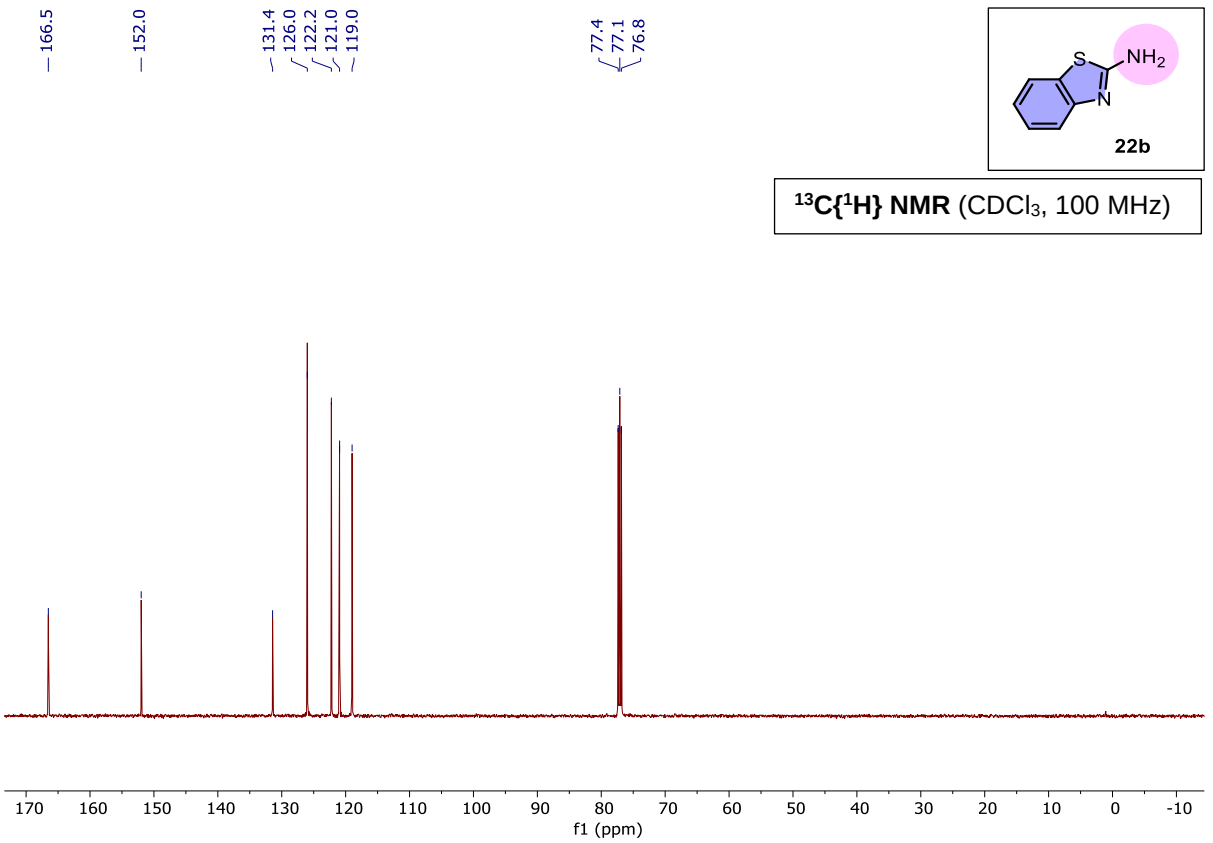
^{1}H NMR ($CDCl_3$, 400 MHz)



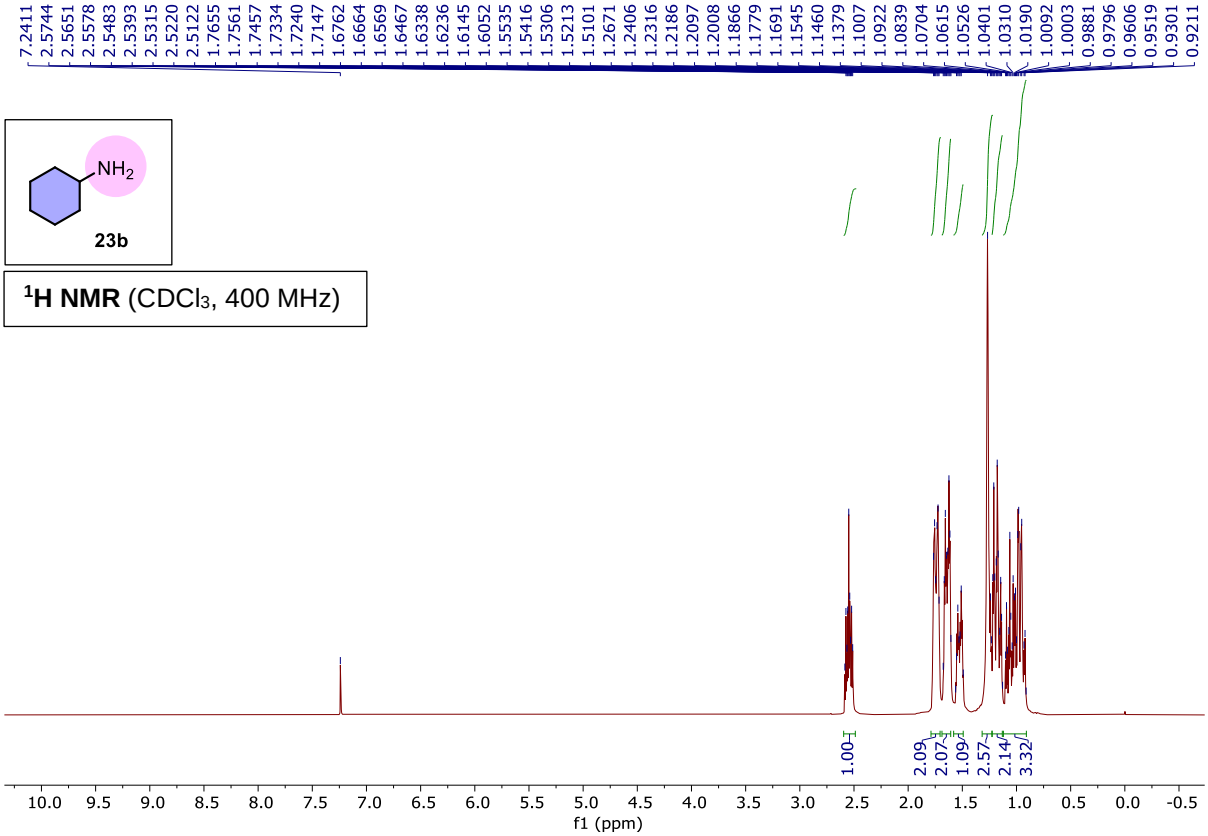
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



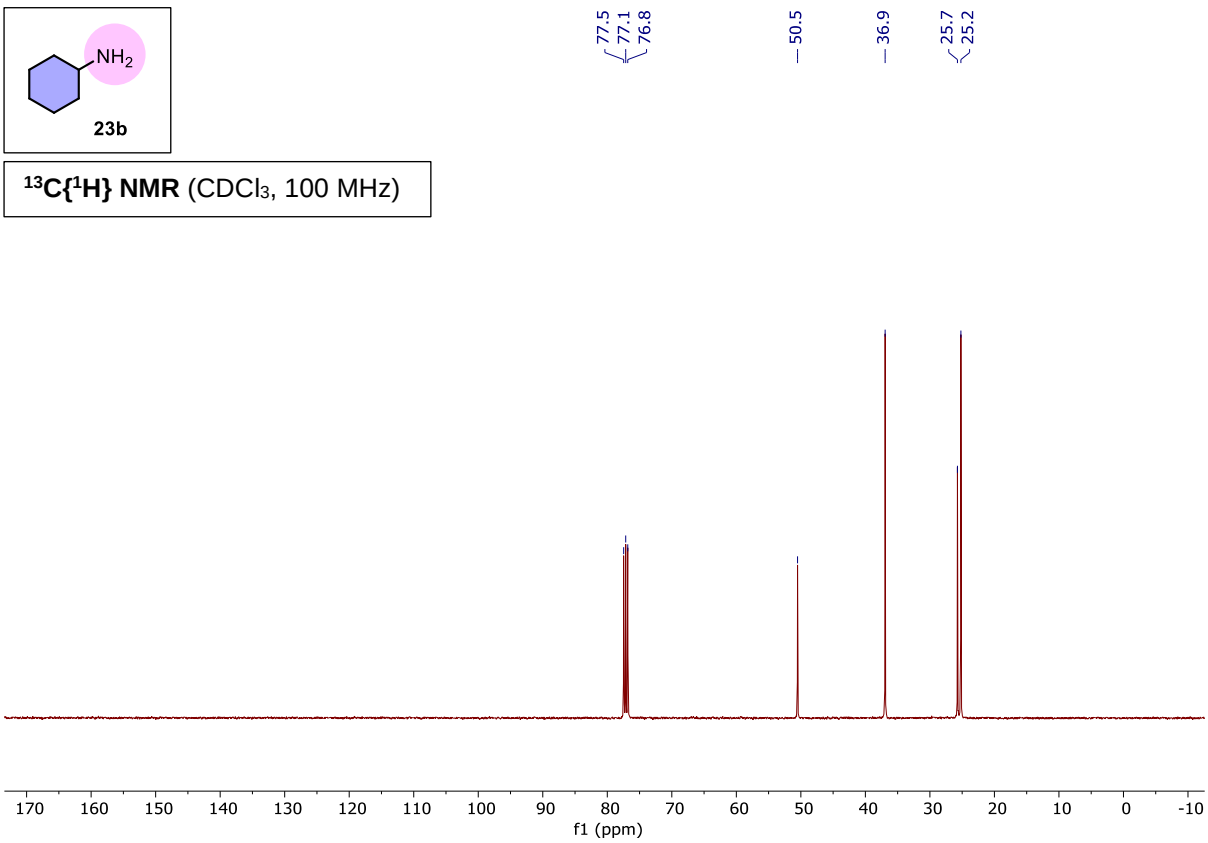
^{1}H NMR ($CDCl_3$, 400 MHz)



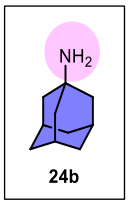
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)

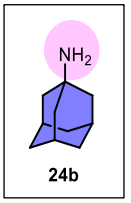


^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



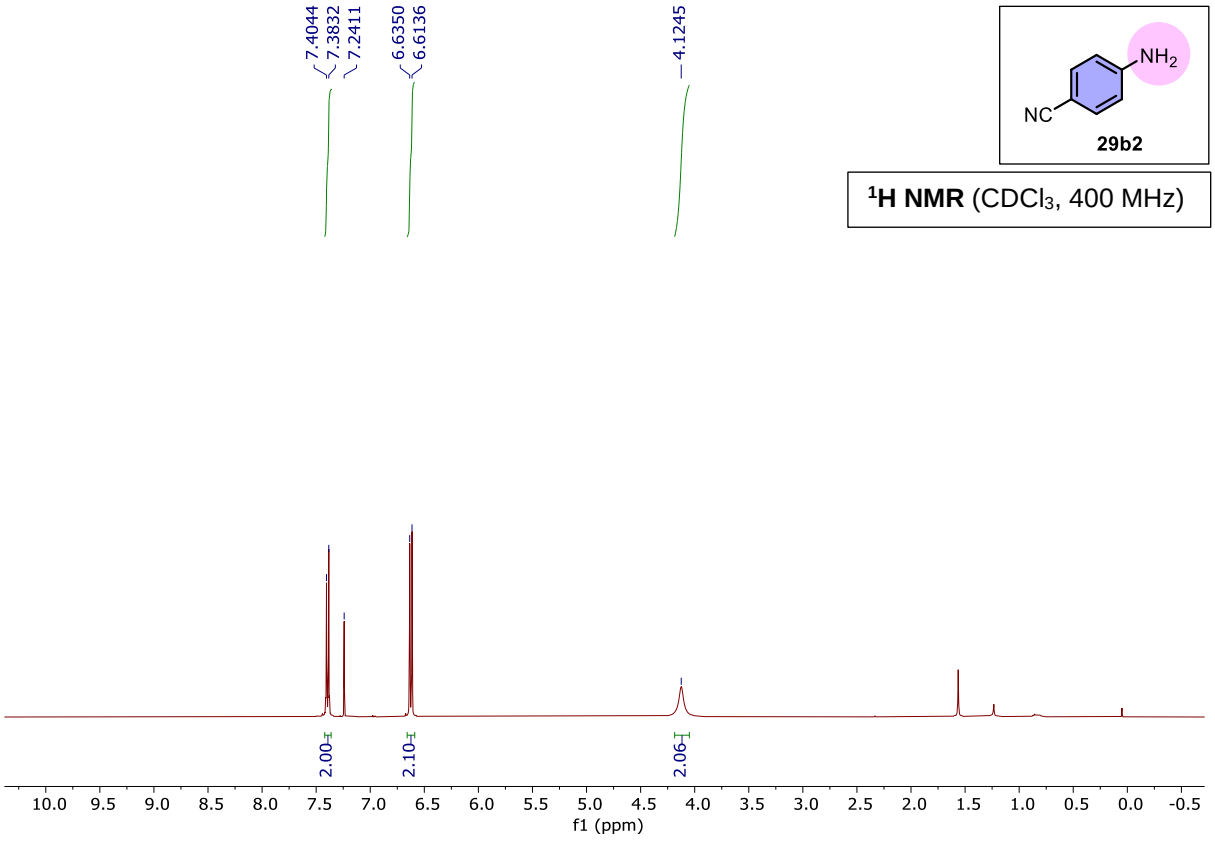
24b

^{1}H NMR ($CDCl_3$, 400 MHz)

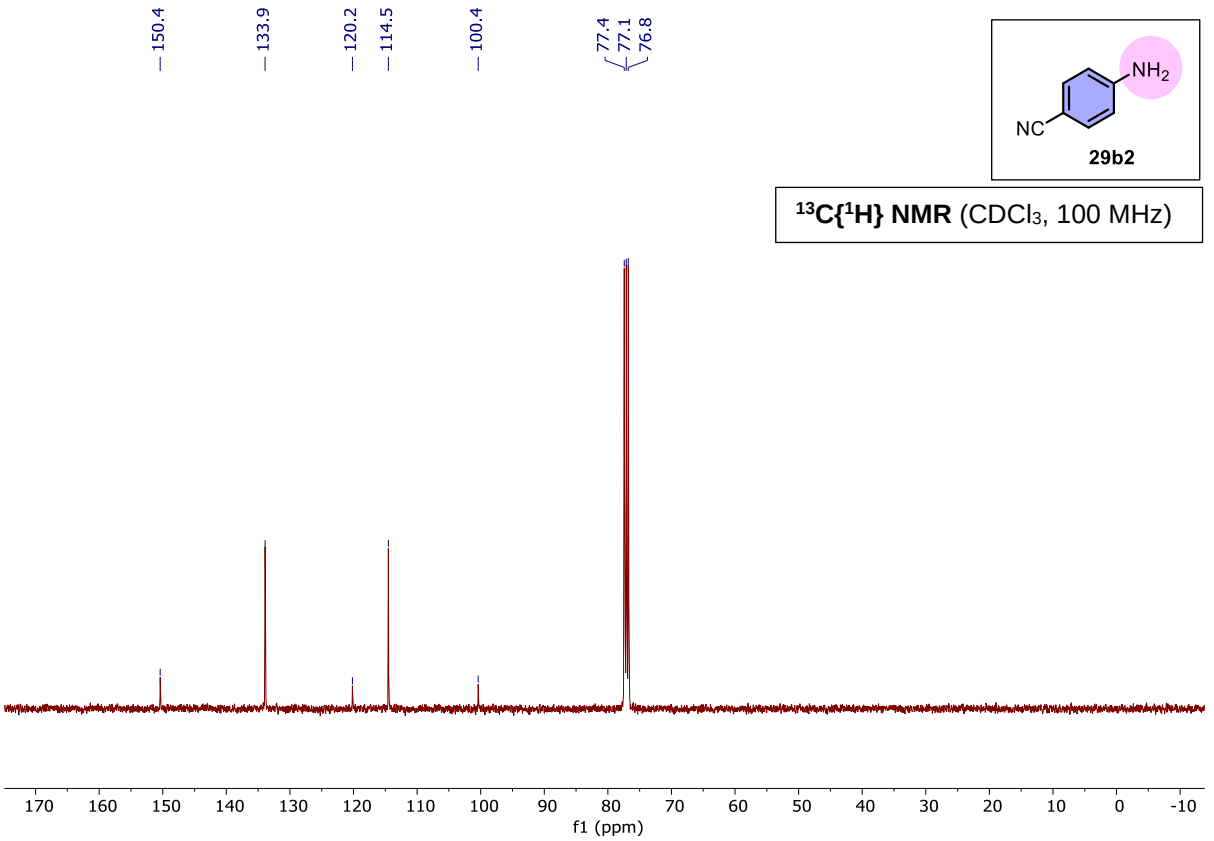


24b

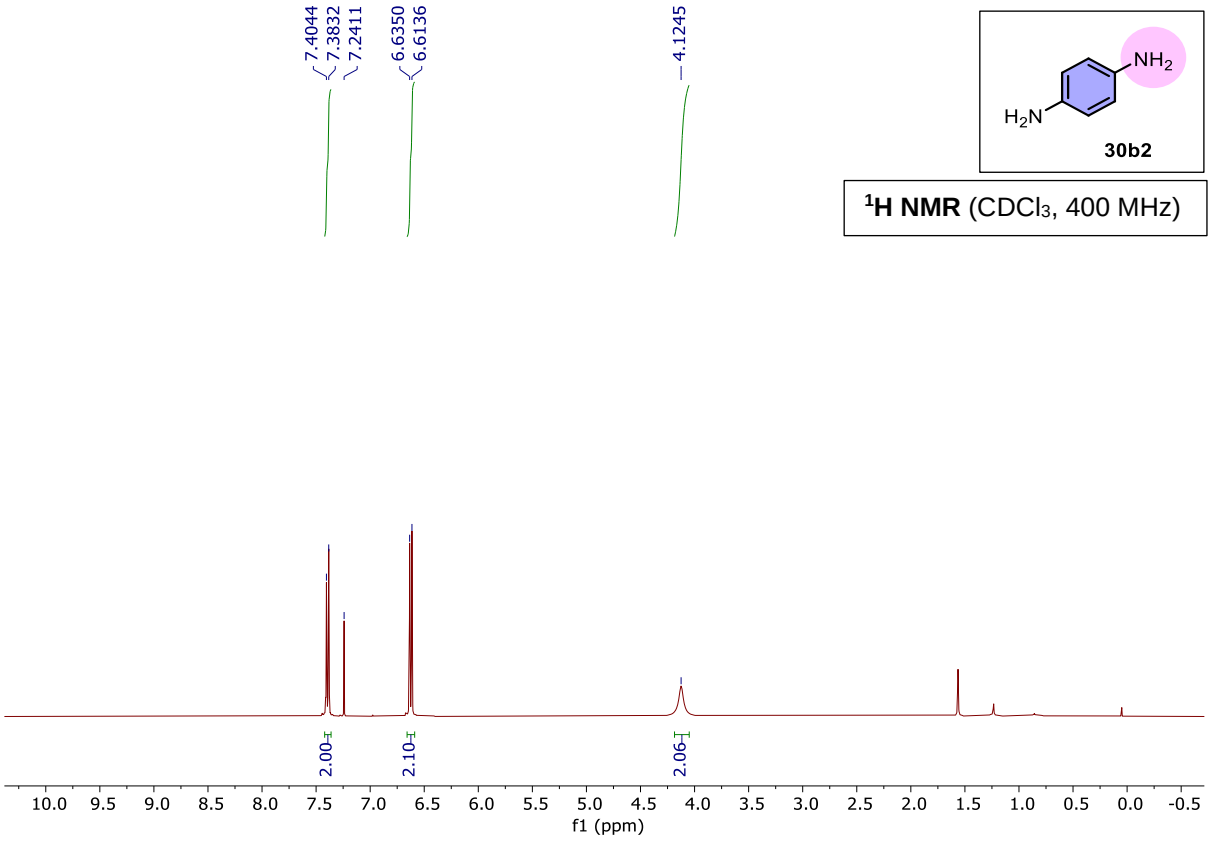
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



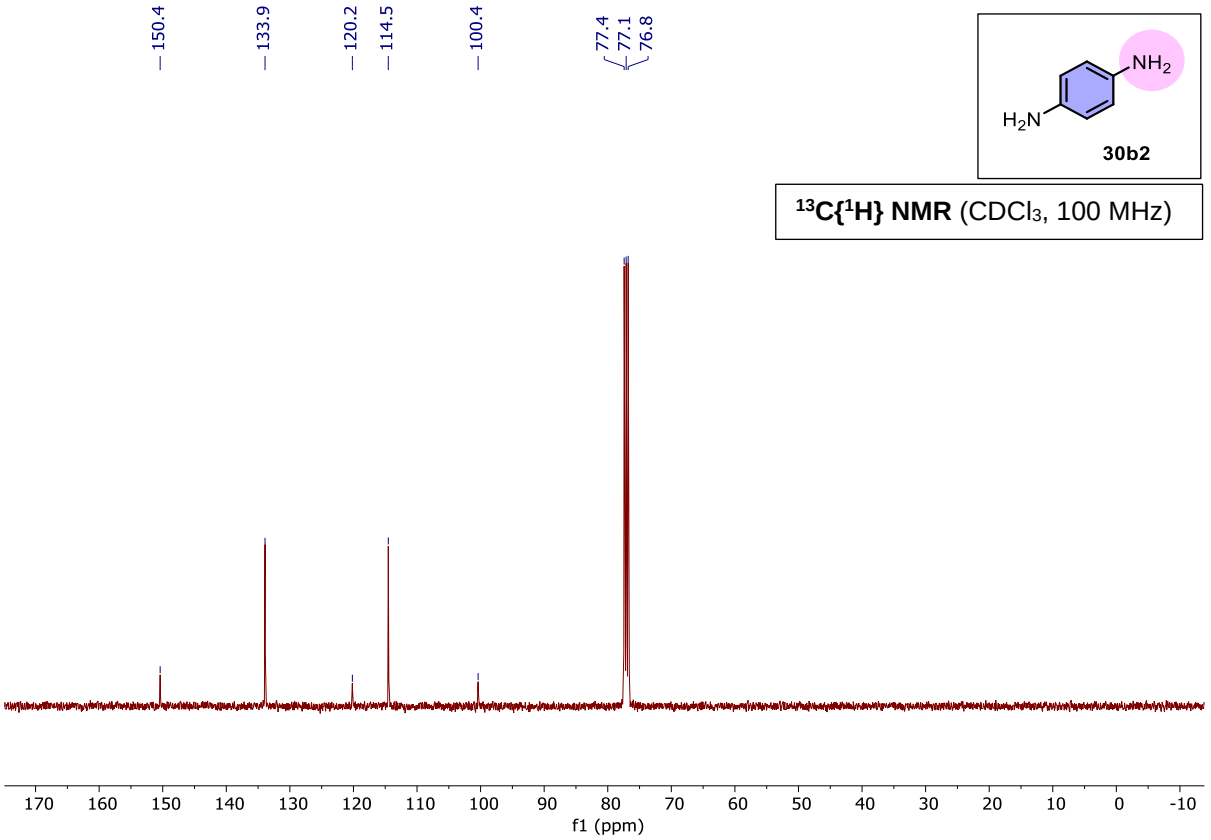
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

Reference:

1. H. Yang, L. Shang, Q. Zhang, R. Shi, G. I. N. Waterhouse, L. Gu and T. Zhang, *Nat. Commun.*, 2019, **10**, 4585.
2. J. Gao, L. Feng, R. Ma, B.-J. Su, A. M. Alenad, Y. Liu, M. Beller and R. V. Jagadeesh, *Chem Catal.*, 2022, **2**, 178-194.
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