Strategies for the Hyperpolarization of Acetonitrile and Related Ligands by SABRE

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Supplementary Information

1. General considerations

Materials

All materials and deuterated solvents were purchased from Sigma-Aldrich and used as received. [Ir(IMes)(COD)Cl][1], **1**, and [Ir(IMes-d_{22})(COD)Cl][2] were synthesized following established procedures.

NMR Equipment

NMR measurements were made using a Bruker 400 MHz Avance III spectrometer equipped with either a TXO flow probe linked directly to the Polarizer[3] (for flow experiments) or a BBI probe (for shake measurements) using 5 mm NMR samples. All measurements were made at 298 K.

*Para*hydrogen was prepared by flowing hydrogen gas over either charcoal at 30 K in a house-built apparatus[4] (used in shake measurements) or an iron oxide catalyst at 36 K in a Bruker-built polarizer (used in flow experiments).

Shake measurements

A typical experiment used, a Young's capped NMR tube containing **1** (~2 mg), MeCN (0.1 M) and pyridine (0.025 M) in d_4-MeOH (0.6 ml). Samples were degassed using Schlenk line techniques before introducing *para*hydrogen into the tube at a pressure of 3 bar. The sample was then shaken in an appropriate region of the fringe field of the magnet to effect polarization transfer for 10 s. After this period, samples were dropped in to the spectrometer and data acquisition begun. Typical NMR spectra are described in the manuscript and presented in sections s5-s17.

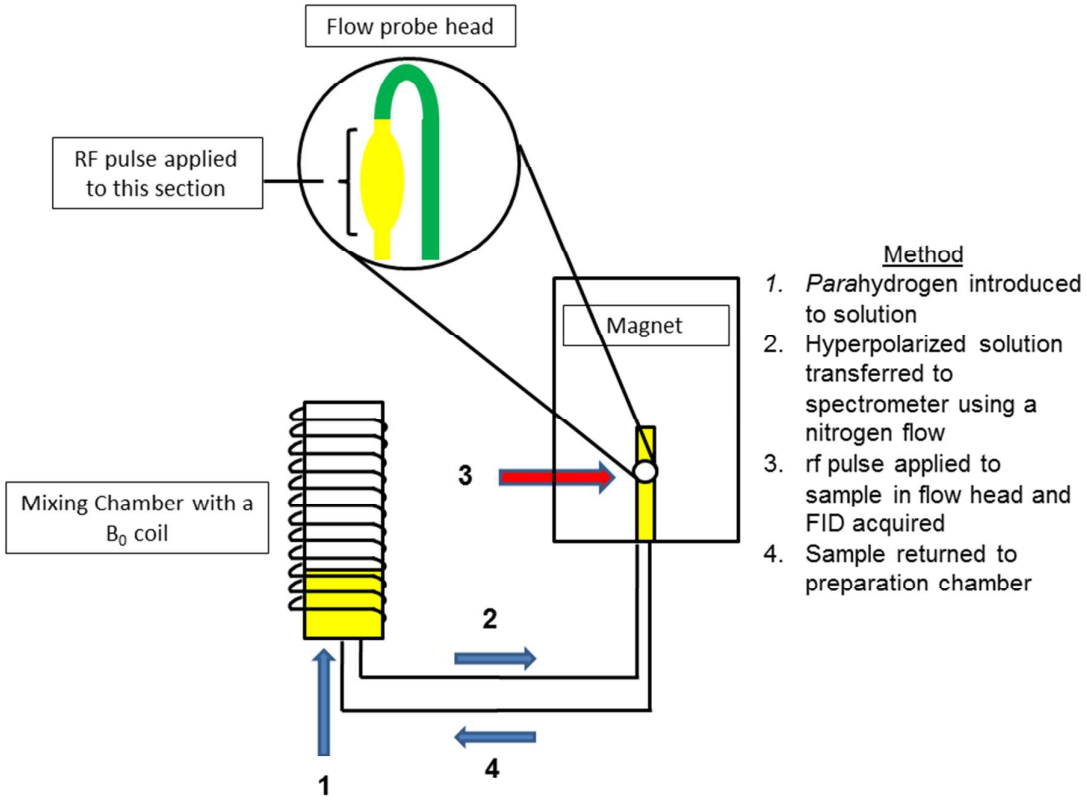
Flow measurements

For flow measurements, samples typically consisted of **1** (10 mg), MeCN (0.1 M) and pyridine (0.025 M) in d_4-MeOH (3 ml).

A schematic representation of the Polarizer used for flow measurements is shown in sScheme 1. The Mixing Chamber (MC) is housed within a tunable copper coil (0 to ±150 G). Whilst the coil on a 0 G setting delivers no field, the resultant field experienced by the sample is not zero and is better approximated by the Earth's field. All magnitudes of the magnetic fields in which polarization transfer occurs (PTF) are stated without correction for this local field. The MC houses the solvent, catalyst and substrates whose amounts are 5 times higher than those used in the shake measurements (although concentrations were kept the same). Liquid and gas flow is computer-controlled via the pulse program. As such, the system is entirely automated.

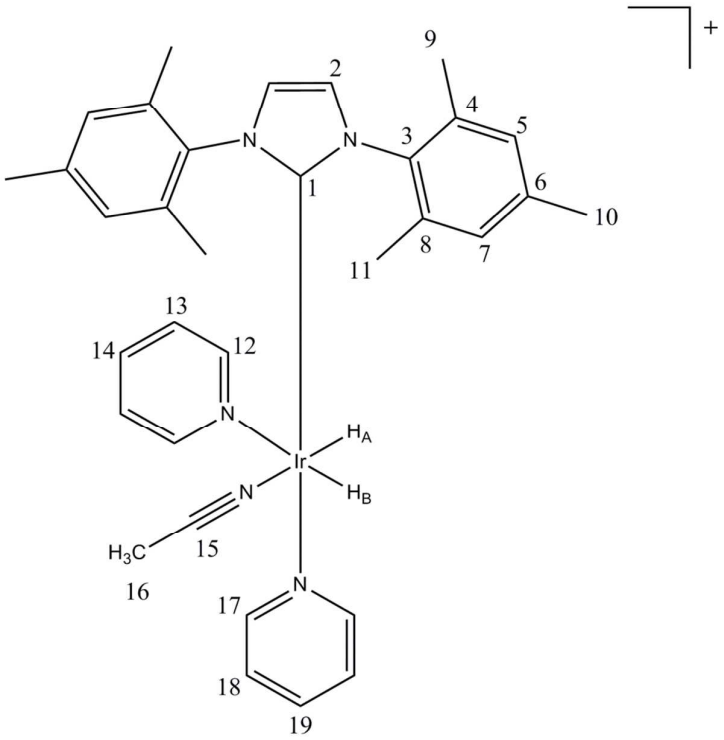
*Para*hydrogen is first introduced into the MC to activate the catalyst for 6 s. Nitrogen gas is used to shuttle the hyperpolarized solution from the MC to the NMR probehead for measurement. The transportation time was calibrated to 2.9 s. A further delay of 0.5 s was allowed for settling of the sample prior to signal acquisition (1 s). Once catalyst activation is complete, the SABRE effect can be detected as enhanced resonances for both the free and bound MeCN.

For experiments that require more than one scan, processes 1-4, as shown in sScheme 1, are repeated n times, where n is the number of scans.



sScheme 1 : Schematic of the Polarizer, the hyperpolarization process and its subsequent NMR analysis.

2. Multinuclear NMR characterisation data for 3 in d_4-MeOH



sFigure 1: Labelling scheme for the structure of 3 (chloride anion omitted)

sTable 1: Multinuclear NMR data for 3 collected in d_4-MeOH.

^{1}H chemical shift / ppm	^{13}C chemical shift /ppm	Nucleus label/number
−20.56		H_A
−22.12		H_B
8.33	155.13	17
8.30	156.46	12
7.82	136.16	14
7.72	136.38	19
7.18	125.47	13
7.08	125.12	18
	137.56	3
7.07	128.37	5
6.86	128.56	7
7.11	122.25	2
2.36	19.86	10
2.2	17.14	11
1.87	16.91	9
2.16	21.94	16
	135.91	8
	135.83	4
	138.5	6
	149.65	1
	117.8	15

Hydride splittings to protons located at positions 12 and 16 were determined to be ~1.2 Hz and ~2.1Hz respectively. The hydride-hydride splitting was found to be −7.56 Hz

^{15}N NMR data

J_{NH} pyridine *trans* to hydride H_B = 20.5 Hz (^{15}N δ 252.5)

J_{NH} MeCN *trans* to hydride H_A = 25 Hz (^{15}N δ 190.6)

^{15}N chemical shift of pyridine *trans* to IMes = δ 231.00

3. T_1 measurements

sTable 2: T_1 values of pyridine and A under specified conditions.

	Vacuum + Py /s			H_2 + Py /s			Vacuum + Py + MeCN /s				H_2 + Py + MeCN /s			
Catalyst	*o*	*p*	*m*	*o*	*P*	*m*	*o*	*p*	*m*	Me	*o*	*m*	*P*	Me
1	29	30	26	13	19	15	20	23	20	8	21	25	20	12

N.B. *o*, *m* and *p* refer to the *ortho*, *meta* and *para* ^{1}H resonances of pyridine, respectively. Me represents the methyl group of **A**.

sTable 3: T_1 values for the labelled ^{13}C nucleus of B or C under specified conditions.

	T_1 of the labelled ^{13}C resonance	
MeCN labelled material	Under vacuum in presence of **1** /s	Under H_2 atmosphere in the presence of **1** /s
B	15.1	13.6
C	15.6	14.8

sTable 4: T_1 values of the methyl protons of B and C under specidied conditions

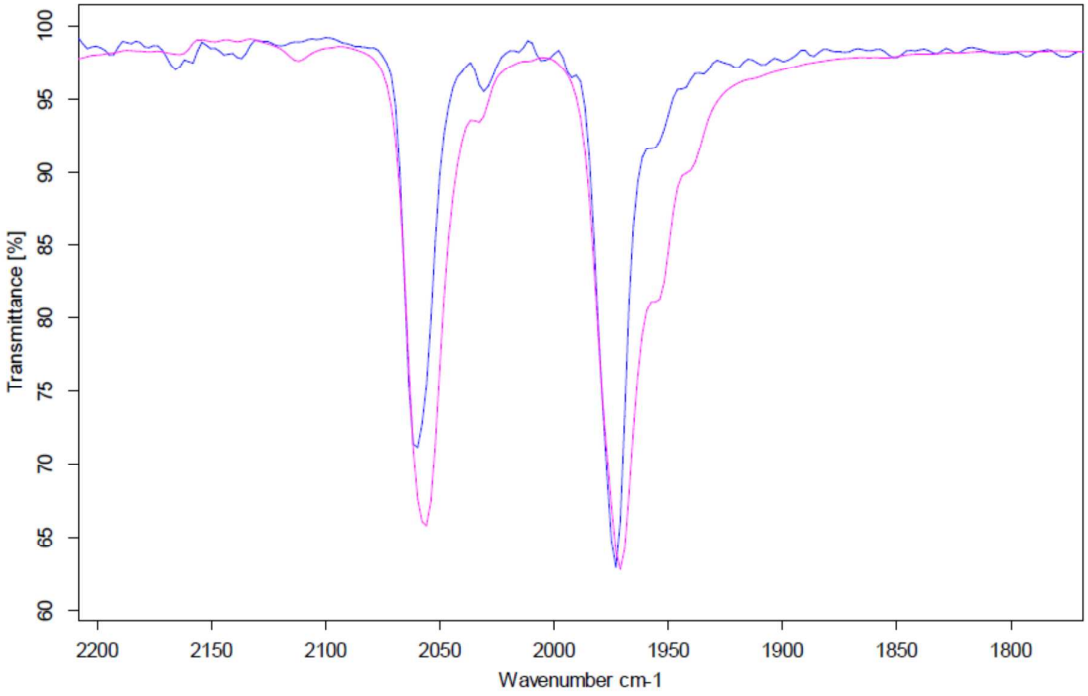
	T_1 of the methyl ^{1}H resonance
MeCN labelled material	Under a H_2 atmosphere in the presence of **1** /s
B	6.64
C	7.07

The T_1 of the methyl protons of **A** in the presence of d_5-pyridine and Ir(d_{22}-IMes)(COD)Cl in MeOH was found to be 16.2 s.

All measurements were made using a sample consisting of **1** (2 mg) or Ir(d_{22}-IMes)(COD)Cl (2 mg), 3.1 µL MeCN, 0.75 µL py in 0.6 ml of d_4-MeOH.

A, B, and C correspond to the acetonitrile isotopomers as shown in Scheme 1 in the main text.

4. IR spectra of $Ir(CO)_2(IMes\text{-}h_{24})Cl$ and $Ir(CO)_2(IMes\text{-}d_{22})Cl$

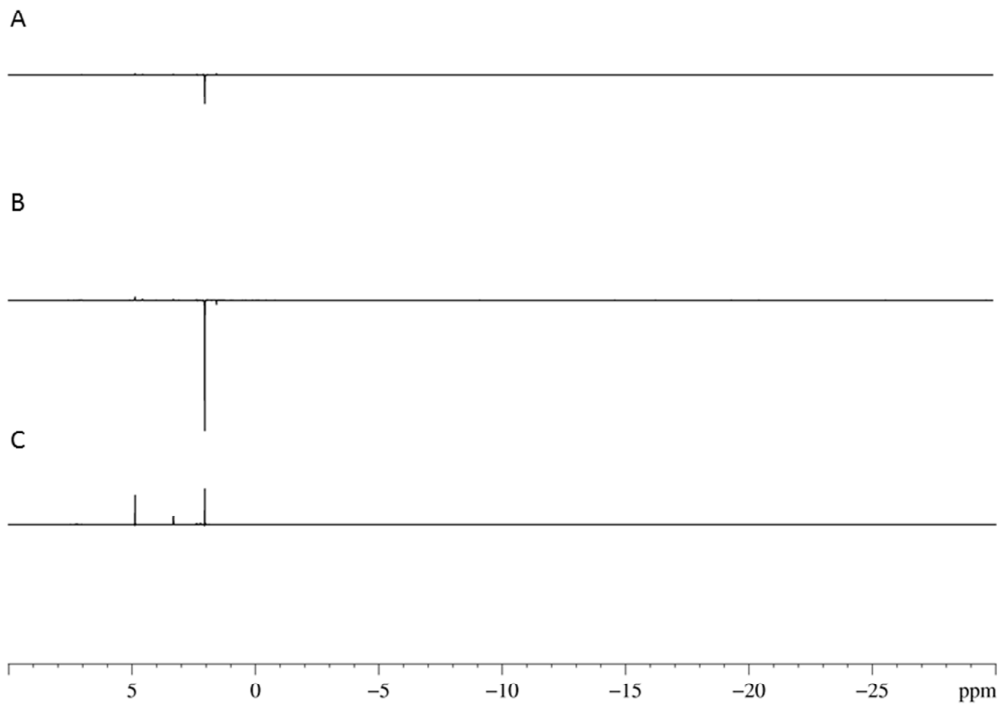


sFigure 2: CO stretching region of the mid-IR region of $Ir(CO)_2(IMes\text{-}h_{24})Cl$ (blue line) and $Ir(CO)_2(IMes\text{-}d_{22})Cl$ (violet line).

IR data was collected using a Bruker Tensor 37 FT-IR spectrometer fitted with a platinum ATR at a resolution of 4 cm^{-1}. The stretching frequencies of CO in $Ir(CO)_2(IMes\text{-}h_{24})Cl$ and $Ir(CO)_2(IMes\text{-}d_{22})Cl$ are 2061 and 1973 cm^{-1} and 2057 and 1971 cm^{-1} respectively. The synthesis of the two carbonyl complexes followed a literature procedure.[5]

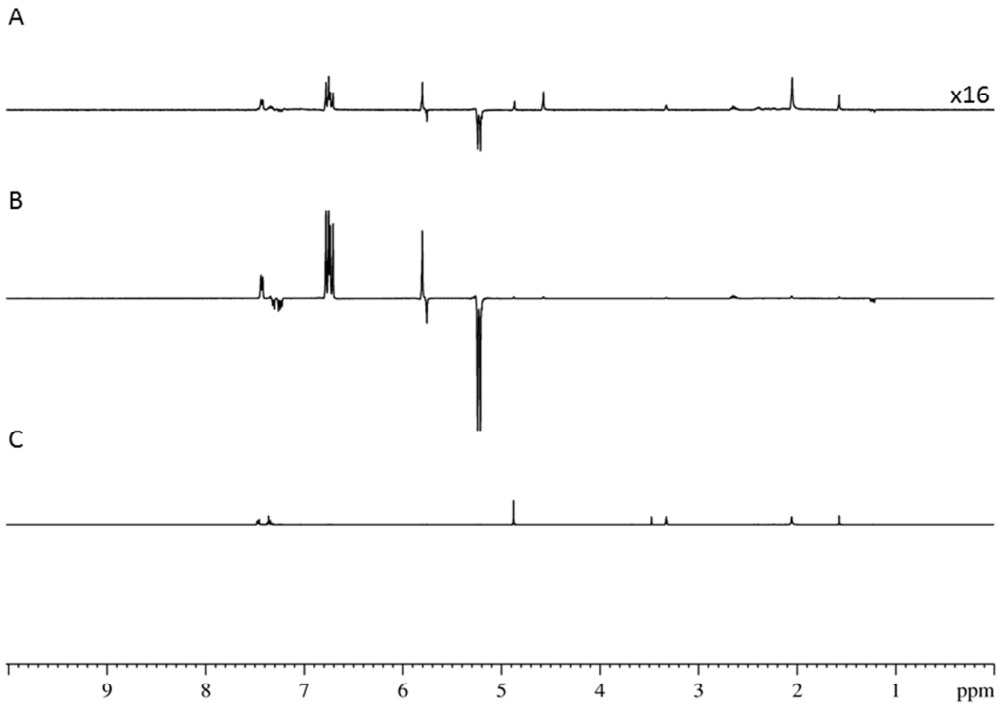
5. ^{1}H polarization of A in the absence of pyridine

Initial experiments involved hyperpolarizing MeCN at 65 G. Initially, the enhancement for pyridine was 8.2-fold but very quickly (~5 mins) dropped to 3.2-fold. After one hour the enhancement was only 2.8-fold.



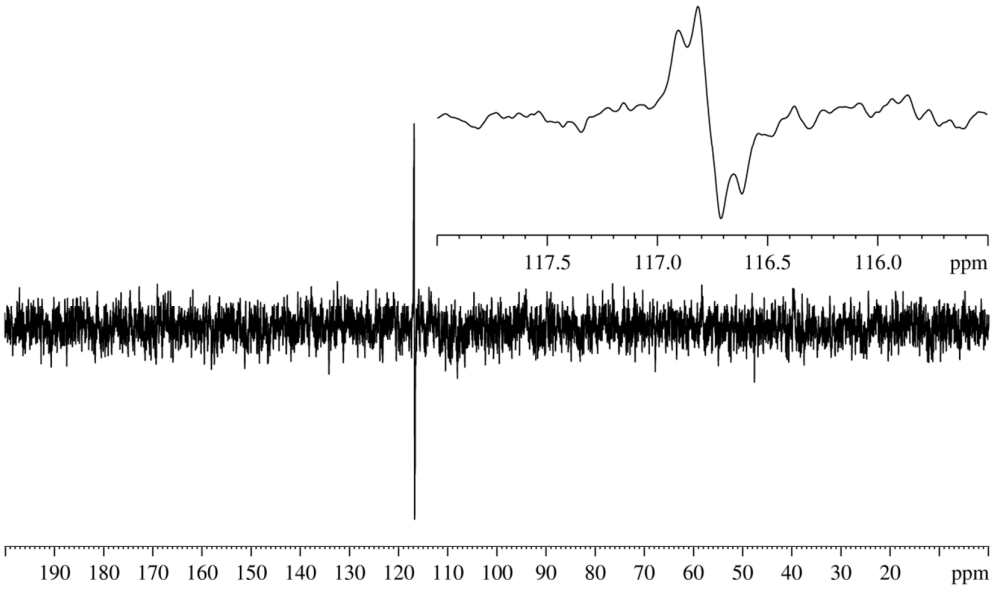
sFigure 3: ^{1}H NMR traces of a sample consisting of A (3.1 µL) and 1 (2 mg) in d_4-MeOH (0.6 ml) after polarization transfer in a PTF of 65 G: after one hour (A); initially (B); and when the sample had fully relaxed back to thermal equilibrium (C).

After one hour, phenylacetylene was added to act as a sacrificial alkyne. This material was observed to hydrogenate to its alkene and alkane derivatives, but the methyl group of MeCN was not observed to be enhanced after subsequent polarization transfer at 65 G.



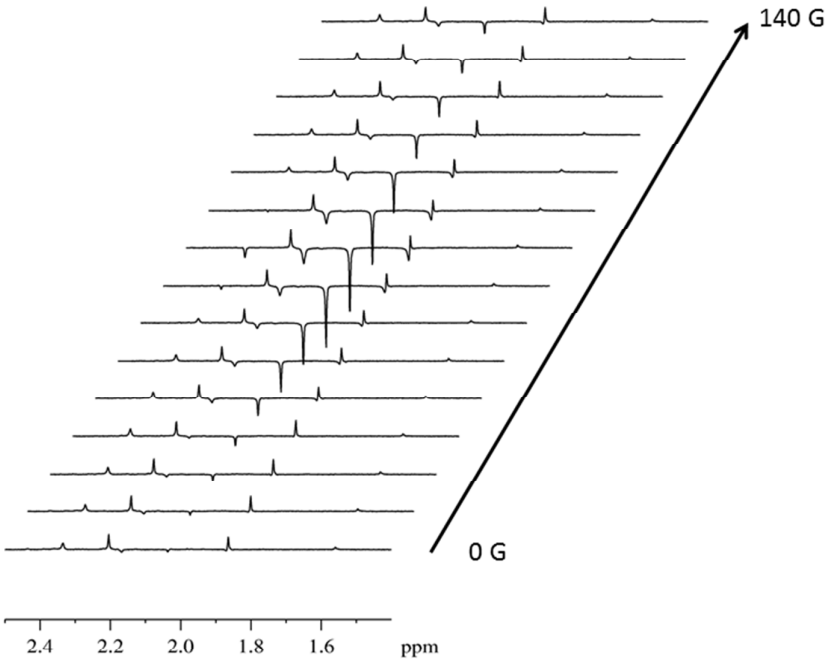
sFigure 4: ^{1}H NMR traces of a sample consisting of A (3.1 µL), phenylacetylene (3.3 µL (10 equivalents)) and 1 (2 mg) in d_4-MeOH (0.6 ml) after polarization transfer in a PTF of 65 G: after one hour (A); initially (B); and when the sample has fully relaxed to thermal equilibrium (C).

6. ^{13}C NMR spectrum of hyperpolarized A



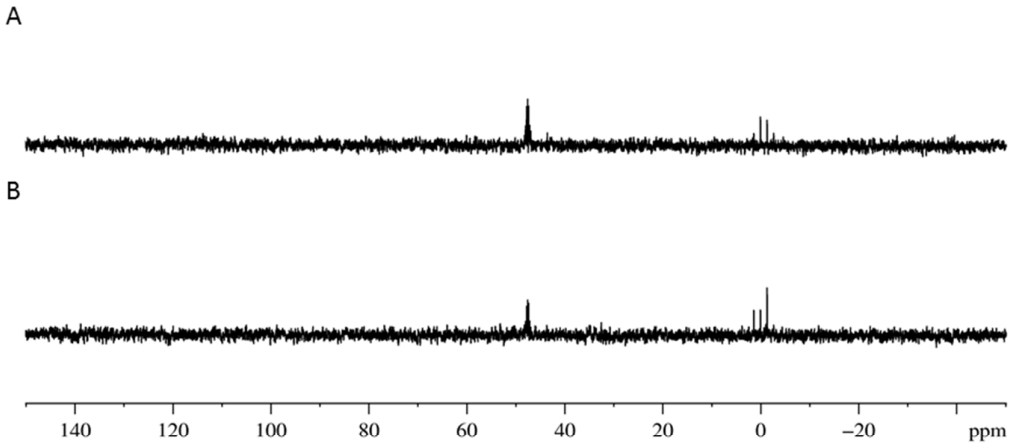
sFigure 5: ^{13}C NMR trace of a sample consisting of A (15.5 µL), d_5-pyridine (3.75 µL) and 1 (10 mg) in d_4-MeOH (3 ml) after polarization transfer in a PTF of 0 G. The insert shows the splitting of the quaternary peak.

7. ^{1}H NMR spectra of hyperpolarized B as a function of the PTF

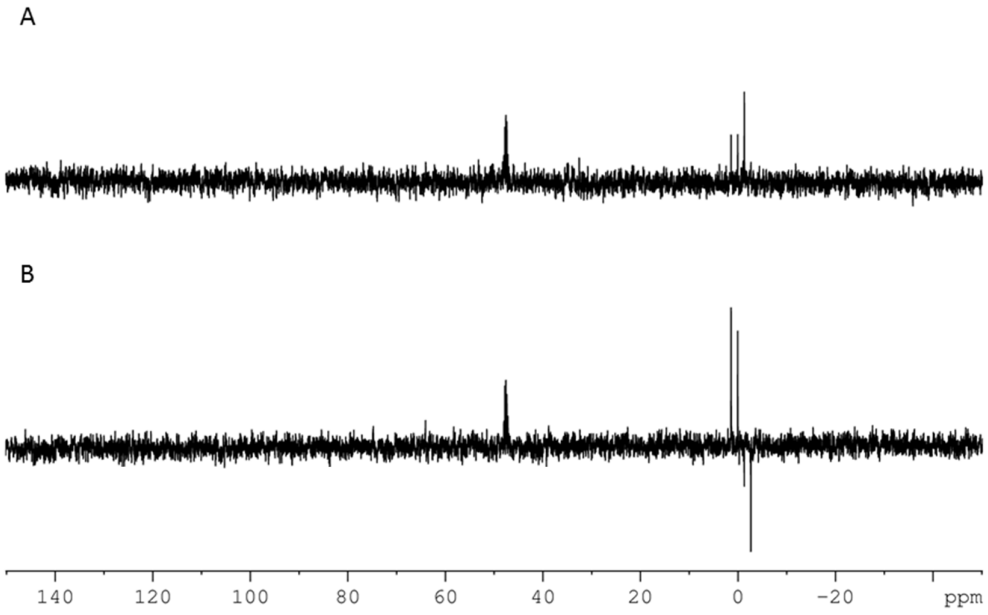


sFigure 6: ^{1}H field plot for a sample consisting of B (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) after polarization transfer at the field indicated. Traces are displayed in 10 G steps.

8. ^{13}C NMR spectra of B

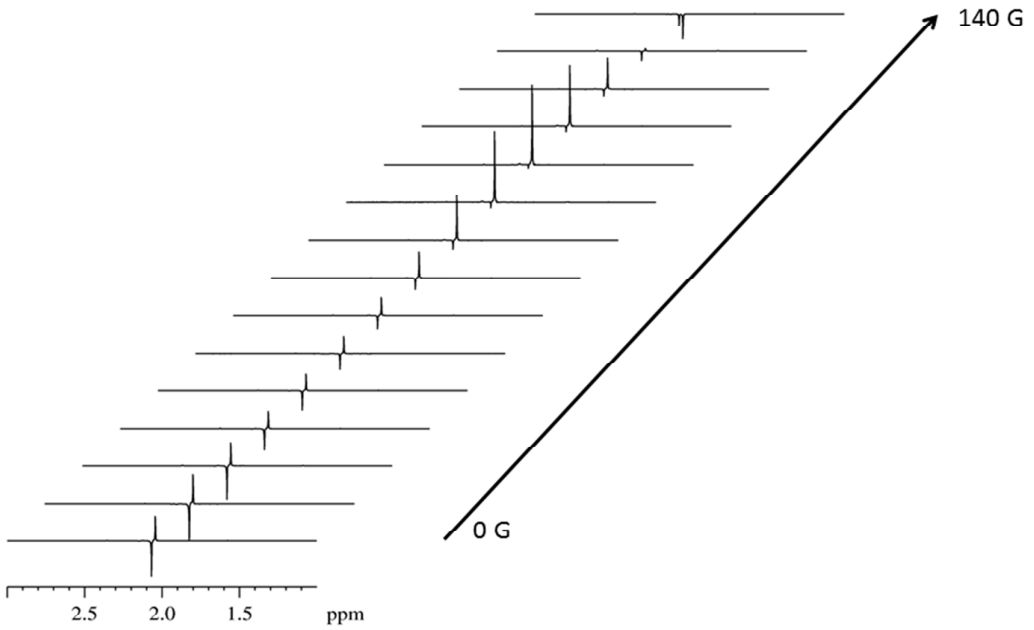


sFigure 7: ^{13}C NMR spectra of a sample consisting of B (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) at thermal equilibrium (A) and after polarization transfer at a PTF of 0.5 G (B). Traces collected using 8 scans.



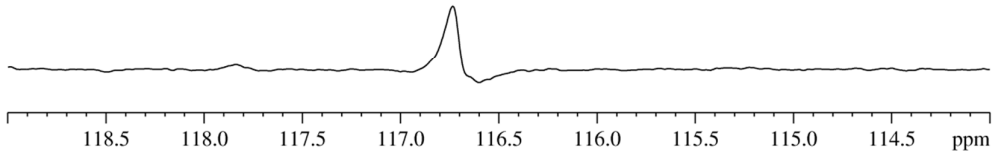
sFigure 8: ^{13}C NMR spectra of a sample consisting of B (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) collected using: A) a π/2 pulse and a PTF of 0.5 G and B) INEPTnd sequence using a total refocusing time of 1/2J (J_{HC} = 135 Hz) and a PTF of 80 G. Traces collected using 8 scans.

9. ^{1}H NMR spectra of hyperpolarized C as a function of PTF

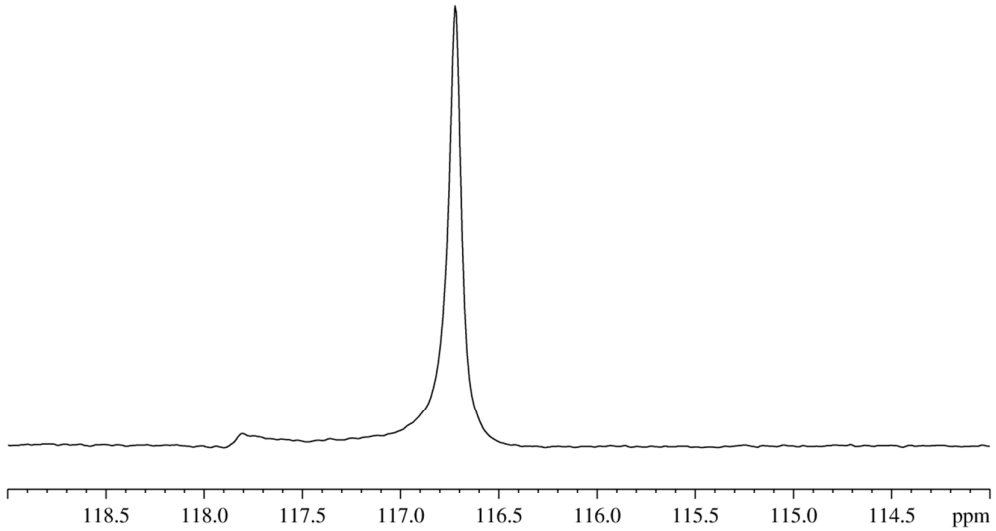


sFigure 9: ^{1}H field plot for a sample consisting of C (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml). Traces are displayed at PTFs in 10 G steps.

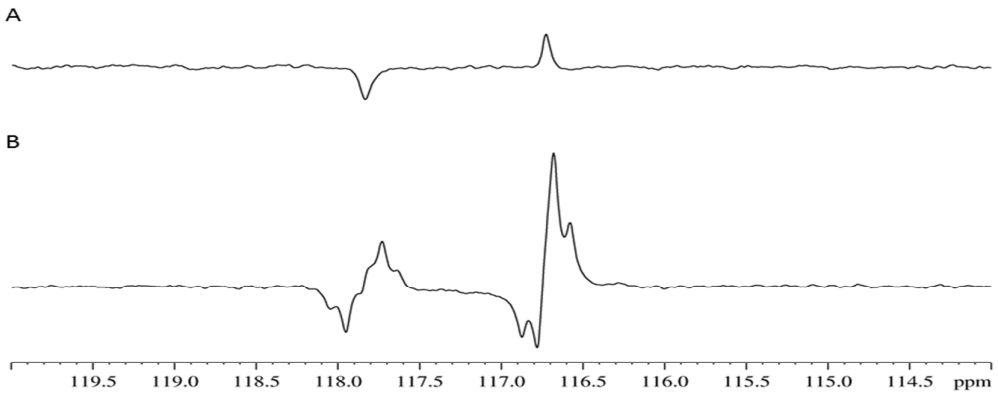
10. ^{13}C NMR measurement of C



sFigure 10 : $^{13}C\{^{1}H\}$ NMR spectrum of a sample consisting of C (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) after polarization transfer at a PTF of 0.5 G. Trace collected using 8 scans.



sFigure 11: Refocused $^{13}C\{^{1}H\}$ NMR spectrum (J = 20 Hz (0.025 s)) of a sample consisting of C (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) after polarization transfer at a PTF of 0.5 G. Trace collected using 8 scans.

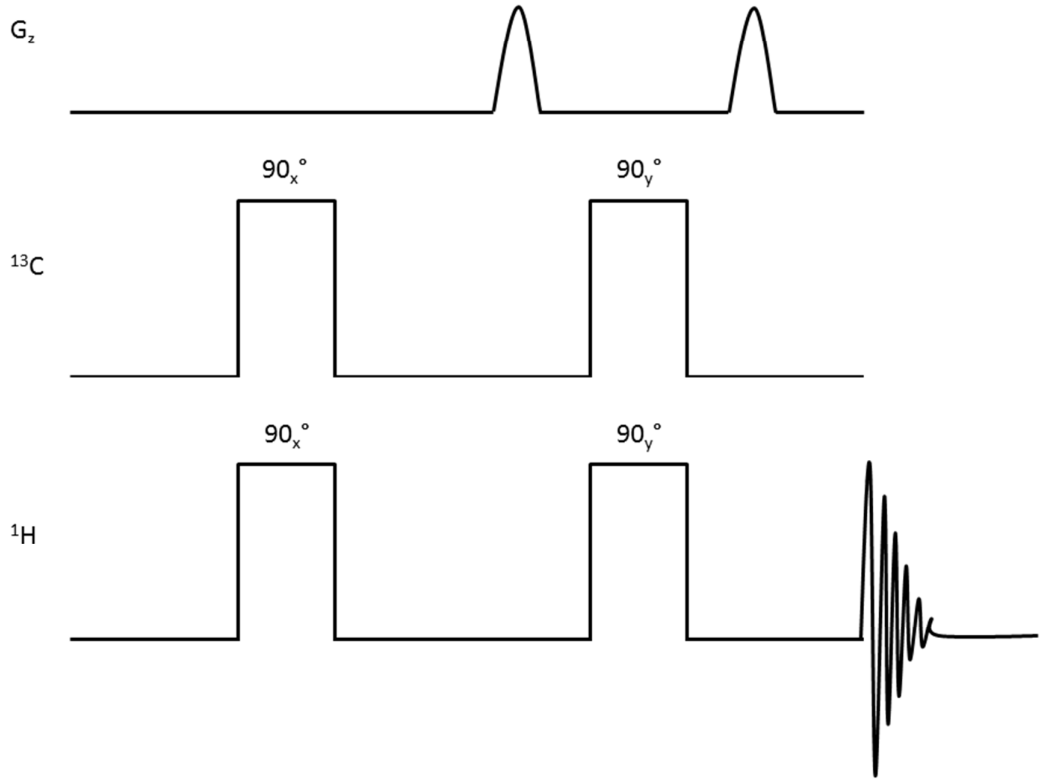


sFigure 12: ^{13}C INEPTrd (A) and INEPTnd (B) NMR traces of a sample consisting of C (15.5 µL), d_5-pyridine (3.75 µL), 1 (10 mg) in d_4-MeOH (3 ml) after polarization transfer at a PTF of 80 G. Traces collected using 8 scans and a value of J=20Hz used for the refocusing time of 1/2J. INEPTrd is an INEPT sequence using refocusing and decoupling during acquisition whereas INEPTnd is an INEPT in which decoupling is not employed.

11. Heteronuclear only *para*hydrogen spectroscopy (OPSY)

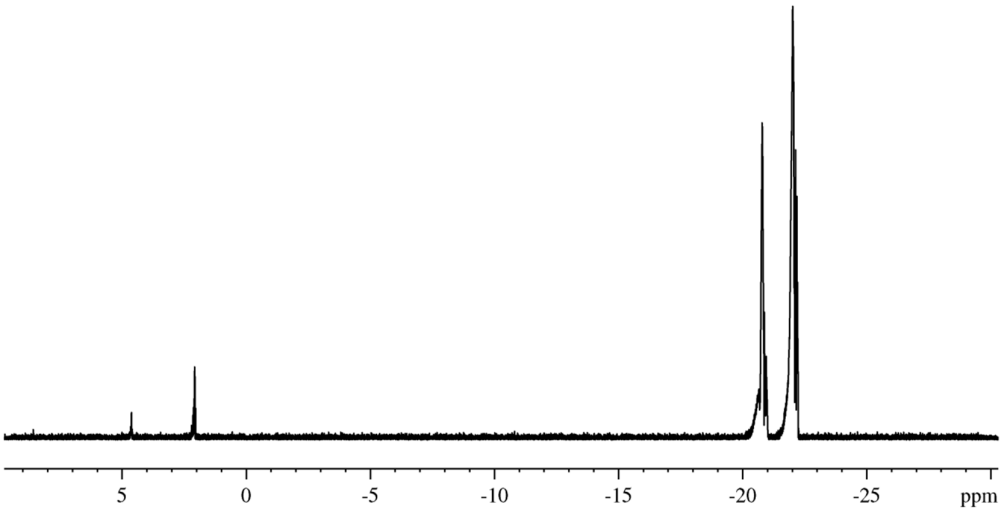
The homonuclear OPSY[6, 7] sequence was converted into a heteronuclear experiment by replacing each proton pulse with simultaneous pulses to proton and carbon. Coherence selection was then achieved by tuning the gradient ratios according to the respective magnetogyric ratios of proton and carbon in an analogous way to that undertaken in traditional HMQC and HSQC[8] experiments. In this way, heteronuclear two- and three-spin order terms can be differentiated and observed as desired in a comparable manner to the homonuclear terms described in the indicated references.[6, 7, 9] More than one solution exists for each pair of gradient ratios depending upon the magnitude and sign of the initial gradient. In our experiment we used the values stated in the main text. Thermal equilibrium control experiments were undertaken to establish the fact that no thermal terms were detectable under these conditions.

12. Heteronuclear OPSY sequence used for exciting ^{1}H and ^{13}C spins simultaneously



sFigure 13 : Schematic of the heteronuclear OPSY pulse sequence for selecting the DQ coherence order that exists between ^{1}H and ^{13}C. The gradient ratios used are 64 : 80 when detecting on ^{1}H or 16 : 80 when detecting on ^{13}C. Although the figure is shown with acquisition occurring on the ^{1}H channel, acquisition can actually be undetaken on either the ^{1}H or ^{13}C channel.

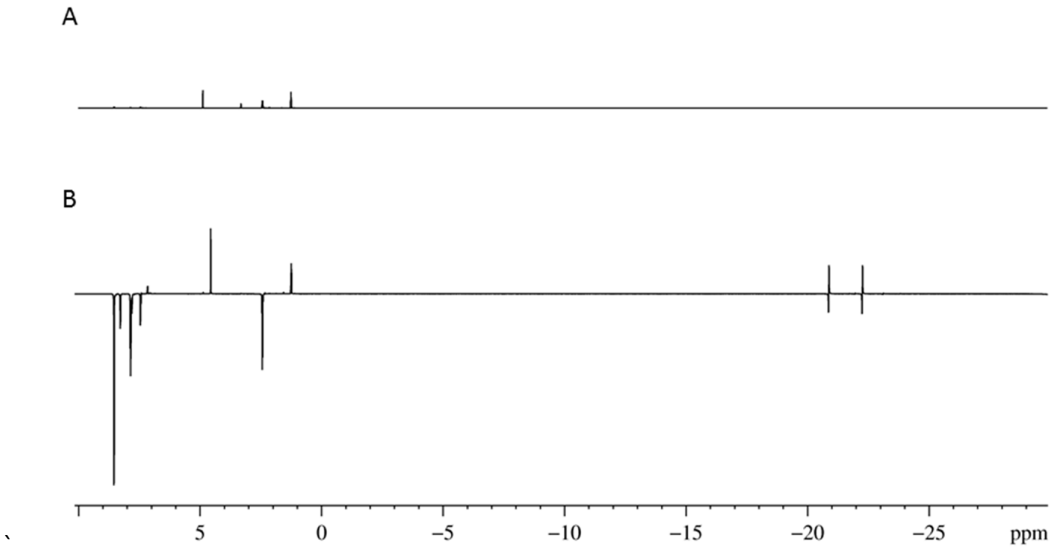
13. ^{1}H NMR spectrum of C acquired using the sequence detailed in sFigure 13



sFigure 14 : ^{1}H NMR trace of C polarized by 1 at a PTF of 80 G. Gradient ratios used were 45.7:80 % to select the TQ coherence.

The corresponding ^{1}H and ^{13}C DQ traces are shown in Figure 4 in the main paper.

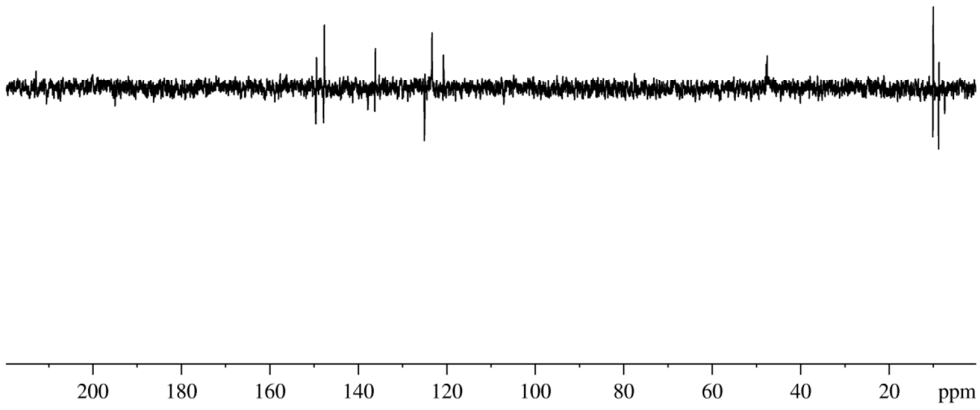
14. Hyperpolarization of propionitrile using 1



sFigure 15: ^{1}H NMR spectra of a sample containing 0.75 µl pyridine, 4.6 µl propionitrile and 1 (2 mg) in d_4-MeOH A) at thermal equilibrium and B) after being shaken in a PTF of 65 G

At a PTF of 65 G, the CH_2 protons of propionitrile (δ 2.43 ppm) are enhanced 10-fold whilst the methyl protons (δ 1.25 ppm) are enhanced only 3-fold.

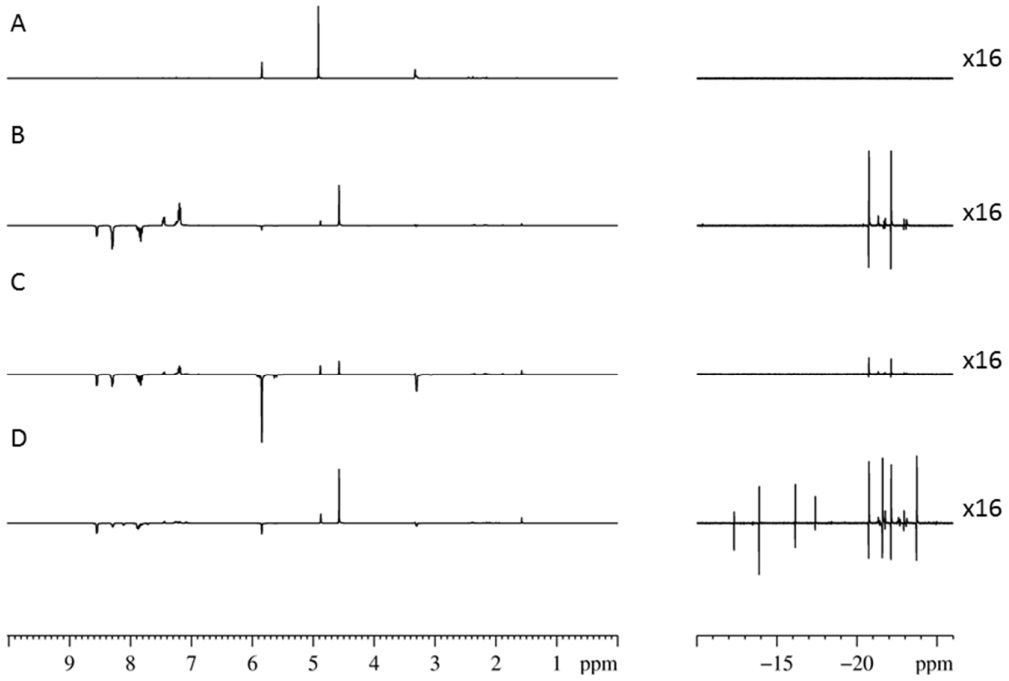
The observed signals for pyridine can be removed by employing d_5-pyridine as discussed in the main text.



sFigure 16: : ^{13}C NMR spectrum of a sample containing 0.75 µl pyridine, 4.6 µl propionitrile and 1 (2 mg) in d_4-MeOH after being shaken in a PTF of 0.5 G

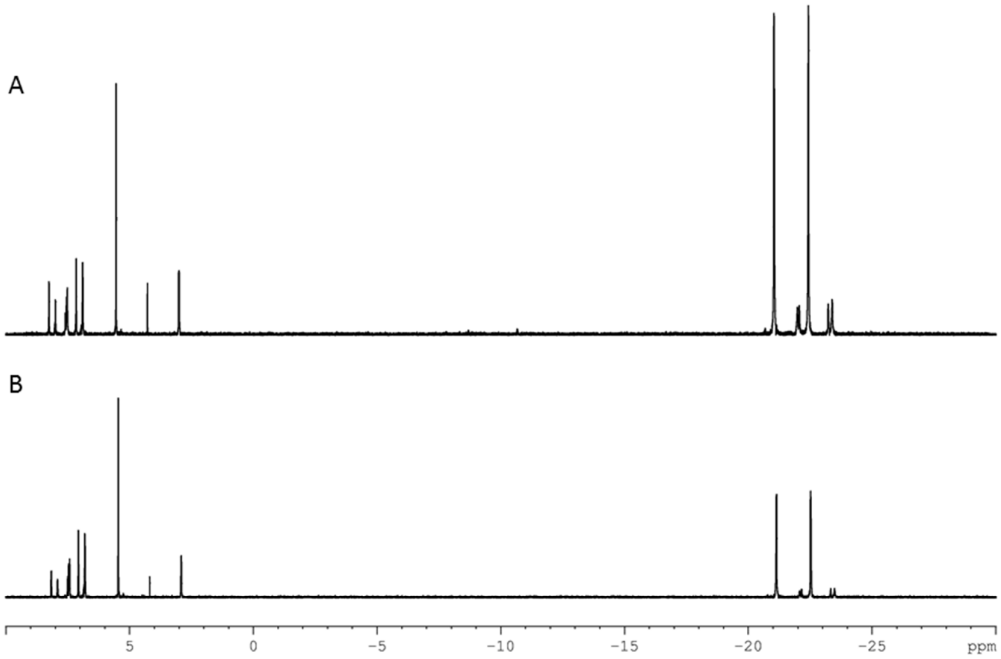
Note the multiplet structure at ~9.4 ppm; this is due to polarization transfer to the CH_3 carbon resonances. The quaternary carbon of the nitrile group is detected at δ 120 ppm. The other peaks in the region of δ 120 – 160 ppm belong to the carbon nuclei of pyridine.

15. Hyperpolarization of *trans*-3-hexenedinitrile using 1



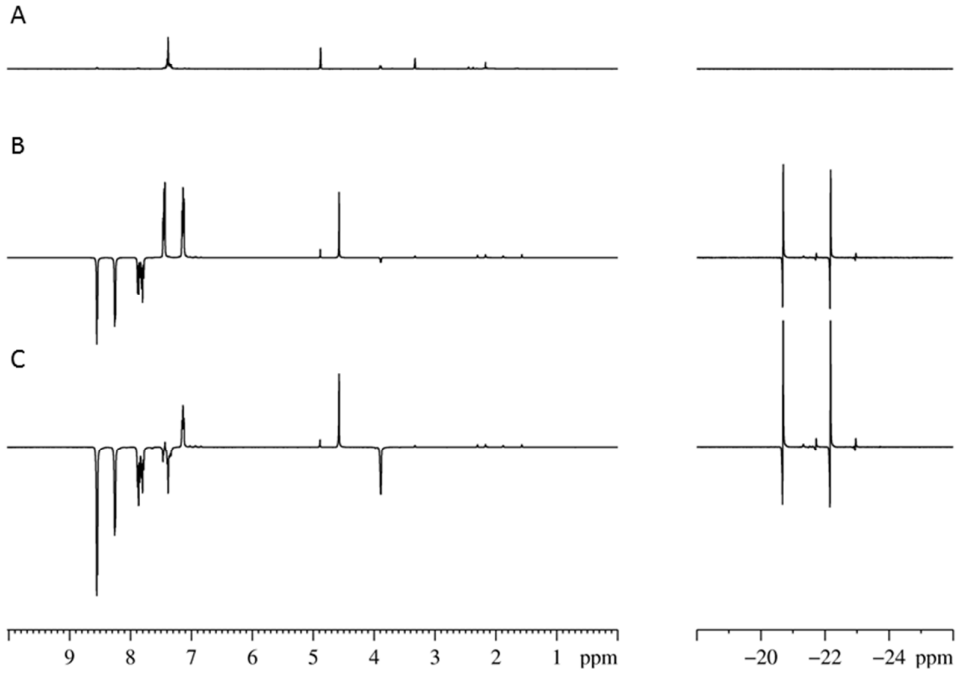
sFigure 17: ^{1}H NMR spectra of a sample containing 0.75 µl pyridine, 6.5 mg *trans*-3-hexenedinitrile and 1 (2 mg) in d_4-MeOH: A) at thermal equilibrium, B) after being shaken in a PTF of 2 G, C) after being shaken in a PTF of 65 G and D) showing the initial complexity of the hydride region immediately after introduction of *para*hydrogen in a PTF of 65 G

After shaking in a PTF of 65 G, the CH_2 and alkenic protons are enhanced by 4- and 10-fold respectively, relative to the thermal trace.



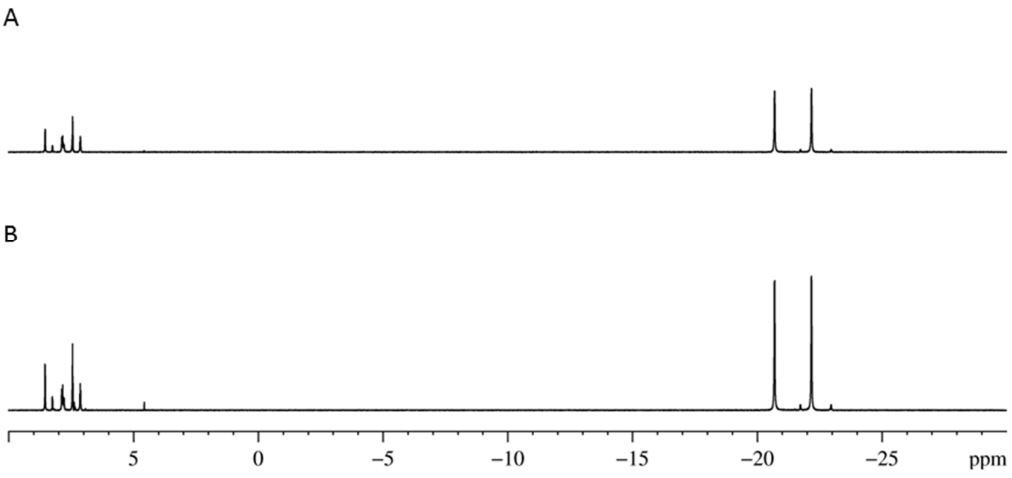
sFigure 18: ^{1}H OPSY-*dq* NMR spectra of a sample containing 0.75 µl pyridine, 6.5 mg *trans*-3-hexenedinitrile and 1 (2 mg) in d_4-MeOH after shaking in a PTF of either 2 G (A) or 65 G(B).

16. Hyperpolarization of benzylcyanide using 1



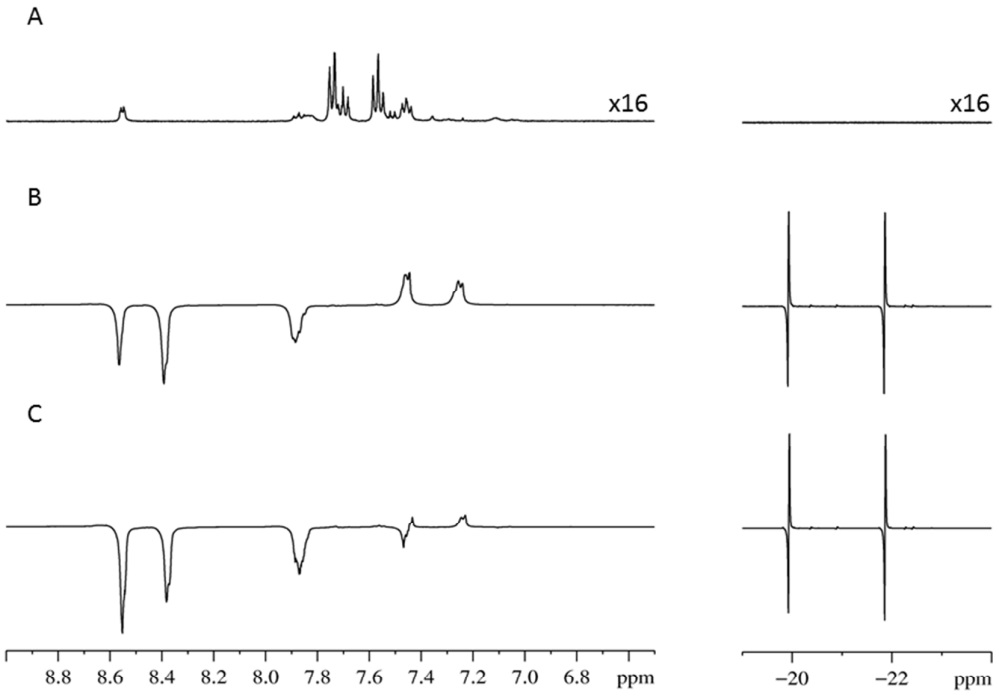
sFigure 19: ^{1}H NMR spectra of a sample containing 0.75 µl pyridine, 7.5 µl benzylcyanide and 1 (2 mg) in d_4-MeOH: A) at thermal equilibrium, B) after being shaken in a PTF of 2 G and C) after being shaken in a PTF of 65 G.

The benzyl protons are enhanced 2-fold at a PTF of 65 G whilst the CH_2 protons are enhanced by 18-fold.

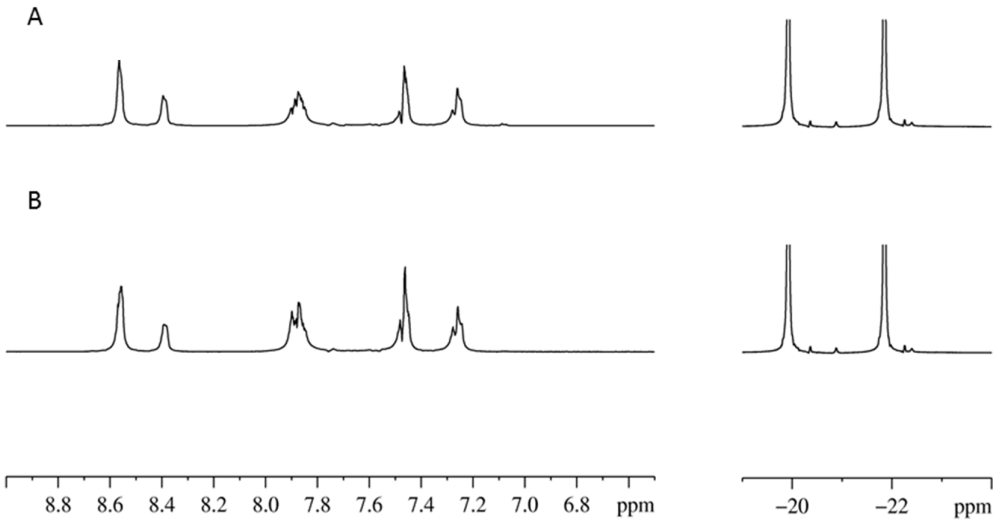


sFigure 20: ^{1}H OPSY-*dq* NMR spectra of a sample containing 0.75 µl pyridine, 7.5 µl benzylcyanide and 1 (2 mg) in d_4-MeOH after shaking in a PTF of either 2 G (A) or 65 G (B).

17. Hyperpolarization of benzonitrile using 1



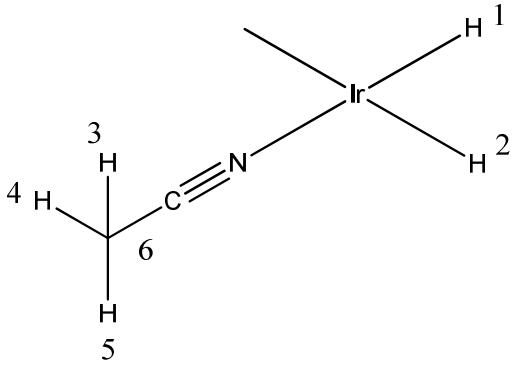
sFigure 21: ^{1}H NMR spectra of a sample containing 0.75 µl pyridine, 6.1 µl benzonitrile and 1 (2 mg) in d_4-MeOH: A) at thermal equilibrium (shown with 16-fold vertical expansion relative to B and C, B) after being shaken in a PTF of 2 G and C) after being shaken in a PTF of 65 G.

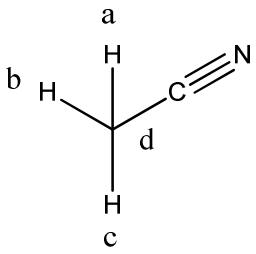


sFigure 22: ^{1}H OPSY-*dq* NMR spectra of a sample containing 0.75 µl pyridine, 6.1 µl benzonitrile and 1 (2 mg) in d_4-MeOH after shaking in a PTF of either 2 G (A) or 65 G(B).

18. Couplings and chemical shifts used to produce the theoretical spectra

The following spectral parameters were used in the theoretical models to produce the reported ^{1}H and ^{13}C NMR spectra. The parameters produce a close match with experiment as discussed in the main paper.





sTable 5: NMR data used in calculatons

	^{1}H	Quaternary ^{13}C	Methyl ^{13}C
v_1	−20.56	−20.56	−20.56
v_2	−22.12	−22.12	−22.12
v_3	2.16	2.16	2.16
v_4	2.16	2.16	2.16
v_5	2.16	2.16	2.16
v_6	N/A	117.8*	21.94*
v_a	2.05	2.05	2.05
v_b	2.05	2.05	2.05
v_c	2.05	2.05	2.05
v_d	N/A	116.7*	1.09*
J_{12}	−7.56	−7.56	−7.56
J_{13}	−2.1	−2.1	−2.1
J_{14}	−2.1	−2.1	−2.1
J_{15}	−2.1	−2.1	−2.1
J_{16}	N/A	−2.0	−4.0
J_{23}	−0.5	−0.2	−0.5
J_{24}	−0.5	−0.2	−0.5
J_{25}	−0.5	−0.2	−0.5
J_{26}	N/A	−0.2	−0.2
$J_{34}(J_{ab})$	0	0	0
$J_{35}(J_{ac})$	0	0	0
J_{36}	N/A	−9.2	136
$J_{45}(J_{bd})$	0	0	0
J_{46}	N/A	−9.2	136
J_{56}	N/A	−9.2	136
Exchange rate (s^{-1})	10.4	10.4	10.4
Residence time (s)	0.096	0.096	0.096

* The corresponding nucleus is either the ^{13}C methyl or quaternary nucleus- this is dependent on the nucleus of interest

19. DFT general considerations

For all structures, the system modelled was the same as the real system i.e. methyl groups on the phenyl rings were modelled as methyl groups rather than hydrogen atoms. The structures were optimised using the PBE0 functional from Adamo[10] and the basis sets from Aldrich described by the def2-SVP label.[11, 12] This basis set family included the ECP for iridium from Andrae.[13] Optimisations were performed in Turbomole 6.4[14] using the RI[15, 16] approximation and associated auxiliary basis sets.[17] Local minima were confirmed by the calculation of analytical second derivatives. Counterpoise corrections[18, 19] were undertaken on the optimised geometries using Gaussian 09C[20] and the same functional and basis set family. Single point energies incorporating the PCM model[21-23] and the SMD model[24] (ε=32.613 for methanol) were subsequently performed in Gaussian 09 using the same basis set family and functional. The thermodynamic corrections calculated in Turbomole were combined with solvation energies to calculate the thermodynamic values given. This approach has been used in the literature previously by Fomine.[25] Additionally, the correction proposed by Sakaki *et. al.* was used[26-28] to correct entropy terms. This results in modified free energy values that lie closer to the true values. The PBE0 functional was chosen due to its success in modelling metal complexes[29], ruthenium-phosphine complexes[30] and second generation ruthenium alkylidiene catalysts.[25]

For the vibrational analysis of Ir(IMes)$(CO)_2$Cl, a scaling factor of 0.9512[31] taken from the literature was applied to all calculated carbonyl stretch frequencies.

20. DFT calculations for complexes 2 and 3

Density functional theory was used to model the energies and reactions of **2** and **3** (sFigure 23). Complex **3** was found to be 31.8 kJ mol^{-1} ($E_{SCF+ZPE}$) more stable than **2**; the enthalpy difference was 25.1 kJ mol^{-1}. These calculations were carried out in the gas phase and so single point energy calculations were undertaken with both the PCM and SMD solvation models to investigate the effect of the methanol solvent. Both calculations revealed the more stable complex to be **3**, with the enthalpy difference rising slightly to 26.5 kJ mol^{-1} for PCM solvation and reducing to 20.0 kJ mol^{-1} for SMD solvation.

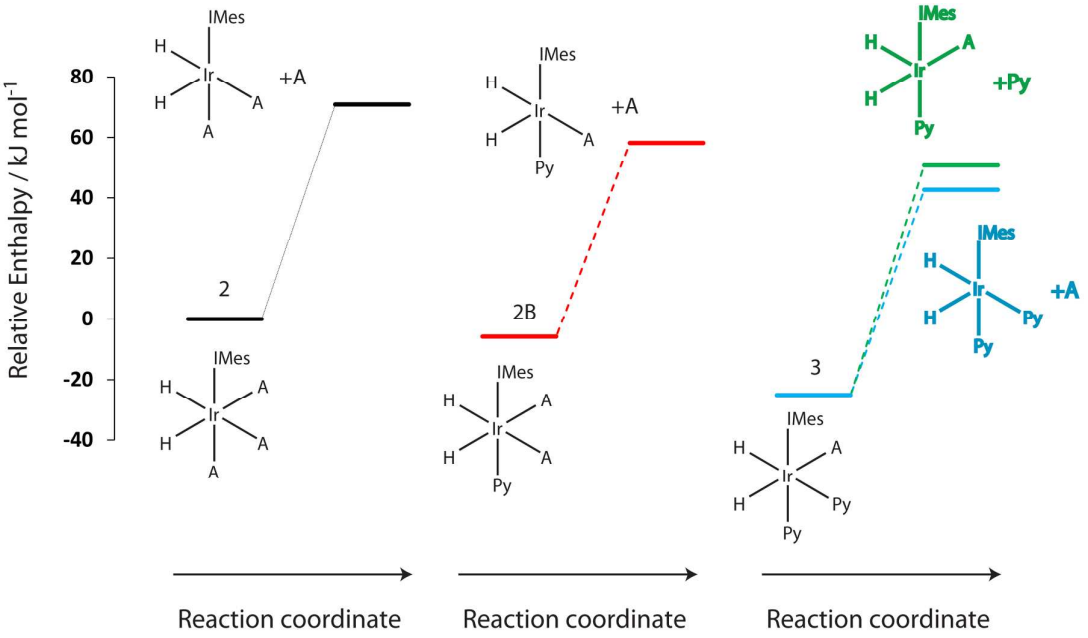
Complex $[Ir(H)_2(IMes)(MeCN)_2(py)]Cl$ (**2B**) was also modelled. This complex can undergo loss of either an acetonitrile ligand *trans* to hydride or a pyridine ligand *trans* to IMes. Loss of **A** proved to be favoured. The resulting 16e$^-$ product $[Ir(H)_2(IMes)(MeCN)(py)]^+$ (**2B–A**) is more stable than $[Ir(H)_2(IMes)(MeCN)_2]^+$ (**2–A**), which is the corresponding product formed by the loss of **A** from **2**. In contrast, **3** can also undergo ligand loss of either **A** or pyridine in the equatorial plane. The loss of **A** is again favoured. The corresponding bond energies are 67.7 and 75.8 kJ mol^{-1} respectively.

sTable 6: Computed zero point corrected SCF energy, enthalpy, Gibbs free energies for A and pyridine loss in 2, 2B and 3

Complex	$[Ir(H)_2(IMes)(MeCN)_2]^+$ **(2–A)** / kJ mol^{-1}	$[Ir(H)_2(IMes)(MeCN)(py)]^+$ **(2B–A)** / kJ mol^{-1}	$[Ir(H)_2(IMes)(MeCN)(Py)]^+$ **(3–A)** / kJ mol^{-1}	$[Ir(H)_2(IMes)(MeCN)_2]^+$ **(3–Py)** / kJ mol^{-1}
Gas phase - $E_{SCF+ZPE}$	62.9	62.5	69.2	74.9
ΔH	70.8	64.1	67.7	75.8
ΔG	58.6	77.8	96.8	95.2
PCM - $E_{SCF+ZPE}$	27.9	26.6	29.4	39.3
ΔH	35.9	28.2	28.0	40.3
ΔG	23.7	41.9	57.0	59.7
SMD - $E_{SCF+ZPE}$	3.4	-1.5	5.8	8.0
ΔH	11.3	0.1	4.3	9.0
ΔG	−0.8	13.8	33.3	28.4

Experimentally, **2** is stable in methanol in solution. The SMD model erroneously predicts that the formation of $[Ir(H)_2(IMes)(MeCN)_2(MeOH)]^+$ via the loss of **A** has a $\Delta G_{corrected}$ of −0.8 kJ mol^{-1} whereas $\Delta G_{uncorrected}$ is −67.6 kJ mol^{-1}. As the true value lies between these two values, the values given by the SMD model can be discounted and are not used in our studies.

The enthalpies of these complexes are also illustrated in sFigure 23, where all enthalpies are relative to that of **2**.

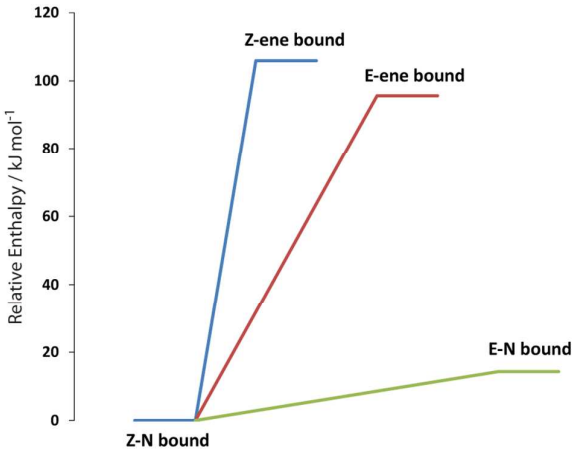


sFigure 23: Relative potential energy profiles for the loss of A or Py from 2, 2B or 3

The results from our DFT calculations are consistent with the observed increase in polarization of **A** in **3** over **2**.

21. DFT calculations for the binding modes of *cis*- and *trans*-3-hexenedinitrile

The coordination of *trans*-3-hexenedinitrile to 3 was modelled theortically and the coordination through the nitrile group was calculated to be −105.9 kJ mol^{-1}(in terms of relative enthalpy) more stable than the coordination through the alkene group. To examine any steric effects, the coordination of the *cis* isomer was also modelled. The nitrile bound *cis*-3-hexenedinitrile was again found to be more stable than via coordination through the alkene, with a difference in enthalpy of −81.3 kJ mol^{-1}. The *cis* isomer was also found to coordinate more weakly through the nitrile group compared to the *trans* isomer by +14.3 kJ mol^{-1}, which arises from the steric crowding of the *cis* isomer relative to the *trans* isomer following ligation to the metal centre. These enthalpies are illustrated in sFigure 24.



sFigure 24: Relative enthalpies for the coordination of *cis*-3-hexenedinitrile and *trans*-3-hexenedinitrile to 3 via either the alkene (ene) or nitrile (N) group. E and Z refer to the *cis*- and *trans*-configuartions of the alkene bond respectively.

22. DFT vibrational calculations for Ir(NHC)$(CO)_2$Cl where NHC= IMes-d_{22} or IMes

The structures of $Ir(CO)_2$(IMes)Cl and Ir(IMes-d_{22})$(CO)_2$Cl were optimised and analytical second derivatives calculated in order to obtain the vibrational frequencies of the complexes. Calculated values for $Ir(CO)_2$ (IMes) Cl were found to be 2090.2 and 1997.1 cm^{-1} whilst for $Ir(CO)_2$(IMes-d_{22})Cl they were 2090.4 and 1996.9 cm^{-1}. The difference between the two CO frequencies in these complexes is small (0.2 cm^{-1}). Thus, a negligible difference in the resulting electron-donating ability of IMes and IMes-d_{22} is predicted. Experimental rate data for ligand loss in $[Ir(H)_2(IMes)(MeCN)_2(py)]^+$ and $[Ir(H)_2$(IMes-d_{22})$(MeCN)_2(py)]^+$ agree with this.

23. Cartesian Coordinates, total electronic energy and zero point energies obtained from DFT calculations

$[Ir(H)_2(IMes)(MeCN)_3]Cl$ (**2**)

SCF-energy: -1425.4289763
SCF + E(vib0): -1424.8676191

Ir	-0.045313802	0.921960036	-0.444779505
H	-1.330032055	0.606218773	-1.283073908
H	0.756645561	0.540559180	-1.742257422
C	-0.739574176	-3.196151636	0.175437250
C	0.612130694	-3.212473669	0.179223894
H	-1.468292396	-3.997690938	0.258025239
H	1.322060894	-4.030016508	0.267916726
C	-0.036850819	-1.049890424	-0.066069806
N	-1.122268897	-1.875471799	0.027631292
N	1.026898969	-1.900005510	0.034162450
C	-2.505912094	-1.501365768	0.005923737
C	-3.169823883	-1.320256378	1.228515210
C	-3.179240713	-1.434855617	-1.223694331
C	-4.530289948	-1.003487707	1.193561037
C	-4.538822984	-1.114581830	-1.202468979
C	-5.231545314	-0.884604181	-0.010321496
H	-5.064315841	-0.870136374	2.139422337
H	-5.077382794	-1.059103279	-2.152695123
C	2.420557799	-1.566717036	0.040348199
C	3.128450143	-1.540874422	-1.171532504
C	3.054738674	-1.388645489	1.277937195
C	4.500507085	-1.285566720	-1.115944159
C	4.433063127	-1.153310302	1.278910019
C	5.173609015	-1.091560100	0.094812402
H	5.065813313	-1.262748718	-2.052086267
H	4.946121182	-1.038420666	2.239014050
C	-2.458578301	-1.515689966	2.537170018
H	-1.483946057	-1.006502293	2.557176183
H	-3.066634007	-1.146310975	3.374918326
H	-2.264546773	-2.583952356	2.729253300
C	-2.473260091	-1.717606759	-2.516381438
H	-3.177519697	-1.703265182	-3.358494029
H	-1.687892731	-0.970024406	-2.709066823
H	-1.983522374	-2.704116740	-2.501370949
C	-6.687632618	-0.519622800	-0.023072366
H	-6.818289518	0.574626097	-0.067017637
H	-7.201743201	-0.941962565	-0.897915301

H	-7.202221704	-0.874307249	0.881382894
C	2.280004115	-1.451351612	2.562391341
H	2.930644836	-1.256246035	3.425440137
H	1.463096066	-0.711786115	2.570756083
H	1.817636589	-2.440221227	2.711452444
C	2.445673980	-1.805730291	-2.480196181
H	1.676361345	-1.045782167	-2.686110876
H	3.167277990	-1.800536634	-3.307601815
H	1.939668366	-2.784169087	-2.478991853
C	6.653792468	-0.839248002	0.113302813
H	7.195687365	-1.610914238	-0.454443499
H	6.899666459	0.128630501	-0.353264666
H	7.053465349	-0.831824328	1.136850042
C	3.980206827	2.480087271	1.529075828
H	4.554691025	2.951112772	0.718298467
H	3.774676500	3.230928207	2.305355674
H	4.581799394	1.666640089	1.959482043
C	2.742154287	1.939436538	1.006257109
N	1.762756283	1.499421423	0.581451711
C	-2.906858102	2.354158501	3.054090744
H	-2.908204196	1.662227021	3.908709911
H	-2.625377885	3.355721590	3.409539097
H	-3.920698516	2.395729528	2.629812105
C	-1.973378248	1.895184287	2.045641703
N	-1.246073623	1.515024854	1.233346350
C	-0.333620971	5.181717714	-2.272771373
H	0.503867738	5.329735179	-2.970056846
H	-1.276629392	5.242436628	-2.835533925
H	-0.316361866	5.983654529	-1.520596445
C	-0.223726748	3.886225058	-1.634103652
N	-0.142279993	2.844151354	-1.145214361

$[Ir(H)_2(IMes)(MeCN)_2]Cl$ (**2–A**)

SCF-energy: -1292.9058820
SCF + E(vib0): -1292.3932215

Ir	0.230262251	-0.634607264	0.576293254
H	0.203187495	-0.250492581	2.105235110
H	1.747529695	-0.614953203	0.760595043
C	-0.466112127	3.425523128	-0.115385004
C	0.881937524	3.490265208	0.014215050
H	-1.208165509	4.200047757	-0.289308891
H	1.564985219	4.334466240	-0.024417953

C	0.290733875	1.325264761	0.240525628
N	-0.808985175	2.092792756	0.025623440
N	1.330521867	2.197555087	0.232204930
C	-2.135882808	1.555011122	-0.033271908
C	-2.681794948	1.233644615	-1.286598361
C	-2.863521935	1.401695349	1.161113602
C	-3.976665281	0.709408363	-1.318637705
C	-4.152989067	0.874295199	1.069771857
C	-4.726274737	0.515751043	-0.155207523
H	-4.418130343	0.457186944	-2.286977602
H	-4.734189742	0.753156769	1.988325743
C	2.709347657	1.859469982	0.435855412
C	3.225116698	1.876385080	1.740245877
C	3.506383592	1.565292226	-0.680627651
C	4.578298882	1.571424851	1.905430471
C	4.851698244	1.266735757	-0.459302595
C	5.407406043	1.261231758	0.824002310
H	4.998391390	1.583816150	2.915048120
H	5.488114707	1.038264437	-1.319005208
C	-1.921749625	1.487016158	-2.556014342
H	-0.888274469	1.116051376	-2.495606690
H	-2.417357690	1.007992953	-3.411244545
H	-1.860435445	2.565608490	-2.774662338
C	-2.291768350	1.821889983	2.483694355
H	-3.022057084	1.672204975	3.289433959
H	-1.386148281	1.247228050	2.731170848
H	-2.008292405	2.886264529	2.478214470
C	-6.109321976	-0.063783136	-0.211288331
H	-6.106249070	-1.117574047	0.112668419
H	-6.796763307	0.475888957	0.456602992
H	-6.523522767	-0.030683782	-1.228429536
C	2.935219298	1.583466459	-2.068467764
H	3.682184413	1.253693247	-2.802712214
H	2.056535002	0.924367263	-2.146825865
H	2.605847964	2.594187787	-2.358729788
C	2.356443456	2.206077540	2.917894564
H	1.570946602	1.445201281	3.052429365
H	2.948652108	2.250453349	3.841104501
H	1.849898055	3.176157817	2.794031173
C	6.851471228	0.911180325	1.034659592
H	7.247788977	1.364420803	1.954030617
H	6.978992510	-0.180467206	1.125849146
H	7.474823649	1.241812609	0.191498054
C	0.429449394	-2.132898989	-3.915619648
H	0.856121602	-3.146371869	-3.923428648

H	-0.572127386	-2.164320825	-4.368586991
H	1.071898589	-1.472542563	-4.516270656
C	0.345594797	-1.639755646	-2.556306575
N	0.284468300	-1.240685509	-1.473174279
C	-0.023628188	-5.038734450	2.034204246
H	0.641022575	-5.697475827	1.456573105
H	0.285799562	-5.057112289	3.089589568
H	-1.053904514	-5.416220929	1.959308885
C	0.048549420	-3.685723582	1.525013117
N	0.110981011	-2.601146494	1.133336025

$[Ir(H)_2(IMes)(MeCN)_2(Py)]Cl$ (**2B**)

SCF-energy: -1540.7554544
SCF + E(vib0): -1540.1492235

Ir	-0.011022233	-0.647234629	0.202642220
H	-1.130629548	-0.507465530	1.296460262
H	1.017134268	-0.545562027	1.388348092
C	-0.628044181	3.530801169	0.392819776
C	0.722934181	3.513195506	0.404248920
H	-1.337180488	4.351054237	0.460679704
H	1.452170270	4.314561582	0.483945750
C	0.021001452	1.358698476	0.213738723
N	-1.043144335	2.215704211	0.274591646
N	1.105522781	2.187497455	0.292579011
C	-2.436666473	1.888275523	0.211457265
C	-3.085184950	1.967794560	-1.028561724
C	-3.133489641	1.615292227	1.399820300
C	-4.460996552	1.716728340	-1.065127258
C	-4.502589651	1.359688074	1.306406238
C	-5.186839002	1.402960713	0.087147762
H	-4.985635636	1.795235526	-2.022731567
H	-5.056574957	1.138687065	2.223301275
C	2.491350354	1.826128646	0.250610831
C	3.164747797	1.542455328	1.449544763
C	3.158320881	1.884412212	-0.981018180
C	4.529996334	1.259125087	1.376811334
C	4.529425314	1.607928895	-0.996627544
C	5.232874522	1.286785785	0.167902930
H	5.065988719	1.029843618	2.302293749
H	5.068315538	1.670648628	-1.947443583
C	-2.336290598	2.342471134	-2.274988192
H	-1.428596916	1.733392116	-2.402125137
H	-2.967167406	2.220557565	-3.166368149

H	-2.011511713	3.395226921	-2.246513185
C	-2.440287718	1.630478243	2.729883449
H	-3.146643194	1.418488551	3.543061248
H	-1.632808121	0.882851567	2.766133170
H	-1.980471546	2.611749058	2.929307526
C	-6.666598769	1.154966896	0.034122370
H	-6.931875208	0.205750084	0.524766890
H	-7.217297017	1.951019456	0.560319531
H	-7.038874938	1.122000773	-0.999272604
C	2.430779392	2.255013079	-2.241096712
H	3.082610011	2.148453625	-3.119061735
H	1.538083747	1.628468767	-2.390918052
H	2.084888758	3.300897732	-2.213662560
C	2.452804443	1.575003978	2.769322553
H	1.630699794	0.843216196	2.795406959
H	3.142937085	1.351870528	3.593397001
H	2.008935329	2.565403391	2.959344552
C	6.709953785	1.019341006	0.137731661
H	7.266742646	1.844785678	0.610018403
H	6.964307698	0.103883177	0.693339472
H	7.085904973	0.913965162	-0.889581924
C	3.690946165	-1.664171123	-2.560031041
H	4.036449155	-2.665572607	-2.265155317
H	3.470043879	-1.664745666	-3.637097146
H	4.490688794	-0.937186280	-2.355076549
C	2.513864692	-1.299462692	-1.799046571
N	1.591437281	-0.993110568	-1.173920634
C	-3.529622385	-1.465792992	-2.846867912
H	-3.256533014	-1.359535666	-3.906637610
H	-3.881953169	-2.492312498	-2.669894308
H	-4.344012984	-0.764704771	-2.611116940
C	-2.393847398	-1.174340774	-1.996708233
N	-1.506709987	-0.923866407	-1.299752935
C	-0.139874972	-5.529368693	0.969899356
C	-0.156128016	-4.627021961	2.030072838
C	-0.116324505	-3.264986600	1.759558433
N	-0.062578549	-2.777580386	0.509315115
C	-0.046681567	-3.648304993	-0.510630555
C	-0.083797339	-5.025381705	-0.326441412
H	-0.170404240	-6.606303589	1.151100500
H	-0.199532918	-4.967148638	3.066040699
H	-0.127174819	-2.524329415	2.559830748
H	-0.002661111	-3.215206377	-1.512072606
H	-0.068924548	-5.687411516	-1.194103136

$[Ir(H)_2(IMes)(MeCN)(Py)]Cl$ (**2B–A**)

SCF-energy: -1408.2300922
SCF + E(vib0): -1407.6728807

Ir	-0.302463724	-0.422487876	0.371553344
H	-1.829806332	-0.409649211	0.443063648
H	-0.393765945	-0.268019852	1.941162609
C	-0.844757626	3.755908070	0.391589392
C	0.497327637	3.671120089	0.220321820
H	-1.501041906	4.616722563	0.485367691
H	1.259600526	4.441034838	0.136756451
C	-0.320014454	1.561763794	0.302567575
N	-1.330163466	2.458702007	0.440779899
N	0.799715138	2.321810060	0.167599214
C	-2.714415953	2.134473757	0.624643280
C	-3.527670017	1.971355574	-0.505144627
C	-3.215930070	2.021164366	1.931076004
C	-4.877848273	1.676583758	-0.299101226
C	-4.571596354	1.725522023	2.080924115
C	-5.420295261	1.551255165	0.982261106
H	-5.526584586	1.545825362	-1.169811736
H	-4.978900839	1.632508056	3.091828072
C	2.103280573	1.753175704	0.003686640
C	2.830734155	1.373110999	1.146169166
C	2.623377463	1.610462971	-1.293437951
C	4.091391713	0.803741325	0.951528794
C	3.889746786	1.036655093	-1.429458957
C	4.639101792	0.625159921	-0.323239360
H	4.669931669	0.502167809	1.829359066
H	4.308369493	0.917207458	-2.432991692
C	-2.966055483	2.103056080	-1.890599231
H	-2.187853178	1.345061192	-2.074591403
H	-3.753277699	1.978095175	-2.645869031
H	-2.500144597	3.088579591	-2.049821727
C	-2.324140032	2.203354018	3.123658951
H	-2.892106471	2.099545793	4.057359679
H	-1.514979085	1.455521645	3.129098809
H	-1.846442141	3.195711186	3.127985780
C	-6.879030351	1.261331444	1.183478242
H	-7.031363711	0.466657275	1.929275970
H	-7.407534709	2.154996753	1.553473481
H	-7.364887409	0.951422519	0.248143288
C	1.863022666	2.092466386	-2.494488936
H	2.302048094	1.697695274	-3.421021973

H	0.803370134	1.802155281	-2.452997629
H	1.888810357	3.192307079	-2.565407979
C	2.291142931	1.601118674	2.528482547
H	1.362127624	1.035519748	2.698495338
H	3.022122950	1.294472471	3.287838818
H	2.057079298	2.664498552	2.694753033
C	6.013884737	0.048182070	-0.492647090
H	6.780676785	0.827691443	-0.350869551
H	6.216173261	-0.740090954	0.246694718
H	6.158202999	-0.372993283	-1.497428324
C	-0.282865930	-1.338981030	-4.266886537
H	0.552525957	-0.850257900	-4.789078477
H	-0.207767810	-2.426389216	-4.412158816
H	-1.229345246	-0.987632986	-4.703431409
C	-0.243294156	-1.019810725	-2.854552656
N	-0.222295731	-0.756474181	-1.728361969
C	0.093967417	-5.273683185	1.115283106
C	-1.021030584	-4.577737938	1.575123620
C	-1.115869699	-3.214359826	1.327122660
N	-0.172869592	-2.538362085	0.650926244
C	0.900024369	-3.211259260	0.205363070
C	1.074587179	-4.572559827	0.418128684
H	0.198364007	-6.345423645	1.299252788
H	-1.816330950	-5.080038364	2.128430150
H	-1.966577272	-2.629174801	1.680428654
H	1.647370306	-2.627997773	-0.340515627
H	1.969791474	-5.068852256	0.039567091

$[Ir(H)_2(IMes)(MeCN)(Py)_2]Cl$ (**3**)

SCF-energy: -1656.0804281
SCF + E(vib0): -1655.4300980

Ir	-0.029341905	0.583797750	-0.452036160
H	-1.398062415	0.229917873	-1.134522901
H	0.627556729	0.362259478	-1.869706974
C	-0.349860532	-3.610612555	-0.122696619
C	0.995798365	-3.509836569	-0.057214374
H	-1.006422186	-4.476123269	-0.120517044
H	1.771348577	-4.267232640	0.015303880
C	0.165905227	-1.394598792	-0.206195175
N	-0.843205332	-2.321689698	-0.211664422
N	1.297534349	-2.159075048	-0.107120181
C	-2.253013990	-2.078991512	-0.299511730
C	-3.006699249	-2.035506599	0.880869814

C	-2.850177329	-1.990520495	-1.568670430
C	-4.388080521	-1.843082596	0.768016902
C	-4.230562250	-1.798301140	-1.625370037
C	-5.018851843	-1.717454800	-0.471105163
H	-4.988678299	-1.803680724	1.681413543
H	-4.708874913	-1.721417269	-2.606218134
C	2.658544599	-1.718949133	-0.043231003
C	3.375334434	-1.523668668	-1.233967196
C	3.264259489	-1.602081190	1.216427796
C	4.721890271	-1.164679553	-1.131154793
C	4.616784281	-1.251544083	1.264704504
C	5.364262100	-1.029191773	0.103734373
H	5.292776133	-1.009645161	-2.051332766
H	5.104609091	-1.169222815	2.241093384
C	-2.367869626	-2.229042002	2.225529879
H	-1.435383154	-1.654775099	2.323758501
H	-3.049162474	-1.925869598	3.032070266
H	-2.110297929	-3.287845025	2.394581245
C	-2.029685940	-2.100822185	-2.818981129
H	-2.666668983	-2.060091121	-3.712307542
H	-1.292583335	-1.283917338	-2.877215989
H	-1.465175987	-3.046256121	-2.848076241
C	-6.505654341	-1.537795880	-0.574133079
H	-6.765046915	-0.723783987	-1.267874853
H	-6.984521163	-2.452426441	-0.959841919
H	-6.957227460	-1.313822075	0.402115955
C	2.494662278	-1.869766205	2.477008814
H	3.046195377	-1.517702438	3.359325938
H	1.508123700	-1.383787023	2.461750750
H	2.311778404	-2.948368464	2.613260817
C	2.729660967	-1.716037775	-2.573119240
H	1.921775571	-0.984319389	-2.728154410
H	3.462254120	-1.603225112	-3.382981215
H	2.277762726	-2.716720663	-2.659997936
C	6.828421680	-0.703079250	0.175101317
H	7.435574451	-1.609886946	0.018102423
H	7.123509351	0.017328258	-0.601954525
H	7.110635532	-0.292741172	1.155497053
C	4.125567642	2.370423330	0.897161626
H	4.638705877	2.644743772	-0.036220214
H	3.970767548	3.277645726	1.498852912
H	4.761257423	1.667333772	1.453789219
C	2.856608060	1.741875764	0.591053109
N	1.848385608	1.238961397	0.328741126
C	-2.454529079	1.622346757	3.828520639

C	-3.121936368	1.555380281	2.608972867
C	-2.401382400	1.238721330	1.461472677
N	-1.082177497	0.999664180	1.479205423
C	-0.441775863	1.064847762	2.655428856
C	-1.084515137	1.369769282	3.850060556
H	-2.991891488	1.866433140	4.747940264
H	-4.194987997	1.741121353	2.536448643
H	-2.888695786	1.162196966	0.487414189
H	0.632287425	0.865742467	2.629060409
H	-0.513804539	1.406895257	4.779835195
C	-0.864336613	5.278715867	-1.758193288
C	-1.046008703	4.228986725	-2.654843168
C	-0.792935970	2.929343219	-2.235109088
N	-0.375908266	2.638413595	-0.991354970
C	-0.201593126	3.651592586	-0.129897854
C	-0.432998374	4.979347518	-0.469346257
H	-1.056104532	6.311307423	-2.058842141
H	-1.382472642	4.406298897	-3.677773673
H	-0.922046016	2.078125587	-2.904518350
H	0.134715976	3.380377080	0.873041938
H	-0.276421181	5.762267379	0.274870306

$[Ir(H)_2(IMes)(Py)_2]Cl$ (**3−A**)

SCF-energy: -1523.5523410
SCF + E(vib0): -1522.9507095

Ir	-0.224803449	0.413767358	-0.478081555
C	-0.489961061	5.224341354	-1.525401030
C	0.484313427	4.742921473	-0.655473305
C	0.506038746	3.385945380	-0.359284925
N	-0.369186609	2.511993098	-0.880554038
C	-1.306485768	2.978570615	-1.723481542
C	-1.401321221	4.320782505	-2.066323860
H	-0.536807339	6.285667807	-1.779649976
H	1.224498734	5.406289685	-0.204929171
H	1.256289359	2.977940032	0.323124317
H	-1.992337436	2.236490658	-2.135374475
H	-2.182580117	4.645089337	-2.755779696
C	-0.599201861	1.793146970	4.328203443
C	-1.731363658	1.601919082	3.540056437
C	-1.573297482	1.169359994	2.228184004
N	-0.370925057	0.923299145	1.685715781
C	0.717434251	1.105683270	2.448429486

C	0.650157138	1.539542700	3.767939803
H	-0.689054290	2.133587697	5.362394443
H	-2.733645942	1.785700118	3.931031602
H	-2.437150162	1.009645881	1.578659492
H	1.683398080	0.883090554	1.983329982
H	1.569017894	1.671673893	4.342029876
H	-1.728271051	0.203067716	-0.656432794
H	-0.146212039	0.176520528	-2.039425162
C	-0.376614353	-3.791193413	-0.399195717
C	0.950858532	-3.597267536	-0.212890431
H	-0.960157103	-4.702695022	-0.494986493
H	1.771666136	-4.302223190	-0.113720704
C	-0.029946871	-1.555466749	-0.326193170
N	-0.962747362	-2.537609420	-0.464984694
N	1.145578345	-2.227243429	-0.168040156
C	-2.370511141	-2.333956212	-0.637501118
C	-3.188990524	-2.289877012	0.501579380
C	-2.891366200	-2.233298968	-1.936471056
C	-4.561031315	-2.110677545	0.311979384
C	-4.270817081	-2.057513356	-2.069956631
C	-5.122189205	-1.988249271	-0.963048855
H	-5.213571570	-2.079919948	1.189295773
H	-4.694294254	-1.982808663	-3.075624400
C	2.404363594	-1.584839050	0.056367670
C	3.145484359	-1.113855814	-1.043652885
C	2.884285745	-1.489134116	1.373042508
C	4.365395306	-0.486533686	-0.781965993
C	4.114736357	-0.856257357	1.576530380
C	4.867246498	-0.342831608	0.516583518
H	4.952960538	-0.114609732	-1.626206195
H	4.502769630	-0.775721877	2.596115532
C	-2.612563483	-2.455968494	1.877698493
H	-1.791523322	-1.746144203	2.062620996
H	-3.380598128	-2.301762899	2.647217232
H	-2.197971090	-3.467101151	2.020869122
C	-1.999594170	-2.316892151	-3.139546996
H	-2.584535901	-2.256982195	-4.066643845
H	-1.263233249	-1.497418952	-3.142443865
H	-1.431624017	-3.260332872	-3.158908739
C	-6.597425386	-1.774854228	-1.138824868
H	-6.836491930	-0.698704451	-1.168387879
H	-6.959657320	-2.213761178	-2.079309965
H	-7.171513977	-2.214392994	-0.310912309
C	2.123700380	-2.078490217	2.526053004
H	2.224097618	-3.176144222	2.546322694

H	2.503837720	-1.699883925	3.484439569
H	1.047137422	-1.860217344	2.467483941
C	2.670095670	-1.318497367	-2.452761468
H	1.711371945	-0.809525560	-2.635541534
H	3.405808159	-0.935658514	-3.171933538
H	2.512884365	-2.387747529	-2.665735551
C	6.194639472	0.316202832	0.751753671
H	6.236720340	1.310719170	0.281763670
H	6.407627483	0.433959037	1.822932743
H	7.010334927	-0.279555958	0.311900949

$[Ir(H)_2(IMes)(MeCN)(Py)]Cl$ (**3–Py**)

SCF-energy: -1408.2300922
SCF + E(vib0): -1407.6728807

Ir	-0.302463724	-0.422487876	0.371553344
H	-1.829806332	-0.409649211	0.443063648
H	-0.393765945	-0.268019852	1.941162609
C	-0.844757626	3.755908070	0.391589392
C	0.497327637	3.671120089	0.220321820
H	-1.501041906	4.616722563	0.485367691
H	1.259600526	4.441034838	0.136756451
C	-0.320014454	1.561763794	0.302567575
N	-1.330163466	2.458702007	0.440779899
N	0.799715138	2.321810060	0.167599214
C	-2.714415953	2.134473757	0.624643280
C	-3.527670017	1.971355574	-0.505144627
C	-3.215930070	2.021164366	1.931076004
C	-4.877848273	1.676583758	-0.299101226
C	-4.571596354	1.725522023	2.080924115
C	-5.420295261	1.551255165	0.982261106
H	-5.526584586	1.545825362	-1.169811736
H	-4.978900839	1.632508056	3.091828072
C	2.103280573	1.753175704	0.003686640
C	2.830734155	1.373110999	1.146169166
C	2.623377463	1.610462971	-1.293437951
C	4.091391713	0.803741325	0.951528794
C	3.889746786	1.036655093	-1.429458957
C	4.639101792	0.625159921	-0.323239360
H	4.669931669	0.502167809	1.829359066
H	4.308369493	0.917207458	-2.432991692
C	-2.966055483	2.103056080	-1.890599231
H	-2.187853178	1.345061192	-2.074591403
H	-3.753277699	1.978095175	-2.645869031

H	-2.500144597	3.088579591	-2.049821727
C	-2.324140032	2.203354018	3.123658951
H	-2.892106471	2.099545793	4.057359679
H	-1.514979085	1.455521645	3.129098809
H	-1.846442141	3.195711186	3.127985780
C	-6.879030351	1.261331444	1.183478242
H	-7.031363711	0.466657275	1.929275970
H	-7.407534709	2.154996753	1.553473481
H	-7.364887409	0.951422519	0.248143288
C	1.863022666	2.092466386	-2.494488936
H	2.302048094	1.697695274	-3.421021973
H	0.803370134	1.802155281	-2.452997629
H	1.888810357	3.192307079	-2.565407979
C	2.291142931	1.601118674	2.528482547
H	1.362127624	1.035519748	2.698495338
H	3.022122950	1.294472471	3.287838818
H	2.057079298	2.664498552	2.694753033
C	6.013884737	0.048182070	-0.492647090
H	6.780676785	0.827691443	-0.350869551
H	6.216173261	-0.740090954	0.246694718
H	6.158202999	-0.372993283	-1.497428324
C	-0.282865930	-1.338981030	-4.266886537
H	0.552525957	-0.850257900	-4.789078477
H	-0.207767810	-2.426389216	-4.412158816
H	-1.229345246	-0.987632986	-4.703431409
C	-0.243294156	-1.019810725	-2.854552656
N	-0.222295731	-0.756474181	-1.728361969
C	0.093967417	-5.273683185	1.115283106
C	-1.021030584	-4.577737938	1.575123620
C	-1.115869699	-3.214359826	1.327122660
N	-0.172869592	-2.538362085	0.650926244
C	0.900024369	-3.211259260	0.205363070
C	1.074587179	-4.572559827	0.418128684
H	0.198364007	-6.345423645	1.299252788
H	-1.816330950	-5.080038364	2.128430150
H	-1.966577272	-2.629174801	1.680428654
H	1.647370306	-2.627997773	-0.340515627
H	1.969791474	-5.068852256	0.039567091

[Ir(IMes)(Py)$_2$(*trans*-3-hexenedinitrile)]Cl *trans*-3-hexenedinitrile bound through alkene

SCF-energy: -1864.5866792
SCF + E(vib0): -1863.8737389

Ir	0.060156938	0.441767672	-0.268371072

C	-0.756047379	5.017079289	-2.004313415
C	-0.311033305	3.984855310	-2.826437591
C	-0.091289653	2.729288675	-2.274923892
N	-0.290664532	2.463510053	-0.971540155
C	-0.721763726	3.460525933	-0.180371552
C	-0.964218083	4.744067428	-0.656029487
H	-0.933978741	6.016639396	-2.407507775
H	-0.130693726	4.141580513	-3.891281881
H	0.254629159	1.896126122	-2.887437762
H	-0.867070533	3.229202010	0.877424875
H	-1.305182061	5.513349810	0.038838551
C	-4.484735984	1.488007048	1.839179278
C	-3.482584734	1.016116671	2.678719973
C	-2.259319576	0.655631180	2.124455754
N	-1.976852931	0.755180184	0.820978099
C	-2.962129491	1.181629608	0.013779342
C	-4.218075387	1.556138645	0.474613804
H	-5.456300999	1.789006163	2.237915860
H	-3.632161473	0.930143302	3.756244388
H	-1.475704968	0.261121487	2.766088090
H	-2.725611809	1.225697743	-1.050498370
H	-4.970881131	1.899554143	-0.237026285
H	-0.888680756	0.041427445	-1.471130083
H	1.242147308	0.289422347	-1.269277210
C	-0.254637632	-3.805774373	-0.235053861
C	1.086573552	-3.700451432	-0.342831603
H	-0.911474034	-4.671091885	-0.227471974
H	1.861789562	-4.453624399	-0.452342025
C	0.254114535	-1.587714149	-0.157420103
N	-0.748616164	-2.518486034	-0.129581887
N	1.386358285	-2.350751901	-0.299216216
C	-2.166648395	-2.311742192	-0.070714951
C	-2.808374760	-2.395181051	1.170957993
C	-2.883965270	-2.189282285	-1.274019331
C	-4.200587756	-2.268485757	1.197613354
C	-4.271248434	-2.068627533	-1.191546972
C	-4.949618313	-2.094633319	0.032587243
H	-4.715157628	-2.322947918	2.161117360
H	-4.843866981	-1.971777307	-2.118607642
C	2.745097364	-1.924680124	-0.476130876
C	3.188800274	-1.601556087	-1.771602190
C	3.630028709	-1.977828369	0.614518696
C	4.521750773	-1.211201531	-1.924826637
C	4.950915189	-1.570948893	0.406371715
C	5.413914865	-1.162436175	-0.847532356

H	4.878098717	-0.945845483	-2.924017436
H	5.642914039	-1.581557431	1.253247129
C	-2.042192346	-2.669380101	2.432727426
H	-1.061379773	-2.172906710	2.438418748
H	-2.607265085	-2.345832119	3.317767035
H	-1.851824016	-3.749627191	2.548659493
C	-2.197581261	-2.246170289	-2.607887154
H	-2.917526305	-2.104727719	-3.424641360
H	-1.416736610	-1.475587898	-2.698514939
H	-1.706464408	-3.220952422	-2.761599587
C	-6.442534279	-1.952498385	0.080413346
H	-6.835902463	-2.125102679	1.091468029
H	-6.753672732	-0.943251043	-0.234819293
H	-6.932792743	-2.664619157	-0.600753589
C	3.220210060	-2.513905756	1.958757292
H	2.137301865	-2.453524949	2.133660607
H	3.496887374	-3.577879825	2.044427114
H	3.739617687	-1.985249027	2.770774415
C	2.281334265	-1.714555639	-2.961843835
H	1.393938034	-1.071386398	-2.861874019
H	2.809765718	-1.435437988	-3.882693874
H	1.916859445	-2.747342806	-3.084109583
C	6.823297937	-0.681464936	-1.022510651
H	6.932093573	0.339725862	-0.620955089
H	7.535596047	-1.318920179	-0.478560831
H	7.117812022	-0.659144388	-2.080504578
C	1.518907782	0.581731471	1.636935005
C	1.786680217	1.614703972	0.765422373
H	2.120995459	-0.322696737	1.557034754
H	1.392895306	2.601653113	1.033005283
C	0.981366553	0.804246806	3.032199411
H	1.846046480	0.812238578	3.721237541
H	0.346080085	-0.027375773	3.377071024
C	3.002166973	1.666189505	-0.133837155
H	2.804923868	2.273114518	-1.031340497
H	3.287794462	0.662275493	-0.477295087
C	0.274766042	2.065533846	3.210334544
N	-0.288194936	3.072640094	3.301139344
C	4.146479187	2.242274528	0.572209514
N	5.056573481	2.675348045	1.141369962

[Ir(IMes)(Py)$_2$(*trans*-3-hexenedinitrile)]Cl *trans*-3-hexenedinitrile bound through nitrile group

SCF-energy: -1864.6267045
SCF + E(vib0): -1863.9148448

Ir	0.301564943	-0.243352779	-0.514898015
C	-1.645964441	-4.604544692	-1.793562813
C	-0.746299135	-3.937629902	-2.621647916
C	-0.230170153	-2.714322029	-2.213788610
N	-0.560797982	-2.144562288	-1.042565976
C	-1.422889570	-2.794091324	-0.245646815
C	-1.991636217	-4.017883432	-0.579466334
H	-2.072602247	-5.565764213	-2.089624069
H	-0.441227260	-4.353673765	-3.583359493
H	0.472205121	-2.155290134	-2.833043252
H	-1.665169543	-2.308075582	0.701597844
H	-2.706513723	-4.484757997	0.101691442
C	1.245110912	-2.332251743	3.959140259
C	1.942107317	-2.707841804	2.814217089
C	1.653545535	-2.074226816	1.609653780
N	0.723152006	-1.114503295	1.502417524
C	0.052244342	-0.756167391	2.606434404
C	0.280118019	-1.333443872	3.850586505
H	1.449294753	-2.809572632	4.920417402
H	2.708626965	-3.484298856	2.844072232
H	2.185777115	-2.329891522	0.691436800
H	-0.699772373	0.026035510	2.478481932
H	-0.294429062	-1.001283414	4.717173460
H	1.682731464	-0.783834788	-1.031795743
H	0.042928795	0.249369005	-1.992816928
C	2.957873911	3.010825037	-0.124381895
C	1.796875484	3.701675032	-0.098106520
H	3.991749537	3.342941113	-0.092495823
H	1.595394935	4.767668363	-0.038854480
C	1.267311221	1.491642401	-0.252278517
N	2.624972631	1.671705405	-0.214971844
N	0.776393275	2.768143965	-0.173286657
C	3.638836631	0.659220838	-0.248346757
C	4.172484835	0.199451414	0.963475870
C	4.123754479	0.220282772	-1.490850423
C	5.184770554	-0.763624292	0.907682924
C	5.135743149	-0.740660164	-1.490851810
C	5.678068686	-1.249485235	-0.305690922
H	5.607669363	-1.136079925	1.845377230
H	5.517945190	-1.098785725	-2.451194098
C	-0.594407431	3.176908883	-0.130336483
C	-1.283868944	3.402646489	-1.330933683
C	-1.179964182	3.422566864	1.121506029
C	-2.606693229	3.847786745	-1.247577143

C	-2.504074331	3.867313486	1.150803743
C	-3.234815136	4.088863267	-0.021760282
H	-3.155576330	4.031101046	-2.175895545
H	-2.971913518	4.065322135	2.120062334
C	3.699475645	0.742291300	2.281057770
H	2.601738860	0.738965749	2.355223782
H	4.104168846	0.154935891	3.116188159
H	4.024350920	1.786068748	2.423143624
C	3.566502811	0.762110570	-2.772965018
H	4.081306526	0.328151930	-3.640256165
H	2.490857589	0.538736116	-2.856122868
H	3.674626349	1.857165833	-2.828829879
C	6.789963861	-2.257164878	-0.342300949
H	6.859929216	-2.820370446	0.598908994
H	6.657775982	-2.974739149	-1.165116738
H	7.761553209	-1.760198404	-0.499842261
C	-0.404768403	3.234401557	2.393079842
H	0.335921141	4.038884958	2.531677687
H	-1.069612130	3.248584873	3.267436585
H	0.157293746	2.288820430	2.393228758
C	-0.625188513	3.185833542	-2.659678329
H	-0.370109108	2.123759034	-2.800695160
H	-1.283187168	3.498233135	-3.481088846
H	0.314183243	3.754759432	-2.739200229
C	-4.636818318	4.624722125	0.034992671
H	-5.219811740	4.340601431	-0.853056268
H	-5.172776058	4.277538426	0.930809673
H	-4.628801754	5.726663138	0.074691146
C	-5.957572277	-1.052990170	-0.300146769
C	-4.893907120	-0.735288295	0.437303897
H	-6.424166648	-0.304363021	-0.950378405
H	-4.443063963	-1.494748025	1.086306450
C	-6.610732146	-2.409221150	-0.324309912
H	-6.772672201	-2.729535658	-1.367747269
H	-7.616070455	-2.363251935	0.130746474
C	-4.240342456	0.619906858	0.449444589
H	-4.382686897	1.124051404	1.422239069
H	-4.665022185	1.289048309	-0.315504170
C	-5.830867928	-3.439353779	0.351030511
N	-5.161738807	-4.223652253	0.875877318
C	-2.803392551	0.507522755	0.221527244
N	-1.671153537	0.348188491	0.045204496

[Ir(IMes)(Py)$_2$(*cis*-3-hexenedinitrile)]Cl *cis*-3-hexenedinitrile bound through alkene group

SCF-energy: -1864. 5907241
SCF + E(vib0): -1863. 8772883

Ir	-0.218735278	0.442393889	-0.483204007
C	-1.835564749	4.927067478	-1.843022656
C	-1.499963512	3.949170459	-2.774390500
C	-1.021146601	2.725792465	-2.327247245
N	-0.860279384	2.436754888	-1.022413599
C	-1.201381239	3.379451608	-0.129973103
C	-1.686953076	4.628389853	-0.493215062
H	-2.203904548	5.903961658	-2.163656062
H	-1.600876068	4.125152756	-3.846583877
H	-0.755839571	1.934643542	-3.028874728
H	-1.073696288	3.123758791	0.921549791
H	-1.931005956	5.356381862	0.281919619
C	-3.029256143	0.857544676	3.674545216
C	-1.686819443	0.506437936	3.791355833
C	-0.922948957	0.384061697	2.636174064
N	-1.416256503	0.597357853	1.406420304
C	-2.717494632	0.910350183	1.297296018
C	-3.552378292	1.054997096	2.399781750
H	-3.657109233	0.969623502	4.561633651
H	-1.225623405	0.329144767	4.764574708
H	0.129059203	0.100449918	2.696411046
H	-3.095908267	1.047454039	0.282553573
H	-4.600936412	1.317128565	2.248153630
H	-1.584748391	-0.018115044	-1.130418036
H	0.281247262	0.227334329	-1.965807335

C	-0.499939301	-3.775864053	-0.153558887
C	0.835891738	-3.693007003	0.020420103
H	-1.169183270	-4.630939027	-0.185849124
H	1.592884285	-4.456998227	0.173806209
C	0.057066485	-1.566354005	-0.237018093
N	-0.962824611	-2.484357192	-0.312581461
N	1.163433219	-2.349789259	-0.033895570
C	-2.359159384	-2.267084967	-0.572074288
C	-3.263341689	-2.312229030	0.496811678
C	-2.792592070	-2.157553976	-1.907337975
C	-4.624403058	-2.150606381	0.210167544
C	-4.158421786	-2.000964178	-2.136523567
C	-5.092819794	-1.982630224	-1.092841191
H	-5.340611862	-2.175781878	1.036727452
H	-4.508135090	-1.907006906	-3.168582930
C	2.549249012	-1.979425426	0.020096168
C	3.271539370	-1.949049763	-1.189264684
C	3.174925977	-1.787625524	1.260125513
C	4.632520012	-1.650176607	-1.128595036
C	4.539932298	-1.479748211	1.262320609
C	5.285253809	-1.397996088	0.085319978
H	5.205705213	-1.622890752	-2.059668684
H	5.035586941	-1.307363388	2.221837486
C	-2.819483355	-2.593601607	1.902798777
H	-1.815731419	-2.201674695	2.113333316
H	-3.521236100	-2.165114215	2.631367151
H	-2.785551684	-3.679989291	2.089949222

C	-1.823486765	-2.220680456	-3.049185043
H	-2.352682038	-2.249517642	-4.010531752
H	-1.154496537	-1.345327569	-3.048523402
H	-1.184218296	-3.115411073	-2.987000562
C	-6.556265355	-1.820250026	-1.383223370
H	-7.155769065	-1.811019349	-0.462805081
H	-6.753208437	-0.883863957	-1.928387968
H	-6.925576877	-2.641956453	-2.016912258
C	2.447765225	-1.936157037	2.567063151
H	1.357975445	-1.978182320	2.440883185
H	2.752543094	-2.867177238	3.072345258
H	2.697032380	-1.110889210	3.251496088
C	2.598441361	-2.226216095	-2.502347059
H	1.777291147	-1.517294421	-2.693842023
H	3.314408495	-2.155282387	-3.331588346
H	2.158000506	-3.235939754	-2.525173776
C	6.741768609	-1.041076586	0.118061751
H	6.874352202	0.052910507	0.081743274
H	7.223020889	-1.393856906	1.040922166
H	7.282107090	-1.466548889	-0.739097561
C	1.990489231	1.138464340	-0.564639607
C	1.610229630	1.211860007	0.766089147
H	2.471328631	0.207919943	-0.863461343
H	1.834917555	0.319379933	1.354135475
C	2.400241346	2.242186955	-1.515642870
H	2.114430168	1.964497172	-2.543168263
H	3.505447075	2.267509123	-1.514299267

C	1.516617561	2.467207139	1.609296701
H	0.642828917	2.443048488	2.281569056
H	1.434547530	3.385657195	1.012098882
C	1.954443815	3.611055921	-1.290125910
N	1.631692213	4.712331340	-1.138293289
C	2.704352870	2.562081121	2.457414968
N	3.645270209	2.577998979	3.131139359

[Ir(IMes)(Py)$_2$(*cis*-3-hexenedinitrile)]Cl *cis*-3-hexenedinitrile bound through nitrile group

SCF-energy: -1864. 6219416
SCF + E(vib0): -1863. 9097439

Ir	0.288969784	-0.304118975	-0.419197854
C	-1.571359519	-4.740196073	-1.558786098
C	-0.765886070	-4.036279522	-2.450260751
C	-0.277296504	-2.789477317	-2.080882262
N	-0.551642797	-2.227571460	-0.891678714
C	-1.329810721	-2.906487281	-0.036028562
C	-1.857121149	-4.159298738	-0.326729321
H	-1.967367159	-5.724432624	-1.819586073
H	-0.510069114	-4.443647413	-3.429811941
H	0.358573335	-2.204801614	-2.746663268
H	-1.531180683	-2.421753988	0.921498450
H	-2.479257103	-4.668018434	0.411875417
C	1.379642353	-2.202981927	4.105061833
C	2.064907168	-2.602512412	2.961023351
C	1.729606932	-2.029049393	1.738570719
N	0.764915373	-1.105875239	1.613597558
C	0.103739352	-0.725434993	2.716371109

C	0.377960246	-1.243177833	3.977523750
H	1.621842531	-2.631371384	5.080524504
H	2.859334312	-3.349717281	3.005609281
H	2.252443796	-2.302472071	0.819937509
H	-0.677395484	0.024920745	2.572223042
H	-0.188879696	-0.894392155	4.842718026
H	1.669776179	-0.828852632	-0.950873328
H	-0.005250444	0.155729906	-1.901258538
C	2.920551008	2.985281413	-0.194072623
C	1.755117340	3.664182126	-0.115717454
H	3.951239929	3.327571864	-0.219917053
H	1.544267580	4.728395870	-0.058133640
C	1.240551987	1.448875454	-0.216962460
N	2.597078963	1.642078539	-0.251458509
N	0.741814649	2.720517663	-0.126471246
C	3.621929979	0.642680731	-0.316370137
C	4.218623577	0.212373594	0.876900614
C	4.057420693	0.191012206	-1.572620760
C	5.243797429	-0.734817026	0.790268462
C	5.084825355	-0.752845639	-1.603532961
C	5.689773086	-1.232373526	-0.436534447
H	5.715764320	-1.084160504	1.713313819
H	5.429387066	-1.120278968	-2.574570175
C	-0.626133671	3.127739776	-0.008136190
C	-1.382711555	3.349596967	-1.168820497
C	-1.134757792	3.389329188	1.273191211
C	-2.691337914	3.815905805	-1.014878385

C	-2.448105470	3.856155847	1.374310474
C	-3.240610912	4.083352696	0.244453843
H	-3.301986599	3.980092911	-1.906820159
H	-2.856436252	4.069308623	2.366976708
C	3.799839121	0.772425176	2.205676688
H	2.705890727	0.783932622	2.320200900
H	4.228621561	0.188537858	3.031248432
H	4.142594184	1.813417760	2.325170049
C	3.432761246	0.701724529	-2.836122984
H	3.922718026	0.271398130	-3.719496987
H	2.361016558	0.449187520	-2.870757138
H	3.507039708	1.798499375	-2.908472087
C	6.817534700	-2.220424054	-0.508328491
H	6.944927778	-2.762458781	0.439305225
H	6.658713224	-2.957304421	-1.309079377
H	7.770409641	-1.709280239	-0.724150299
C	-0.289250343	3.207856730	2.500774392
H	0.453850349	4.016670838	2.597008206
H	-0.905874698	3.222861900	3.409875272
H	0.276300190	2.264725762	2.475262582
C	-0.807054700	3.105186109	-2.531391778
H	-0.562298416	2.040311698	-2.669445195
H	-1.514837181	3.404672010	-3.315160652
H	0.126796494	3.669991455	-2.680238527
C	-4.628433356	4.642268103	0.370264236
H	-5.281396705	4.282941706	-0.438103209
H	-5.085506967	4.388184388	1.338142368

H	-4.606299677	5.742819687	0.304129288
C	-6.031596337	-0.801455861	-0.760726734
C	-5.076447770	-0.547416909	0.139054880
H	-6.503956565	-1.787576088	-0.694234242
H	-4.856485943	-1.348933293	0.852090324
C	-6.616958372	0.014743339	-1.880081505
H	-7.708524404	0.092401095	-1.729102187
H	-6.500409458	-0.544582541	-2.825538783
C	-4.266641126	0.708094680	0.335000854
H	-4.466335681	1.137860623	1.332650805
H	-4.505016622	1.497818058	-0.391157747
C	-6.112238383	1.363213315	-2.105259590
N	-5.730028827	2.437725648	-2.300328834
C	-2.831988893	0.463770354	0.244515937
N	-1.696412506	0.269731301	0.137273907

[Ir(IMes)(CO)$_2$]Cl

SCF-energy: -1713.1197939
SCF + E(vib0): -1712.6996611

Ir	-0.075704140	0.371587952	-0.443745196
C	-0.762838855	-3.875137483	-0.540939240
C	0.489710808	-3.873296803	-0.021704729
H	-1.432538848	-4.689586450	-0.801945207
H	1.149207998	-4.685990780	0.269219052
C	-0.124316881	-1.723196971	-0.318534234
N	-1.123321430	-2.551584965	-0.711004187
N	0.861899625	-2.548750840	0.111296972
C	-2.407403072	-2.149049949	-1.213366797
C	-3.453555325	-1.936154957	-0.302932633
C	-2.592772068	-2.054982269	-2.602116719
C	-4.698274963	-1.565759998	-0.818415093
C	-3.857141149	-1.679264517	-3.060601730
C	-4.917678011	-1.417312540	-2.189310845
H	-5.523688499	-1.394652281	-0.121200302
H	-4.015743910	-1.594806341	-4.139548605

C	2.124436381	-2.142798493	0.663554006
C	3.247601952	-2.091750557	-0.178207847
C	2.209015072	-1.883329018	2.039763301
C	4.464302074	-1.710324713	0.391218909
C	3.452514856	-1.508915677	2.555362994
C	4.587005493	-1.401603971	1.748502333
H	5.346881755	-1.657101939	-0.252533427
H	3.534253156	-1.301058209	3.626208192
C	-3.267145553	-2.095084221	1.178264639
H	-2.840700542	-1.185797911	1.628796349
H	-4.231715110	-2.281146423	1.670238076
H	-2.592316362	-2.927549811	1.425810840
C	-1.481169004	-2.346391682	-3.563476864
H	-1.845820453	-2.315250902	-4.598874759
H	-0.668618915	-1.607610446	-3.457698629
H	-1.040547260	-3.340827489	-3.388403286
C	-6.253402954	-0.976003305	-2.713919098
H	-7.069849799	-1.259724904	-2.034330757
H	-6.284431120	0.120951446	-2.823760657
H	-6.462478822	-1.407482257	-3.703699585
C	1.019236366	-2.000351063	2.947504836
H	1.340817783	-2.144643046	3.988059134
H	0.401410270	-1.089946533	2.919270769
H	0.367635569	-2.842573623	2.672070750
C	3.152863693	-2.430616273	-1.634774041
H	2.502994301	-1.709698279	-2.158644160
H	4.145430109	-2.407159127	-2.103994534
H	2.726487386	-3.433912387	-1.793763911
C	5.900922847	-0.952732111	2.319778283
H	6.015778652	0.139491202	2.217914558
H	5.980924572	-1.191590407	3.390104549
H	6.749546060	-1.418651141	1.798017189
C	-0.823459755	0.579771452	1.210117437
O	-1.294776314	0.726094078	2.254220128
C	0.039702428	2.250573843	-0.706982704
O	0.119757579	3.374984023	-0.884374412
Cl	0.900084986	0.146719017	-2.615724295

[Ir(IMes-d_{22})(CO)$_2$]Cl

SCF-energy: -1713.1197939
SCF + E(vib0): -1712.7703845

Ir	-0.075704145	0.371587978	-0.443745228
C	-0.762838914	-3.875137779	-0.540939282

C	0.489710845	-3.873297099	-0.021704729
H	-1.432538959	-4.689586810	-0.801945266
H	1.149208088	-4.685991140	0.269219074
C	-0.124316891	-1.723197104	-0.318534260
N	-1.123321515	-2.551585161	-0.711004240
N	0.861899693	-2.548751035	0.111296982
C	-2.407403257	-2.149050113	-1.213366892
C	-3.453555589	-1.936155105	-0.302932655
C	-2.592772264	-2.054982428	-2.602116915
C	-4.698275323	-1.565760120	-0.818415156
C	-3.857141445	-1.679264644	-3.060601963
C	-4.917678386	-1.417312651	-2.189311014
H	-5.523688923	-1.394652387	-0.121200312
H	-4.015744217	-1.594806463	-4.139548923
C	2.124436545	-2.142798657	0.663554059
C	3.247602201	-2.091750716	-0.178207863
C	2.209015241	-1.883329161	2.039763454
C	4.464302413	-1.710324846	0.391218941
C	3.452515121	-1.508915794	2.555363190
C	4.587005842	-1.401604077	1.748502465
H	5.346882162	-1.657102066	-0.252533448
H	3.534253426	-1.301058309	3.626208467
C	-3.267145802	-2.095084379	1.178264729
H	-2.840700759	-1.185798001	1.628796476
H	-4.231715433	-2.281146598	1.670238203
H	-2.592316558	-2.927550033	1.425810946
C	-1.481169115	-2.346391861	-3.563477134
H	-1.845820596	-2.315251077	-4.598875108
H	-0.668618968	-1.607610568	-3.457698894
H	-1.040547340	-3.340827743	-3.388403546
C	-6.253403431	-0.976003379	-2.713919304
H	-7.069850338	-1.259724999	-2.034330910
H	-6.284431601	0.120951456	-2.823760874
H	-6.462479314	-1.407482363	-3.703699866
C	1.019236446	-2.000351216	2.947505064
H	1.340817883	-2.144643210	3.988059441
H	0.401410302	-1.089946618	2.919270991
H	0.367635596	-2.842573840	2.672070957
C	3.152863932	-2.430616459	-1.634774168
H	2.502994492	-1.709698411	-2.158644324
H	4.145430426	-2.407159312	-2.103994692
H	2.726487592	-3.433912651	-1.793764049
C	5.900923296	-0.952732185	2.319778458
H	6.015779112	0.139491213	2.217914727
H	5.980925027	-1.191590497	3.390104808

H	6.749546573	-1.418651247	1.798017327
C	-0.823459819	0.579771494	1.210117527
O	-1.294776415	0.726094131	2.254220303
C	0.039702433	2.250574017	-0.706982757
O	0.119757590	3.374984283	-0.884374481
Cl	0.900085055	0.146719028	-2.615724497

Ligands

MeCN

SCF-energy: -132.4921811
SCF + E(vib0): -132.4467809

N	3.549862271	2.112563390	-2.236035740
C	3.618907604	2.010891956	-1.085719275
H	4.755926364	1.930346602	0.682902298
C	3.706661507	1.879005777	0.358733475
H	3.146635208	2.686925608	0.851008755
H	3.286950117	0.914611076	0.679075971

Pyridine

SCF-energy: -247.8110426
SCF + E(vib0): -247.7215867

H	3.651501843	2.709308324	-3.324664712
C	3.584513036	2.682770921	-2.230414206
N	2.499774697	2.107276337	-1.718059015
C	2.391502597	2.060514463	-0.392742395
H	1.489092618	1.581792603	0.006163110
H	3.208771386	2.512960630	1.558831607
H	5.257655988	3.601349667	0.578284326
C	4.482188175	3.181128918	-0.067511317
C	3.350352082	2.580059146	0.477786534
C	4.604030575	3.234777162	-1.453835999
H	5.472683322	3.695687508	-1.929532775

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