Supporting Information for

Practically Convenient and Industrially-aligned Methods for Iridium-catalysed Hydrogen Isotope Exchange Processes

A. R. Cochrane,[a] C. Idziak,[a] W. J. Kerr,[a]* B. Mondal,[a] L. C. Paterson,[a] T. Tuttle,[a] S. Andersson[b] and G. N. Nilsson[b]

[a]*Department of Pure and Applied Chemistry, WestCHEM, University of Strathclyde, 295 Cathedral Street, Glasgow G1 1XL, U.K.; Tel: (+44)-141-548-2959; Fax: (+44)-141-548-4822; E-mail: w.kerr@strath.ac.uk*

[b]*Medicinal Chemistry, AstraZeneca, R&D Mölndal, SE-431 83 Mölndal, Sweden.*

General

All solvents were purified prior to their use. Dichloromethane and 2-methyltetrahydrofuran were dried by heating to reflux over calcium hydride, and then distilled under nitrogen. Diethyl ether was dried by heating to reflux over sodium wire, and then distilled under nitrogen. Acetone and *tert*-butylmethyl ether were dried by heating to reflux over calcium sulfate, and then distilled under nitrogen. Acetanilide, benzamide, and benzanilide were purified by recrystallisation from ethanol.

IR spectra were obtained on an A2 Technologies ML FTIR machine. ^{1}H and ^{13}C spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz and 100 MHz, respectively. Chemical shifts are reported in ppm. Coupling constants are reported in Hz and refer to $^{3}J_{H\text{-}H}$ interactions unless otherwise specified. Acquisition details for ^{1}H NMR are: Pulse Programme: 30°; Number of Data Points: 32768; Number of Scans: 16; Frequency Width: 8278.146 Hz; Acquisition Time: 1.98 sec; Relaxation Time (D1): 2 sec; and Pulse Length: 4 μsec. For two samples (acetophenone and 2-phenylpyridine) additional spectra were collected where the D1 value was increased ten-fold (to 20 sec) with no changes to the proton integrations used to establish levels of D incorporation.

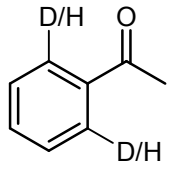
Typical procedure for the deuteration of substrates using iridium(I) complexes:

To a flame-dried, 100 mL, three necked round bottomed flask, fitted with two stopcock valves and a suba seal, was added the iridium(I) complex, substrate, and dry solvent. The suba seal was replaced with a glass stopper, fitted with a Teflon sleeve, and the solution was placed in a dry ice/acetone slurry bath and cooled to -78 °C. The flask was evacuated three times, filled with nitrogen in the first two instances, and with deuterium in the third. The flask was then removed from the slurry bath and placed in a water bath set at 25°C. (NOTE: the glass stopper must be physically restrained as the reaction mixture warms to room temperature). The solution was then stirred vigorously for the allotted reaction time. The flask was evacuated to remove excess deuterium from the system. The contents of the flask and washings were then transferred to a single necked flask, and concentrated *in vacuo*. The catalyst was precipitated from the residue by addition of diethyl ether (~10 mL) and the solution filtered through a short plug of silica. The solvent was then removed under reduced pressure. The level of isotope incorporation achieved was determined by ^{1}H NMR analysis of the reaction products. As such, the relevant integral for the residue proton signal from the site of incorporation was compared against that of a site where exchange would not be expected to occur.

Following the above typical procedure, results are reported as a) amount of substrate, b) amount of catalyst, c) solvent, volume of solvent, d) reaction time, and e) level of incorporation.

***Spectral and experimental details*:**

Acetophenone ***1***:[1]



δ_H(400 MHz, $CDCl_3$): 7.93 (2 H, d, *J* = 7.5 Hz, ArC*H*), 7.54 (1 H, t, *J* = 7.4 Hz, ArC*H*), 7.40 (2 H, t, *J* = 7.4 Hz, ArC*H*), and 2.58 (3 H, s, CH_3).
Incorporation expected at δ_H 7.93.
Determined against integral at δ_H 2.58.

Table 1, Entry 1, Run 1

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) Et_2O, 4 ml, d) 16 h, and e) 93%.

Table 1, Entry 1, Run 2

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) Et_2O, 4 ml, d) 16 h, and e) 94%.

Table 1, Entry 2, Run 1

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 16 h, and e) 90%.

Table 1, Entry 2, Run 2

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 16 h, and e) 92%.

Table 1, Entry 3, Run 1

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) acetone, 2.5 ml, d) 16 h, and e) 41%.

Table 1, Entry 3, Run 2

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) acetone, 2.5 ml, d) 16 h, and e) 45%.

Table 1, Entry 4, Run 1

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) 2-MeTHF, 2.5 ml, d) 16 h, and e) 95%.

Table 1, Entry 4, Run 2

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) 2-MeTHF, 2.5 ml, d) 16 h, and e) 94%.

Table 2, Entry 1

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.0065 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 2 h, and e) 92%.

Table 2, Entry 2

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 97%.

Table 2, Entry 3

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.01 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 91%.

Table 2, Entry 4

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 94%.

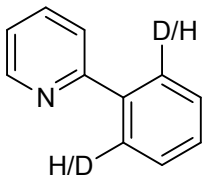
Table 2, Entry 5

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2a**, 0.0065 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 2 h, and e) 95%.

Table 2, Entry 6

a) acetophenone, 0.026 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 96%.

*2-Phenylpyridine **11***:[2]



δ_H(400 MHz, $CDCl_3$): 8.71 (1 H, d, *J* = 4.7 Hz, ArC*H*), 8.01 (2 H, d, *J* = 6.9 Hz, ArC*H*), 7.75-7.71 (2 H, m, ArC*H*), 7.51-7.41 (3 H, m, ArC*H*), and 7.27-7.22 (1 H, m, ArC*H*).

Incorporation expected at δ_H 8.01.

Determined against integral at δ_H 7.75-7.71.

Figure 2 (Et_2O)

a) 2-phenylpyridine, 0.033 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 96%.

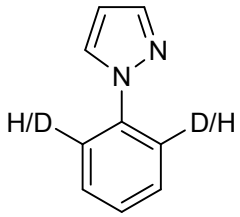
Figure 2 (t-BuOMe)

a) 2-phenylpyridine, 0.033 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 97%.

Figure 2 (2-MeTHF)

a) 2-phenylpyridine, 0.033 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 96%.

N-*Phenylpyrazole **12***:[3]



δ_H(400 MHz, $CDCl_3$): 7.92 (1 H, d, *J* = 4.0 Hz, ArC*H*), 7.75-7.70 (3 H, m, ArC*H*), 7.45 (2 H, t, *J* = 8.0 Hz, ArC*H*), 7.29 (1 H, t, *J* = 8.0 Hz, ArC*H*), and 6.47 (1 H, t, *J* = 2.0 Hz, ArC*H*).
Incorporation expected at δ_H 7.75-7.70.
Determined against integral at δ_H 6.47.

Figure 2 (Et_2O)

a) *N*-phenylpyrazole, 0.031 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 94%.

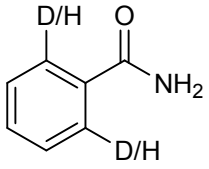
Figure 2 (t-BuOMe)

a) *N*-phenylpyrazole, 0.031 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.001 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 82%.

Figure 2 (2-MeTHF)

a) *N*-phenylpyrazole, 0.031 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 94%.

*Benzamide **13***:[4]



δ_H(400 MHz; [D_6]acetone): 7.92 (2 H, d, *J* = 7.5 Hz, ArC*H*), 7.49 (1 H, t, *J* = 7.5 Hz, ArC*H*), and 7.41 (2 H, t, *J* = 7.5 Hz, ArC*H*).

Incorporation expected at δ_H 7.92.

Determined against integral at δ_H 7.49.

Figure 2 (Et_2O)

a) benzamide, 0.026 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) Et_2O, 4 ml, d) 16 h, and e) 29%.

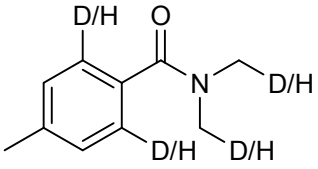
Figure 2 (t-BuOMe)

a) benzamide, 0.026 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 16 h, and e) 57%.

Figure 2 (2-MeTHF)

a) benzamide, 0.026 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) 2-MeTHF, 2.5 ml, d) 16 h, and e) 89%.

N,N,*4-Trimethylbenzamide **14***:[5]



δ_H(400 MHz, $CDCl_3$): 7.33 (2 H, d, *J* = 8.1 Hz, ArC*H*), 7.20 (2 H, d, *J* = 7.9 Hz, ArC*H*), 3.05 (6 H, br s, NCH_3), and 2.38 (3 H, s, CH_3).

Incorporation expected at δ_H 7.33 and 3.05.

Determined against integral at δ_H 2.38.

Figure 2 (Et_2O)

a) *N*,*N*,4-trimethylbenzamide, 0.035 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 83% at δ_H 7.33 (*ortho*) and 13% at δ_H 3.05 (NMe).

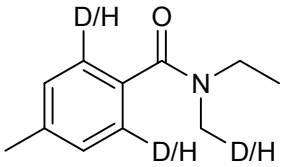
Figure 2 (t-BuOMe)

a) *N*,*N*,4-trimethylbenzamide, 0.035 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 96% at δ_H 7.33 (*ortho*) and 18% at δ_H 3.05 (NMe).

Figure 2 (2-MeTHF)

a) *N*,*N*,4-trimethylbenzamide, 0.035 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 95% at δ_H 7.33 (*ortho*) and 22% at δ_H 3.05 (NMe).

N-*Ethyl*-N*,4-dimethylbenzamide **15***:



FTIR (DCM): 3682, 3445, 3046, 2980, 2930, 2874, 1910, 1613, 1516 cm^{-1}.

δ_H(400 MHz, [D_6]acetone): 7.28 (2 H, d, *J* = 8.0 Hz, ArC*H*), 7.23 (2 H, d, *J* = 7.9 Hz, ArC*H*), 3.38 (2 H, br s, NCH_2), 2.96 (3 H, s, NCH_3), 2.35 (3 H, s, CH_3), and 1.12 (3 H, br s, NCH_2CH_3).

Incorporation expected at δ_H 7.28 and 2.96.

Determined against integral at δ_H 2.35.

δ_C(100 MHz, $CDCl_3$): 171.3, 138.7, 133.4, 128.4, 126.0, 45.4, 36.3, 20.8, and 11.6.

HRMS (ESI): m/z calcd for $C_{11}H_{16}NO$ $[M+H]^+$: 178.1226; found 178.1226.

Figure 2 (Et_2O)

a) *N*-ethyl-*N*,4-dimethylbenzamide, 0.038 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 91% at δ_H 7.28 (*ortho*) and 22% at δ_H 2.96 (NMe).

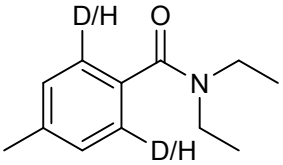
Figure 2 (t-BuOMe)

a) *N*-ethyl-*N*,4-dimethylbenzamide, 0.038 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 95% at δ_H 7.28 (*ortho*) and 31% at δ_H 2.96 (NMe).

Figure 2 (2-MeTHF)

a) *N*-ethyl-*N*,4-dimethylbenzamide, 0.038 g, 0.215 mmol, b) complex **2b**, 0.0068 g, 0.0065 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 91% at δ_H 7.28 (*ortho*) and 17% at δ_H 2.96 (NMe).

N,N-*Diethyl-4-methylbenzamide* ***16***:[6]



δ_H(400 MHz, [D_6]acetone): 7.27-7.22 (4 H, m, ArC*H*), 3.38 (4 H, br s, NCH_2CH$_3$), 2.36 (3 H, s, ArCH_3), and 1.14 (6 H, s, NCH$_2$CH_3).

Incorporation expected at δ_H 7.27-7.22.

Determined against integral at δ_H 2.36.

Figure 2 (Et_2O)

a) *N*,*N*-diethyl-4-methylbenzamide, 0.041 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) Et_2O, 4 ml, d) 16 h, and e) 74%.

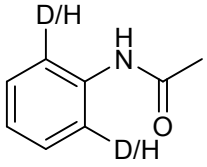
Figure 2 (t-BuOMe)

a) *N*,*N*-diethyl-4-methylbenzamide, 0.041 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 16 h, and e) 54%.

Figure 2 (2-MeTHF)

a) *N*,*N*-diethyl-4-methylbenzamide, 0.041 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) 2-MeTHF, 2.5 ml, d) 16 h, and e) 85%.

*Acetanilide **17***:[7]



δ_H(400 MHz, MeOD): 7.50 (2 H, d, *J* = 7.9 Hz, ArC*H*), 7.32 (2 H, t, *J* = 7.9 Hz, ArC*H*), 7.11 (1 H, t, *J* = 7.4 Hz, ArC*H*), and 2.12 (3 H, s, CH_3).

Incorporation expected at δ_H 7.50.

Determined against integral at δ_H 2.12.

Figure 2 (Et_2O)

a) acetanilide, 0.029 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) Et_2O, 4 ml, d) 16 h, and e) 51%.

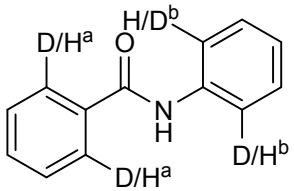
Figure 2 (t-BuOMe)

a) acetanilide, 0.029 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 16 h, and e) 57%.

Figure 2 (2-MeTHF)

a) acetanilide, 0.029 g, 0.215 mmol, b) complex **2b**, 0.011 g, 0.01 mmol, 5 mol%, c) 2-MeTHF, 2.5 ml, d) 16 h, and e) 70%.

*Benzanilide **18***:[8]



δ_H(400 MHz, [D_6]acetone): 9.50 (1 H, s, N*H*), 7.99 (2 H, dd, *J* = 7.0 Hz, ^4J = 1.5 Hz, ArC*H*), 7.86 (2 H, d, *J* = 8.0 Hz, ArC*H*), 7.60-7.50 (3 H, m, ArC*H*), 7.36 (2 H, t, *J* = 7.0 Hz, ArC*H*), and 7.11 (1 H, t, *J* = 7.3 Hz, ArC*H*).

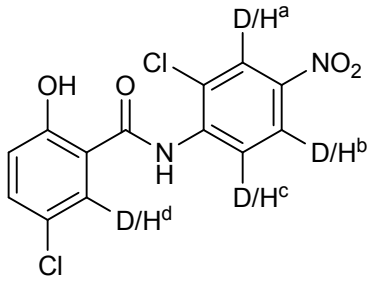
Incorporation expected at δ_H 7.99 and 7.86.

Determined against integral at δ_H 7.11.

Scheme 5

a) benzanilide, 0.042 g, 0.215 mmol, b) complex **2b**, 0.0065 g, 0.0068 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 93% at δ_H 7.99 (D^a) and 12% at δ_H 7.86 (D^b).

*Niclosamide **20***:[9]



δ_H(400 MHz, [D_6]DMSO): 11.37 (1 H, br s, ArO*H*), 8.81 (1 H, d, *J* = 9.2 Hz, ArC*H*), 8.41 (1 H, d, ^4J = 2.8 Hz, ArC*H*), 8.29 (1 H, dd, *J* = 9.2 Hz, ^4J = 2.8 Hz, ArC*H*), 7.95 (1 H, d, ^4J = 2.8 Hz, ArC*H*), 7.53 (1 H, dd, *J* = 8.8 Hz, ^4J = 2.8 Hz, ArC*H*), and 7.08 (1 H, d, *J* = 8.4 Hz, ArC*H*).

Incorporation expected at δ_H 8.81, 8.41, 8.29, and 7.95.

Determined against integral at δ_H 7.53.

Table 6, Entry 1

a) Niclosamide, 0.016 g, 0.05 mmol, b) complex **2b**, 0.0026 g, 0.0025 mmol, 5 mol%, c) DCM, 2.5 ml, d) 1 h, and e) 40% at δ_H 8.81 (D^c), 55% at δ_H 8.41 (D^a), 44% at δ_H 8.29 (D^b), and 58% at δ_H 7.95 (D^d).

Table 6, Entry 2

a) Niclosamide, 0.016 g, 0.05 mmol, b) complex **2b**, 0.0016 g, 0.0015 mmol, 3 mol%, c) Et_2O, 4 ml, d) 1 h, and e) 63% at δ_H 8.81 (D^c), 75% at δ_H 8.41 (D^a), 70% at δ_H 8.29 (D^b), and 76% at δ_H 7.95 (D^d).

Table 6, Entry 3

a) Niclosamide, 0.016 g, 0.05 mmol, b) complex **2b**, 0.0026 g, 0.0025 mmol, 5 mol%, c) *t*-BuOMe, 4 ml, d) 2 h, and e) 37% at δ_H 8.81 (D^c), 83% at δ_H 8.41 (D^a), 48% at δ_H 8.29 (D^b), and 87% at δ_H 7.95 (D^d).

Table 6, Entry 2

a) Niclosamide, 0.016 g, 0.05 mmol, b) complex **2b**, 0.0016 g, 0.0015 mmol, 3 mol%, c) 2-MeTHF, 2.5 ml, d) 1 h, and e) 28% at δ_H 8.81 (D^c), 89% at δ_H 8.41 (D^a), 55% at δ_H 8.29 (D^b), and 97% at δ_H 7.95 (D^d).

Theoretical details

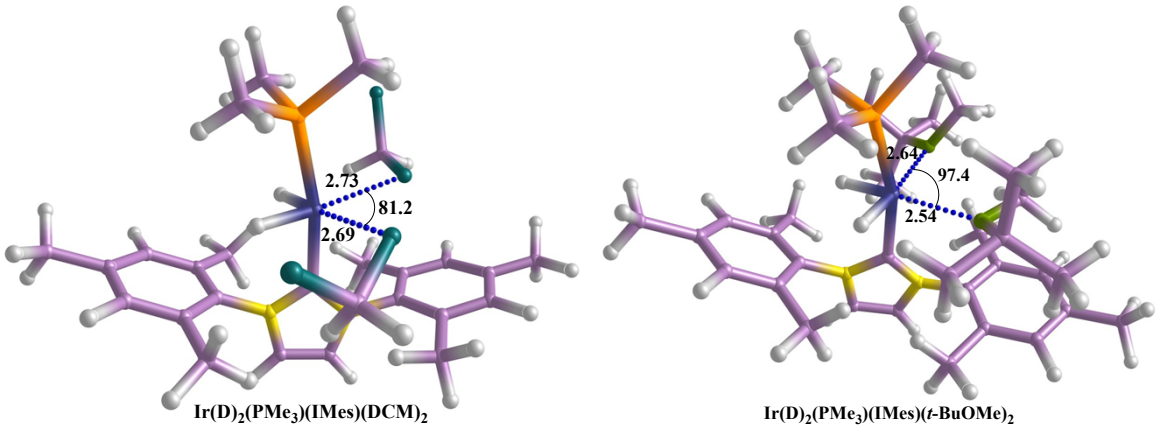
All of the geometry optimisations have been performed at Density Functional Theory (DFT) level with M06 density functional.[10] In conjunction with M06 functional, valence double-ζ basis set 6-31G(*d*,*p*) with polarisation on all atoms[11] was used for main group elements. Stuttgart RSC effective core potential and the associated basis set was used for Ir.[12] Consecutive frequency calculations were also performed at the same level of theory to characterise the structures as minima. All calculations were performed in Gaussian 09 suite of the quantum chemistry program.[13]

Solvent and substrate binding enthalpies (ΔH) were calculated according to the following equations, using the absolute enthalpies (H) of the corresponding species as described in Schemes 3 and 4:

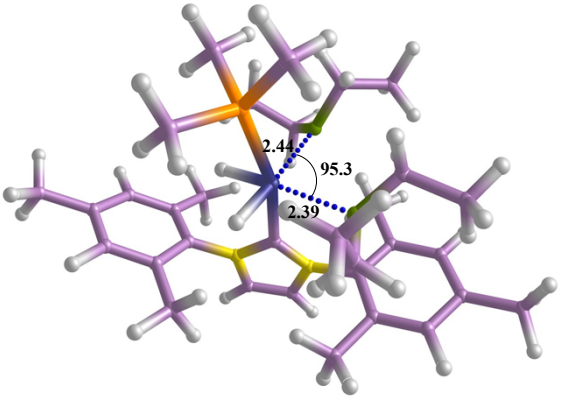
$\Delta H_{sol} = H_{solvent\text{-}complex} - (H_{catalyst} + 2\times H_{solvent})$

$\Delta H_{exc} = (H_{substrate\text{-}complex} + H_{solvent}) - (H_{solvent\text{-}complex} + H_{substrate})$

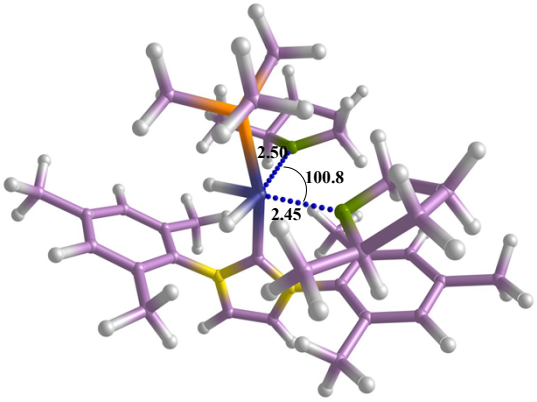
Optimised structures of the Ir species with two solvent molecules coordinated at the metal center (distances are in Å and angles in degrees). H (Grey), C (Purple), N (Yellow), P (Orange), O (Light Green), Cl (Dark Green), and Ir (Blue).



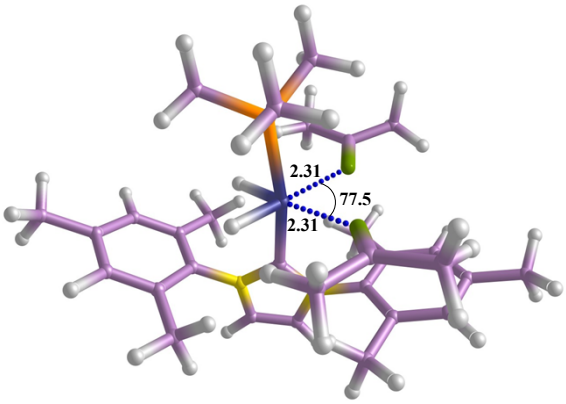
$Ir(D)_2(PMe_3)(IMes)(DCM)_2$ $Ir(D)_2(PMe_3)(IMes)(t\text{-}BuOMe)_2$



$Ir(D)_2(PMe_3)(IMes)(Et_2O)_2$

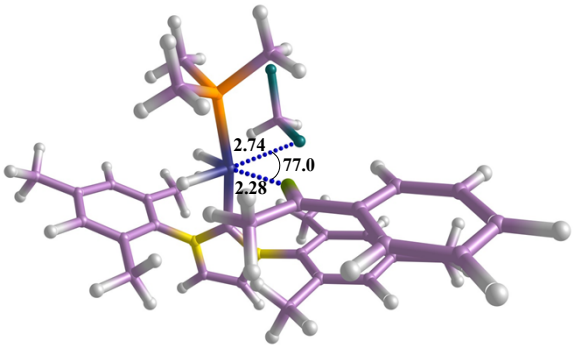


$Ir(D)_2(PMe_3)(IMes)(2\text{-}MeTHF)_2$

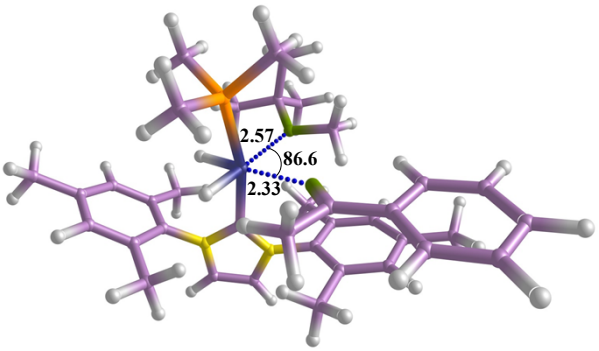


$Ir(D)_2(PMe_3)(IMes)(acetone)_2$

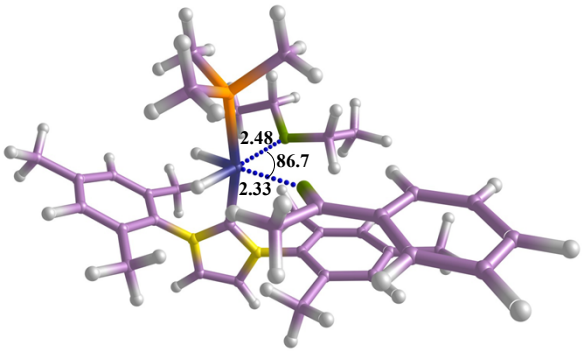
Optimised structures of the Ir species with one solvent and substrate molecule coordinated at the metal center (distances are in Å and angles in degrees). H (Grey), C (Purple), N (Yellow), P (Orange), O (Light Green), Cl (Dark Green), and Ir (Blue).



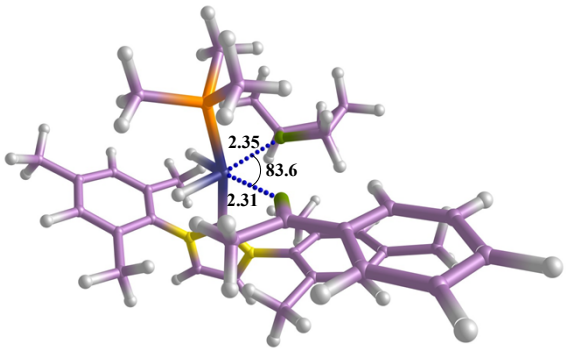
$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(DCM)$



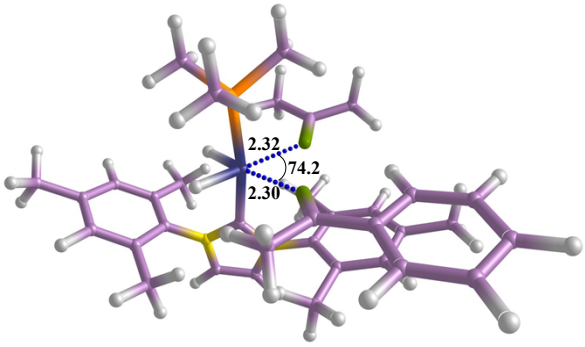
$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(t\text{-}BuOMe)$



$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(Et_2O)$



$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(2\text{-}MeTHF)$



$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(acetone)$

Gas-phase optimised Cartesian coordinates at M06/[6-31G(d,p) for H, C, O, N, P, Cl + Stuttgart RECP and associated basis set for Ir] level of theory for all the species involved.

Solvents

DCM

```
C,-1.5429470296,-2.1502878541,2.7744345052
H,-1.5745572763,-2.1146624405,3.8631828579
H,-1.3925424387,-3.1700670809,2.4208440198
Cl,-3.1035117148,-1.5711711441,2.1538337096
Cl,-0.1702145406,-1.1645664804,2.2251699075
```

t-BuOMe

```
C,-0.8824554837,0.2423461233,-0.0204127743
C,-0.3160079369,1.0444096781,-1.1805969168
H,-0.6211862612,0.612949602,-2.1408447663
H,-0.6706726452,2.0797881179,-1.131450848
H,0.7783912324,1.0557102101,-1.131861821
C,-0.3562137325,-1.1874012978,-0.0690651682
H,0.7341187891,-1.1920957968,0.0456752049
H,-0.7914918317,-1.8168714569,0.7157658301
H,-0.6041755787,-1.6488846498,-1.0321501563
C,-2.4058723024,0.2616642488,-0.0678949521
H,-2.8534484352,-0.3599267283,0.7163002559
```

H,-2.7739483553,1.2878034992,0.0487173325
H,-2.7588874556,-0.1245058489,-1.0313400424
O,-0.3942361972,0.931564357,1.1324864493
C,-0.756734196,0.4227851338,2.3837851599
H,-0.2941607385,1.0702343825,3.1346299089
H,-1.8450875989,0.4329167256,2.5548249422
H,-0.3934267679,-0.6033134327,2.5540916118

Et_2O

O,-0.1226441421,-0.7343966546,-0.1962810539
C,1.2146500766,-0.6569961198,0.2257365398
H,1.2689125175,-0.7083193121,1.3300795889
C,-0.9129695539,0.2926795181,0.3450026748
H,-0.5033516945,1.2799564485,0.0573901982
H,-0.8839064568,0.2527031299,1.450802162
C,-2.3244774289,0.131655033,-0.1592454595
H,-2.7285975579,-0.8402978252,0.1412609497
H,-2.9742838711,0.9167486127,0.2402918981
H,-2.3473052586,0.1845499994,-1.2524092094
H,1.6491495685,0.3191463885,-0.0632368594
C,1.9844477306,-1.7916574706,-0.4008048851
H,1.9382354995,-1.7270428848,-1.4925704766
H,3.0352858368,-1.7666793228,-0.0953344945
H,1.5579123342,-2.7539198701,-0.100142073

2-MeTHF

C,-1.2449372757,0.3699780309,0.1753558633
O,0.1430362366,0.3086684008,-0.0806478338
C,0.7015485689,1.6238225786,-0.0371996441
C,-0.4778933805,2.5786277489,0.195309652
C,-1.6705212207,1.7544448082,-0.2771408367
H,-1.7326139822,-0.4494194811,-0.3651866425
H,-1.453822668,0.2369754538,1.252849997
H,1.4150934155,1.672646236,0.8011419825
H,-0.5829539779,2.8101475804,1.2628875653
H,-0.3553491949,3.525831602,-0.3414847873
H,-2.6253363252,2.0795092196,0.1477378865
H,-1.7539400298,1.7832450724,-1.3713701897
C,1.4325377109,1.8767722158,-1.3381278758
H,1.9852119372,2.8228578834,-1.3019456573
H,2.1410479573,1.0675512162,-1.5411577295
H,0.7218030386,1.9211120838,-2.1732233299

Acetone

```
C,0.3912177301,2.3701535035,2.4629312451
O,0.6889446659,1.6964185375,1.5013232442
C,-1.0423434047,2.6876212851,2.8075632563
H,-1.1997077104,3.773009216,2.8233360321
H,-1.7135268069,2.2291337442,2.0787733613
H,-1.2830822931,2.3215642931,3.8131167456
C,1.4302602379,2.9454475613,3.3924917242
H,1.3495089747,4.0388354466,3.4251323951
H,1.2657408962,2.5885219341,4.4165152206
H,2.4301337102,2.6602494784,3.0597007755
```

Substrate

PhCOMe (1)

```
C,2.9479720888,-2.36986956,-1.0996225441
C,3.9103710685,-1.8671197362,-0.2196458965
C,5.1920751329,-2.3943111258,-0.2030214964
C,5.5267239541,-3.4332945962,-1.0688704189
C,4.5768036802,-3.9411587556,-1.9486806636
C,3.2918113511,-3.4121604938,-1.9648589911
H,3.6198136671,-1.056543412,0.4437174355
H,5.9357042114,-1.9983029594,0.4842311253
H,6.5315734421,-3.8489900732,-1.058172299
H,4.8372885148,-4.751960398,-2.6246560682
H,2.5566559328,-3.817002473,-2.6570652725
C,1.5867567985,-1.7587813936,-1.0678807398
C,0.5382260278,-2.2908786421,-2.0107692367
H,-0.3877344517,-1.7351197524,-1.8537862667
H,0.8559007388,-2.1819161377,-3.0543507509
H,0.3567852356,-3.3578052771,-1.835906181
O,1.3294686071,-0.8518592141,-0.2984577354
```

Catalyst

$Ir(D)_2PMe_3(IMes)$ (8)

```
Ir,-0.3200615983,0.3007417479,-0.2851788206
H,0.9778554754,1.1427042819,-0.396706292
P,-1.5492213918,2.2928091993,-0.312541403
C,1.8385441091,-3.4173423774,-0.1564210942
C,0.5308331826,-3.7609252676,-0.2501668844
H,2.7341891694,-4.0214595171,-0.1174985273
H,0.0505152623,-4.7263642248,-0.3158385985
N,1.9030846123,-2.0272954222,-0.1149558594
N,-0.1721801801,-2.565093542,-0.2638485007
C,0.6665874892,-1.4989200233,-0.1817492102
```

H,-0.0076678296,0.6350433516,1.1983361009
C,-2.193240064,2.8238760705,-1.9422887088
H,-2.7570203662,3.7601179929,-1.8572576165
H,-1.3595830819,2.9715882448,-2.6368335744
H,-2.8510349688,2.0482806094,-2.3500679698
C,-3.045205086,2.2637804298,0.7382393067
H,-3.5759368573,3.222270927,0.6993441908
H,-3.7130085882,1.4638421837,0.3985284145
H,-2.7563560271,2.052230646,1.7730712289
C,-0.647641156,3.7653263098,0.2800241037
H,0.2240546633,3.9437789907,-0.357571146
H,-1.2916349627,4.6520816343,0.2714440801
H,-0.2929504824,3.5852178615,1.3000990229
C,3.1149996247,-1.2620524447,-0.0037024647
C,3.7398980869,-0.8243067504,-1.1735062694
C,3.6057608897,-0.9754495763,1.2735922911
C,4.9133659786,-0.0864000071,-1.0363124585
C,4.780525903,-0.2329427987,1.3562280574
C,5.4508176669,0.2131493684,0.215802984
H,5.4234464807,0.263587307,-1.933829792
H,5.1853587439,0.0042534104,2.3402212925
C,-1.5728750526,-2.2633678973,-0.2791359418
C,-2.391040238,-2.6774553097,0.7834675873
C,-2.0533960565,-1.4280847383,-1.3115885892
C,-3.7169437569,-2.2585386362,0.7784415548
C,-3.3945679632,-1.0225979815,-1.2477046617
C,-4.238495959,-1.4302897261,-0.220344833
H,-4.3647782903,-2.5697067614,1.5980617534
H,-3.7899068576,-0.3964449259,-2.0488873072
C,-1.8497292449,-3.5002532896,1.9121320381
H,-0.8920214026,-3.1043249691,2.2734715223
H,-2.550548925,-3.5077155773,2.7510233147
H,-1.6821692879,-4.5446171047,1.6222539526
C,-1.211053425,-1.0353371162,-2.5018544302
H,-1.8552285735,-0.7685317346,-3.3455285799
H,-0.5545574557,-0.1309353365,-2.3718362417
H,-0.5312998781,-1.8369654173,-2.8091704628
C,-5.6738548881,-1.0048503688,-0.1791275161
H,-5.8854960864,-0.2195278505,-0.911678614
H,-6.3398749476,-1.8482236372,-0.3965081593
H,-5.9492647103,-0.6296212486,0.8130865429
C,3.1542372677,-1.1132428699,-2.5221608279
H,2.9098316878,-2.175383015,-2.6489703531
H,2.2238398205,-0.5482436246,-2.6740896734
H,3.848208122,-0.8306833348,-3.3185254713
C,2.8831427098,-1.4369126711,2.502591859
H,1.8638291535,-1.0292846634,2.5422326321
H,2.792980999,-2.5300065702,2.5402712994
H,3.4077181148,-1.1160612906,3.4066627595

C,6.7339324618,0.9760549356,0.3370325024
H,7.5859819291,0.2926308719,0.4398306195
H,6.9197300053,1.5971430583,-0.5447421221
H,6.73429323,1.624771915,1.2190859039

Catalyst-*bi*-Solvent Complex (9)

$Ir(D)_2(PMe_3)(IMes)(DCM)_2$

C,0.1692460797,0.0762388565,-0.1319359361
C,0.0876393531,0.0962501611,1.2575132601
C,1.2265729499,0.0628176845,2.0640974351
C,2.4691786672,0.0210656805,1.4303098068
C,2.5983909535,-0.0257493639,0.03508778
C,1.433968543,0.0123201297,-0.7238901078
N,3.6689584612,-0.0220732794,2.2202563176
C,4.2146831271,-1.225317839,2.63933304
C,5.370435815,-0.9286899378,3.2701252387
N,5.5061237864,0.4518110069,3.2217014591
C,4.4541879648,1.0402099336,2.5747976569
C,6.7048331141,1.0994661656,3.6703849756
C,6.8120588745,1.5358399709,4.9904397412
C,8.0063403626,2.1530573266,5.3732238802
C,9.0746426459,2.2990783,4.493631315
C,8.9407746735,1.802234195,3.1921577109
C,7.7680226775,1.1951367704,2.7598112045
Ir,3.9870921937,3.0350670554,2.1410959391
Cl,3.8235879906,3.8711129481,4.7000169583
C,2.5218614515,2.9375072668,5.5334785823
Cl,0.9144526578,3.5682730594,5.1947526165
C,5.7329188071,1.2892420573,6.0009385138
C,7.6455795965,0.6383397911,1.372252536
C,10.3531691315,2.9497015289,4.9246592392
C,1.0849454084,0.1017730808,3.5556941795
C,3.9433874419,-0.1068388369,-0.6203322051
C,-1.0663167393,0.075101881,-0.9787905134
P,3.1308265821,5.0927318814,1.3872338313
C,1.3522283427,5.3143053557,1.7451879923
C,3.8526061924,6.6471932391,2.0337724598
C,3.2134029905,5.3205808261,-0.424684025
Cl,6.4567166716,4.191421192,2.362736649
C,7.2142263458,4.0841703,0.7331237395
Cl,7.0255361451,5.5724298969,-0.1957222245
H,2.5336230155,2.5058203224,1.9877847515
H,3.7184705761,-2.1657863035,2.4449069589
H,6.1145552835,-1.5503809207,3.748277411
H,4.1026195694,2.6327149861,0.6371993584
H,3.322039003,7.5131732928,1.6207462601

H,3.7691140792,6.6699242024,3.1261124621
H,4.9115556067,6.7141148506,1.7640270298
H,2.7597538619,6.2747461332,-0.7167691909
H,4.2588816741,5.3038703499,-0.7532901705
H,2.6794357048,4.4997103876,-0.914805897
H,1.2011382192,5.3418914331,2.8297651453
H,0.9792153841,6.2469649171,1.3059000937
H,0.7877921058,4.4677615424,1.3403754622
H,6.7222466283,3.2627175469,0.2086896667
H,8.2752095038,3.8897621335,0.8988598398
H,2.5907943253,1.9102643108,5.1683250062
H,2.7273905107,3.0122873073,6.6021520386
H,8.1077670348,2.5098829646,6.3984415445
H,9.7819791689,1.8838648518,2.5014627549
H,-0.8922296803,0.1289221564,1.7348419489
H,1.5118932006,-0.0242128931,-1.8108907986
H,11.1944329419,2.250488912,4.8521837612
H,10.5972998967,3.8080548237,4.2879298178
H,10.2991170017,3.3033278445,5.9582859462
H,7.6361610199,-0.4595053084,1.380057725
H,6.7100951497,0.9470631082,0.8850245181
H,8.4878598002,0.9499234276,0.7462023771
H,5.6173579024,2.1456294167,6.6746956192
H,4.7666125993,1.0749302319,5.5305350505
H,5.9854408166,0.422319168,6.625158712
H,1.9819979582,-0.2598814746,4.0719977169
H,0.8789150303,1.1269085444,3.8959640267
H,0.2395607445,-0.5120204685,3.8832806892
H,4.5030142733,0.8313040457,-0.4964674796
H,4.563335597,-0.9043957246,-0.1909740528
H,3.8434934889,-0.2979360113,-1.6925071312
H,-0.9473495544,0.709143276,-1.8639154232
H,-1.2926352389,-0.9366081999,-1.3375994751
H,-1.9393060097,0.4273211204,-0.4208386543

Ir(D)$_2$(PMe$_3$)(IMes)(*t*-BuOMe)$_2$

C,5.1468082497,-1.6092260754,-0.7325901493
C,4.1522507339,-1.9333835359,-1.6581434067
C,2.8554748276,-2.246740607,-1.2658442288
C,2.5458645989,-2.1922009987,0.1034574959
C,3.529467722,-1.9443014978,1.0646448936
C,4.8184957747,-1.6426201431,0.6183157243
N,1.1790880048,-2.433350919,0.4954612694
C,0.7408283691,-3.6803091873,0.9151082299
C,-0.6003913141,-3.6030820402,1.0285999704
N,-0.9696016718,-2.3100194335,0.6692196471
C,0.1324300265,-1.5541268688,0.3517357933
C,-2.3572659149,-2.0467875114,0.3598161969

C,-3.2295986696,-1.5272496288,1.3207760686
C,-4.5744270238,-1.3789960275,0.9773076761
C,-5.0639399603,-1.748057235,-0.2724493259
C,-4.1734879821,-2.3138114702,-1.1852796774
C,-2.8232306746,-2.4795537296,-0.8918034825
Ir,0.4488666483,0.4596778725,-0.0921197018
P,1.3974843379,2.5325547676,-0.701695273
C,2.0997714902,2.4971926936,-2.3986033528
C,-2.7621101216,-1.1276228805,2.6822660535
C,-1.9171243206,-3.1391440833,-1.8842651841
C,-6.4983779429,-1.532525337,-0.6439911244
C,1.8438501277,-2.6581423539,-2.2917213434
C,3.2793630173,-1.9935613066,2.5417766771
C,6.5428923357,-1.3086831052,-1.1849930061
C,0.5105718029,4.1452453321,-0.6637239778
C,2.9144455018,2.9602843958,0.2361085707
O,-1.7430420856,0.7209181433,-1.3665428261
C,-2.7392955984,1.2446056048,-0.5095778389
C,-1.9470723532,0.9706244632,-2.7892535281
C,-1.7307932323,2.4425593914,-3.1059516792
O,-0.4049060926,1.3639595175,2.2446909518
C,0.2992140305,1.1344077336,3.5087887472
C,1.6458103268,1.8393073047,3.4637715883
C,-1.0120230546,2.6376570755,2.1413977526
H,1.0949162974,-0.0397900684,-1.4038112717
H,1.4327517046,-4.4933537722,1.084976682
H,-1.3426265383,-4.3384094358,1.3070211336
H,1.818897045,0.2450221268,0.6082404818
H,1.1089736423,4.9188655063,-1.1595591427
H,-0.4628074314,4.0749342138,-1.1599476402
H,0.3459714958,4.4484433605,0.375459348
H,3.4051338713,3.8340166463,-0.2086388323
H,2.6725082204,3.1825714353,1.279671848
H,3.6023383763,2.1071582131,0.2130457705
H,1.3257144378,2.3471763977,-3.1571396105
H,2.6330756255,3.4305115941,-2.6142320684
H,2.8037173659,1.6585646347,-2.4580798251
H,-2.7966950441,2.3431506225,-0.5645906656
H,-2.4674650292,0.9503901218,0.5085605939
H,-1.2703900603,2.7976242231,1.0922184518
H,-0.3330965156,3.4452637508,2.4528135543
H,1.5399065701,2.9229159446,3.3268578757
H,2.1813541117,1.6873105141,4.4082224475
H,2.258465028,1.4351328256,2.6486850954
H,-1.8520680653,2.6140591506,-4.1816053652
H,-2.4540144371,3.0890548584,-2.5940574003
H,-0.7197909502,2.7563363768,-2.827038784
H,-5.2598698106,-0.966969346,1.7181447778
H,-4.5439377243,-2.6452080401,-2.1567416586

H,4.4028963682,-1.9693034491,-2.7189676921
H,5.5924162709,-1.4429115125,1.3605670229
H,-2.1973829779,-1.9343234211,3.1662150725
H,-2.0987712425,-0.2547877951,2.6271817331
H,-3.609796813,-0.8774512229,3.3274022801
H,-2.3716918477,-3.1491033413,-2.880560047
H,-0.949544036,-2.6307730662,-1.9511077362
H,-1.7101519252,-4.1824911695,-1.6098147462
H,-7.1159383671,-1.3110731835,0.2316383339
H,-6.5966113906,-0.688898612,-1.3402923915
H,-6.9201078597,-2.4098817288,-1.1463661575
H,1.2928864936,-3.5529947876,-1.9759166877
H,1.1030711422,-1.8690745475,-2.479879987
H,2.3334096701,-2.8860739703,-3.2430859218
H,2.3538490711,-2.514725588,2.8033127999
H,4.1073108103,-2.5036707163,3.0457760059
H,3.2193416246,-0.9841812777,2.9688051139
H,7.1051087694,-0.7599964299,-0.4230279492
H,7.0937732786,-2.2338908618,-1.3952312714
H,6.5476719919,-0.7174275703,-2.1069167271
H,-1.9296460137,2.6983575102,2.7432455314
H,-3.7283057688,0.820687248,-0.7234514517
C,0.5028512692,-0.3640154476,3.6158837285
H,1.2216977319,-0.5798989282,4.4148586768
H,-0.4287705684,-0.8812543147,3.8584872563
H,0.8965073604,-0.7634638175,2.6765830073
C,-0.5291013583,1.6158667135,4.6937824928
H,-1.5406211074,1.1926988639,4.6694666276
H,-0.0492654932,1.272602354,5.6170113006
H,-0.6031178921,2.7066749886,4.7550634786
C,-0.9196050065,0.1156940725,-3.5060729444
H,-1.0766663053,-0.9449384764,-3.2763865927
H,-1.0116196088,0.251134148,-4.5894539994
H,0.1000561345,0.3852418804,-3.2094193625
C,-3.3455588421,0.5427255582,-3.2167639906
H,-3.4072104967,0.5686685286,-4.3100912156
H,-3.5553439335,-0.4793551349,-2.8830279776
H,-4.1296234109,1.2059858703,-2.834794639

$Ir(D)_2(PMe_3)(IMes)(Et_2O)_2$

C,0.0091238327,0.2036009488,0.1662321841
C,0.0502748453,0.1197817609,1.5582123933
C,1.2511393751,0.0006542847,2.2555548003
C,2.4358248573,-0.0048303098,1.5114250066
C,2.4370926465,0.0097548648,0.1128872383
C,1.211640755,0.1334483695,-0.538164435
N,3.6926718675,-0.0530810511,2.2064927714
C,4.374306526,-1.2427140981,2.4091613909

C,5.4622379235,-0.9438003394,3.1469680887
N,5.4269352475,0.4259207783,3.3839023985
C,4.3327044567,1.0069716141,2.7981394679
C,6.335608576,0.9898585713,4.3483043314
C,7.5270051438,1.5916666005,3.9303263794
C,8.4234101728,2.0103286839,4.912106868
C,8.1711870061,1.8241384092,6.2721180998
C,6.9794893595,1.2047250728,6.6452051815
C,6.051939008,0.7665299161,5.7003563323
Ir,3.6342050982,2.9696878934,2.6928526637
P,2.3333766775,4.8918906019,2.3360393119
C,0.576480581,4.5484148251,2.7283165745
C,7.8560011921,1.7540075475,2.4800400206
C,4.8220523844,0.0268188646,6.1352782299
C,9.1507290781,2.2989733443,7.3019218138
C,1.2561333362,-0.1353794713,3.7477642238
C,3.7051515216,-0.141630412,-0.6697726097
C,-1.2985998978,0.2992835543,-0.55861243
C,2.5940735668,6.5210825449,3.1538544091
C,2.1986174887,5.4147444287,0.5820334482
O,4.6822949557,3.6118114603,4.7507397274
C,5.505292541,4.7783152289,4.7405954022
C,6.3924082378,4.931137697,5.9542562929
C,3.9365314418,3.3775809533,5.9464288189
C,2.8949503023,4.429361778,6.2472638621
O,5.4471421503,3.7576401,1.2591796985
C,5.697614626,3.014114006,0.0592803157
C,4.641070167,3.2044376869,-1.0020975055
C,5.8254416534,5.1335545198,1.1679691472
C,7.3100944007,5.3432770644,1.364239433
H,2.4185065158,2.4738149349,3.5271490112
H,4.0087804354,-2.1778183473,2.0087275206
H,6.2572610175,-1.5596552436,3.5436500421
H,2.8644528181,2.4879683647,1.4219115409
H,1.8039679953,7.2212953856,2.8568844055
H,2.5754114411,6.4133155179,4.2429502093
H,3.5609986645,6.9467048856,2.8628397654
H,1.4555979877,6.2138885883,0.4752288827
H,3.163880535,5.7795348153,0.2154325691
H,1.895004303,4.5571721806,-0.0278497867
H,0.4566320856,4.3664104456,3.8015944231
H,-0.0672927951,5.3844474245,2.4312736589
H,0.274058443,3.6400139652,2.1945085029
H,4.6376363561,3.2662117195,6.7867097256
H,4.8779736795,5.6755571345,4.5996068302
H,6.1239397151,4.6553555828,3.8424363864
H,3.4627475295,2.4031175882,5.7874900555
H,5.253414869,5.6462478134,1.9508735878
H,5.4947480123,5.5437995165,0.2005250142

H,6.693239533,3.284882914,-0.3235404507
H,5.7527562529,1.9650858053,0.3763233963
H,4.5545694127,4.2502304627,-1.3184960865
H,4.9048520458,2.6198517021,-1.8906153789
H,3.6626920426,2.8639747517,-0.6426311278
H,7.904463329,4.8448271479,0.5905449238
H,7.5457635934,6.4117163882,1.3186486678
H,7.639524227,4.9616042477,2.3385451235
H,7.1171751844,5.7304745397,5.7671557967
H,5.8380079557,5.2013112287,6.8593763969
H,6.9435487253,4.0030766105,6.141397194
H,2.3722830399,4.1748661173,7.175234315
H,3.3335148535,5.4251721065,6.3843341257
H,2.1472779376,4.4824290824,5.4472661749
H,9.3627116803,2.4700468712,4.6023621727
H,6.7727162817,1.0361257758,7.7027417751
H,-0.8841792593,0.129367283,2.1202147536
H,1.1941774211,0.1575965425,-1.6282186472
H,7.6869165049,0.8263002029,1.9186105928
H,7.2288836791,2.5300386278,2.0275577186
H,8.9034165471,2.0429685694,2.3483883525
H,4.5605445153,0.2787598265,7.1682487757
H,3.9570438116,0.2425103419,5.4962667439
H,4.9789606317,-1.0591712211,6.0957144645
H,10.1840541033,2.1335850123,6.9792140697
H,9.0408038384,3.3764355552,7.484404449
H,9.0073764434,1.7899968721,8.2599610432
H,1.916755002,-0.9475640223,4.0768318562
H,1.6080375895,0.7830031831,4.238025789
H,0.2501590398,-0.3491288212,4.1203376363
H,4.5118930753,0.4845096421,-0.2720271583
H,4.0674971036,-1.1775215894,-0.6429782844
H,3.5503290333,0.1217512448,-1.7205766497
H,-1.2084883939,0.8876040455,-1.4776871887
H,-1.6591418011,-0.6959439358,-0.847226242
H,-2.07336252,0.7556670414,0.0656799488

$Ir(D)_2(PMe_3)(IMes)(2\text{-}MeTHF)_2$

C,5.2769444965,-0.8436232282,-0.9336926535
C,4.8103342801,-1.2349105122,0.3225439072
C,3.5321012375,-1.7601536885,0.4959704755
C,2.7090634883,-1.8584990831,-0.6308503657
C,3.1478279672,-1.519470741,-1.9126873498
C,4.4377917248,-1.0054148453,-2.0360962311
N,1.363353962,-2.3189097009,-0.4469255959
C,1.0401016963,-3.6645193245,-0.3818502912
C,-0.2850639186,-3.7332029642,-0.1384929605
N,-0.7419629309,-2.4236115327,-0.058029919

C,0.2681851989,-1.5207641389,-0.243119079
C,-2.1203411325,-2.1247885245,0.1907371969
C,-3.0229594954,-2.1932249819,-0.8718269773
C,-4.3644942944,-1.9166800131,-0.6020670739
C,-4.8063760806,-1.6050055003,0.682888496
C,-3.8762588619,-1.6010305812,1.7261261956
C,-2.5289161421,-1.8784992396,1.5065842436
Ir,0.3161701845,0.5628235794,-0.2776415272
O,-1.9880593453,0.9753374896,-1.0282401505
C,-2.9239283922,1.5622553483,-0.1138032197
C,-4.1548019932,1.9470812182,-0.9309797098
C,-3.605860594,1.9923959058,-2.3497211229
C,-2.6166609377,0.8443650935,-2.3249076693
C,-2.5686656049,-2.5850582912,-2.2457374589
C,-1.5532939932,-1.9662053774,2.6397969824
C,-6.2508755191,-1.3122748388,0.9538916018
C,3.0556880109,-2.2152779251,1.8419890824
C,2.2701766165,-1.6864981527,-3.1145167627
C,6.668706858,-0.3144307605,-1.1010660941
P,0.8294962917,2.8348917023,-0.5112614
C,2.6214481992,3.0994715836,-0.7763849656
C,0.1127107301,3.7367540662,-1.9364579276
C,0.4450543211,3.9945119267,0.8609608744
O,0.0814617716,0.9390168631,2.1827389689
C,1.1058204463,0.7301420917,3.1903489016
C,0.6026485031,1.503698806,4.3967061748
C,-0.9029290137,1.3190097963,4.3024470795
C,-1.134215386,1.388938036,2.802131748
H,0.6618321082,0.4372134878,-1.7893586435
H,1.789415961,-4.431971029,-0.5161264198
H,-0.9543904497,-4.5729163887,-0.0131888951
H,1.8280405518,0.3894517013,0.0266834405
H,0.4188937188,4.7894426498,-1.9268356957
H,0.4543886465,3.275709772,-2.8694501868
H,-0.9807943123,3.6771683846,-1.8978031815
H,0.940575712,4.960437073,0.7078694392
H,-0.637334008,4.1616798158,0.9066759534
H,0.7693120003,3.5653408919,1.8141712552
H,2.9342280848,2.5227119557,-1.6539115826
H,2.8510905771,4.1598919914,-0.9338117021
H,3.1854414735,2.7271107012,0.0852701703
H,-1.9621633964,0.7531606701,2.4628802846
H,-1.4752330951,2.0748164588,4.8474791771
H,-1.1890227247,0.3343375514,4.6936181095
H,0.8740203962,2.5650159286,4.2948808965
H,1.0356731555,1.1354201023,5.3316746352
H,-3.1554353722,0.8362190971,0.678476535
H,-2.4390123042,2.4405363091,0.3403269823
H,-3.1819866694,-0.1022438609,-2.3222997776

H,-3.0767755343,2.9367249533,-2.5480744978
H,-4.3726560062,1.8653396154,-3.1202449335
H,-4.6029982925,2.8871459016,-0.5972929191
H,-4.9204951951,1.163722831,-0.8554152622
H,-5.0848294415,-1.9511975974,-1.4208033492
H,-4.2156887039,-1.4006121105,2.7436224038
H,5.4629680362,-1.1378997816,1.191051887
H,4.801468775,-0.7311021687,-3.0269040997
H,-1.6415627443,-2.0716350217,-2.5336113615
H,-2.360970791,-3.6615158104,-2.3015383595
H,-3.3358771591,-2.3641641358,-2.994787916
H,-1.105546608,-2.9669092892,2.6995597805
H,-0.7280651163,-1.2534458037,2.5174616728
H,-2.0495333127,-1.7689564191,3.5957407994
H,-6.3678474689,-0.4144883797,1.5719908758
H,-6.8130109498,-1.162409342,0.0266301708
H,-6.7262315643,-2.1373561614,1.4979350123
H,1.6862947627,-2.6136490646,-3.0713436385
H,1.5522049597,-0.8595327905,-3.1960845583
H,2.8654238152,-1.7015075272,-4.0322221048
H,2.0422706874,-1.8522997857,2.0611924754
H,3.0152351608,-3.3106504644,1.901357263
H,3.7271359143,-1.8695847741,2.6345849234
H,7.3810442374,-1.1324206956,-1.2661831813
H,6.7441072729,0.3580705756,-1.9615665421
H,7.0032482517,0.2287822301,-0.2112437065
C,-1.6059829471,0.8242143873,-3.4375584099
H,-0.9048484826,-0.0107006833,-3.3339599668
H,-2.1305084994,0.7094649965,-4.393135073
H,-1.0317281028,1.7562508081,-3.4714351884
H,-1.3291025585,2.4197989537,2.4689131862
C,2.4663615187,1.1606900183,2.7072525352
H,3.1957513638,0.9949237664,3.5094273678
H,2.7936316098,0.5976910754,1.826895155
H,2.4740441937,2.2310486033,2.4639561719
H,1.1209746963,-0.3501334537,3.4257255405

Ir(D)$_2$(PMe$_3$)(IMes)(acetone)$_2$

C,0.1025892125,0.1337538341,0.0028747884
C,0.079621999,0.0635147415,1.3961569012
C,1.2502051777,-0.0353616364,2.1450168364
C,2.4636321928,-0.0508574658,1.4528862275
C,2.5341409899,-0.0061496936,0.0583633183
C,1.3370355456,0.0932931304,-0.6467459577
N,3.685538052,-0.1059835192,2.2028424329
C,4.2968202525,-1.3005800802,2.5510657889
C,5.4120063236,-0.9796810587,3.2403016956
N,5.457214851,0.4075369813,3.2972077086

C,4.3916300744,0.972874154,2.655847802
C,6.5075780658,1.1125046371,3.9710801508
C,7.6620067457,1.4509671121,3.2602799205
C,8.6619135367,2.1420686189,3.9399555513
C,8.5415689099,2.4696291921,5.2915385806
C,7.3861214589,2.0833509365,5.9699945648
C,6.3552424372,1.3987944749,5.3293473532
Ir,3.8789502883,2.9625980023,2.3354661848
O,6.0166152215,3.6972451602,1.8607727879
C,6.6322701417,3.9034228674,0.8201055792
C,6.0957977453,3.5436771305,-0.5282332995
C,7.8379263004,1.0426925254,1.8290373093
C,5.1312477781,0.9596668696,6.074464722
C,9.6509169394,3.1831826254,6.002416432
C,1.2103959977,-0.1082756893,3.6410176347
C,3.8532974078,-0.0475024736,-0.6511739089
C,-1.1725958832,0.2030980903,-0.7808640583
P,2.9985320775,5.0428874264,1.7593477622
C,2.1960921993,6.0082263029,3.0966218968
O,4.5833383399,3.7996369409,4.3735595209
C,4.047139246,4.0022544287,5.4584502881
C,2.6420793244,3.5936056262,5.7662635606
C,4.1501516964,6.2873046465,1.0563515694
C,1.6855614431,4.9487166717,0.4914069952
C,4.8034671381,4.7180003063,6.5332934667
C,7.976234787,4.557709383,0.874291389
H,2.4130505386,2.5472497339,2.7073247902
H,3.8713446278,-2.253838787,2.2703324005
H,6.1796100063,-1.5878713916,3.6981332335
H,3.4214100299,2.4775165747,0.9192092703
H,3.6260943689,7.2213521176,0.8225317571
H,4.9509766931,6.4929458172,1.7755395327
H,4.5976573698,5.8971818335,0.1348946841
H,1.2528934966,5.9335170268,0.2806456323
H,2.1082603813,4.5312641011,-0.429211581
H,0.9026623402,4.2654714659,0.837599011
H,2.9354607302,6.2590196918,3.865938798
H,1.7682433222,6.9385680207,2.705258881
H,1.3977372614,5.4128275796,3.5523827614
H,8.6668837377,4.1214332497,0.1439099239
H,7.8593454744,5.6165305893,0.6040471678
H,8.3879339759,4.4968221614,1.884864545
H,6.2885126039,4.3437425899,-1.2528884609
H,6.6351084724,2.6591833333,-0.8959291733
H,5.0280182367,3.3083799325,-0.4748237967
H,4.6629448253,4.237021554,7.5080987998
H,5.8642994562,4.7706815354,6.2795560558
H,4.406110833,5.7375851898,6.6302805163
H,2.1559161872,3.1663410733,4.884681257

H,2.64387478,2.8586357152,6.5815735522
H,2.0730520387,4.4569694818,6.1340106675
H,9.5707821165,2.4191150566,3.4029692817
H,7.2876028554,2.3147452611,7.0316585961
H,-0.8786382179,0.0795707855,1.916257732
H,1.3679054358,0.1329589901,-1.7360599653
H,10.4580645067,2.488869342,6.2669014432
H,10.0937970507,3.9636245448,5.3742983116
H,9.3042147779,3.6482466442,6.9306605948
H,5.0804530634,1.4316454403,7.0622001456
H,4.2108438182,1.1926898597,5.5221968747
H,5.1293627199,-0.1262274017,6.2355221917
H,8.1159196477,-0.0166903305,1.7511584582
H,6.9153021202,1.1681147078,1.2485339149
H,8.6395584072,1.6180660445,1.3522442368
H,1.7148720736,0.7563542782,4.0929391044
H,0.1788822387,-0.1280721207,4.004161388
H,1.7165623659,-1.0047656461,4.0209930147
H,4.4912589247,0.7953541725,-0.3505095718
H,4.4114813937,-0.9645364575,-0.4233372013
H,3.7155438061,-0.0020038077,-1.7353880339
H,-1.0274436025,0.7024507509,-1.7442728297
H,-1.5568933491,-0.8025977313,-0.9924751014
H,-1.9553739792,0.73760841,-0.2326874905

Catalyst-Solvent-Substrate Complex (10)

$Ir(D)_2(PMe_3)(IMes)(PhCOMe)(DCM)$

Ir,0.6834858405,0.5543655555,-0.0145261324
H,1.5488680908,0.4161355489,-1.2991753818
P,0.8591311786,2.8680332588,-0.3459356334
C,1.8345039338,-3.5785461888,0.0929425112
C,0.5416258088,-3.7601202998,0.434823009
H,2.6492781552,-4.2749466951,-0.0475940507
H,-0.0285643348,-4.6500188242,0.6625912696
N,2.0113268345,-2.2148398503,-0.0834572414
N,-0.0440481616,-2.5015416222,0.4595017
C,0.8548990731,-1.521205059,0.1405599727
H,2.0996793853,0.5982212351,0.6567064495
C,-0.5102640156,3.9389320644,0.2335441915
H,-0.3552488927,4.9752895564,-0.0888046312
H,-1.4596301489,3.5734991206,-0.1758347882
H,-0.5738066397,3.9117900656,1.3255906461
C,2.3499185925,3.6514499506,0.3625099774
H,2.3861626327,4.7207864042,0.1239864745
H,2.3530282627,3.5212065974,1.4498339264
H,3.2366764194,3.155466975,-0.0466467348

C,0.9763824854,3.3459883767,-2.1117422399
H,0.0531345587,3.0681070432,-2.6320831682
H,1.1276252684,4.4270937653,-2.2145683191
H,1.8117289325,2.816779103,-2.5819194135
C,-3.540752558,0.7904865593,-1.8526694002
C,-4.1863865319,0.9951821637,-0.6248685202
C,-5.5686159697,1.0789283935,-0.5700746289
C,-6.321433246,0.9308513449,-1.7347036194
C,-5.6901180068,0.715361908,-2.9570747714
C,-4.3044014899,0.6547454615,-3.0190919566
H,-3.5832594863,1.0834806153,0.2766093799
H,-6.0652995985,1.2536277098,0.3812125683
H,-7.4061521873,0.9885671674,-1.6893788259
H,-6.279281605,0.5999200542,-3.8626599127
H,-3.820031193,0.4938250207,-3.9797647052
C,-2.0725483874,0.6844918833,-1.8737952867
C,-1.343398993,0.6389890595,-3.1821375797
H,-0.2665672191,0.5610945362,-3.0035916137
H,-1.6703933675,-0.2155938456,-3.7859270766
H,-1.5567304617,1.5396575868,-3.7712651241
O,-1.4629504794,0.6368450494,-0.8000634502
Cl,-0.7938445688,0.9078680137,2.2675708634
C,0.4272726857,1.1941447448,3.5543763024
H,1.3317283558,0.6635704177,3.2524411565
H,0.0106143566,0.8020762552,4.4830673166
Cl,0.8064273846,2.9064162096,3.7709414039
C,3.2634429999,-1.6582625046,-0.5124238456
C,4.2057387504,-1.2903645635,0.4513198207
C,3.4995659634,-1.5236005405,-1.8833103112
C,5.404668026,-0.7377638926,0.0069165116
C,4.7150044438,-0.968982472,-2.2785208141
C,5.6762271727,-0.5662014682,-1.3508526449
H,6.1514246127,-0.4382009646,0.742651736
H,4.9208209366,-0.8559148893,-3.3433566491
C,-1.4405226043,-2.3303536376,0.7424702443
C,-2.3418657936,-2.3437339353,-0.3262129616
C,-1.8601076079,-2.2233585202,2.0715105283
C,-3.6955390539,-2.1858062022,-0.0395234614
C,-3.2235695667,-2.0595154261,2.3088979532
C,-4.1541090304,-2.0389704516,1.269625369
H,-4.413984849,-2.1761675031,-0.8613411078
H,-3.5705664081,-1.9592761269,3.3380503525
C,6.988481225,-0.003705857,-1.8052618483
H,7.4076901952,0.6881533358,-1.0675987941
H,7.7261136768,-0.8018191296,-1.9558497471
H,6.8902079491,0.528455335,-2.7570333061
C,3.9314709936,-1.4706680305,1.9128172983
H,4.7853719466,-1.1464265318,2.5143565478
H,3.0538018109,-0.8873114661,2.2233070598

H,3.7219268961,-2.5175996953,2.1656917446
C,2.4762918813,-1.9444701859,-2.8943339904
H,1.6140176846,-1.2626619088,-2.8933060245
H,2.900855832,-1.9476678849,-3.9023446803
H,2.0839935912,-2.9481763227,-2.6878366725
C,-0.8877803547,-2.318693016,3.2079362747
H,-0.640207702,-3.36538775,3.4287782545
H,0.0594232549,-1.8110152293,2.9863111238
H,-1.3120062893,-1.8864080757,4.1205158745
C,-1.8664178116,-2.545299919,-1.7321643487
H,-2.6860438698,-2.4066235,-2.4458825601
H,-1.0560860975,-1.850746436,-1.9884393924
H,-1.4674170987,-3.5573974346,-1.8788417042
C,-5.616290226,-1.8904555784,1.5598405245
H,-6.1791776888,-1.6285262852,0.6578819222
H,-6.037033171,-2.8248730912,1.9511539749
H,-5.7988633126,-1.1178436347,2.3158458364

Ir(D)$_2$(PMe$_3$)(IMes)(PhCOMe)(*t*-BuOMe)

C,5.7073495211,0.2484771591,-1.1083251525
C,4.8051520611,0.3856160162,-2.1656015168
C,3.6000781209,-0.3114271095,-2.1970380376
C,3.3074178565,-1.1494416328,-1.1168401833
C,4.1955164657,-1.3460941952,-0.0570099374
C,5.3883380875,-0.624775941,-0.0690001278
N,2.0406777746,-1.8213997356,-1.0846885878
C,1.8523261356,-3.0909099285,-1.6061622037
C,0.5598933253,-3.4115549086,-1.3867977012
N,-0.0115098872,-2.330650146,-0.7280877513
C,0.8932477162,-1.3274618376,-0.5246186626
C,-1.3987811481,-2.3223916495,-0.3665735869
C,-1.7705230144,-2.8420525169,0.8780458365
C,-3.1253895448,-2.8451666721,1.2006446058
C,-4.0922363261,-2.3585873863,0.3183716891
C,-3.6802011388,-1.8791736155,-0.9238564824
C,-2.3362413903,-1.8658813276,-1.2958631274
Ir,0.7272035811,0.5891330346,0.2790758348
O,-1.4892051227,0.9894219581,-0.3535540584
C,-2.0632606774,1.5147180629,-1.3121189737
C,-1.2954663226,2.0574776245,-2.4795762249
C,-0.7364095492,-3.3643716245,1.8254193897
C,-1.9279199479,-1.4143554424,-2.6648067732
C,-5.5427087268,-2.3660014039,0.694488686
C,2.6544748683,-0.1677421458,-3.3509380076
C,3.8870838188,-2.3150235925,1.0428156582
C,7.0119732691,0.9854428102,-1.1178136923
P,0.9968273135,2.8499425839,0.8430426975

C,1.4587393342,3.8630623049,-0.6160482012
C,-0.4062874846,3.818906391,1.5259231273
C,2.3936184031,3.2608869039,1.9584239932
C,-3.535988008,1.6181833946,-1.3050520344
C,-4.2386177079,1.2526300534,-0.1486293184
C,-5.6234159821,1.3048307468,-0.1236839816
C,-6.324829216,1.7043155086,-1.2600331912
C,-5.6382559312,2.0677115356,-2.4155998681
C,-4.2503461976,2.0331056452,-2.4369153092
O,-0.2171988813,-0.1682164849,2.5538475795
C,0.4411561966,-0.064628354,3.850844002
C,1.9152049197,-0.2938841611,3.5815970521
C,-1.6128484883,0.0727217371,2.567676453
H,1.3329013137,1.0414019654,-1.0747685664
H,2.6600411123,-3.6319956508,-2.0786859057
H,-0.0178075538,-4.2937108104,-1.6251207173
H,2.2081347417,0.3873575258,0.7241020231
H,-0.1470920188,4.8810035873,1.6106460565
H,-1.2746760931,3.7135432866,0.8646714042
H,-0.6872129929,3.442336568,2.5148826445
H,2.49265686,4.3465039952,2.0756009288
H,2.2731474941,2.8046553731,2.945526312
H,3.3107976072,2.8606023203,1.5102757493
H,0.6497041964,3.8593252848,-1.3539514429
H,1.667876423,4.8986354455,-0.3228348579
H,2.3518662171,3.4293822632,-1.0803506541
H,-3.6783635455,0.923886996,0.7223406014
H,-6.1613713186,1.0283125885,0.7799908099
H,-7.4113300237,1.7379171205,-1.2432008522
H,-6.1859731235,2.3815284598,-3.2999872351
H,-3.7260477221,2.3230249349,-3.344664238
H,-0.2293284506,1.857800741,-2.3447183341
H,-1.6298398968,1.6051972657,-3.4199058285
H,-1.4630827758,3.1384583322,-2.572269318
H,-1.8414828874,1.1438659529,2.6855791176
H,-2.0071398752,-0.2628678175,1.6063822203
H,2.316992829,0.4507399945,2.8857222278
H,2.4781734907,-0.2418691817,4.5202585818
H,2.0736259608,-1.2864388413,3.1441150357
H,-3.4341568555,-3.2350637545,2.1716648239
H,-4.4271068403,-1.509922351,-1.6290846676
H,5.054434492,1.0471554678,-2.9959930732
H,6.0918850418,-0.7573222096,0.7535049135
H,4.1299407043,-3.3426862829,0.7412203761
H,4.4716750139,-2.09032693,1.9406163883
H,2.8231983732,-2.3038847787,1.3093019954
H,3.0734223802,0.4896065969,-4.1182622666
H,2.4366592598,-1.1353055389,-3.8207526129
H,1.6901687879,0.2507495802,-3.0324176201

H,7.4028244695,1.1274435499,-0.1052141484
H,7.7705895824,0.4300577276,-1.6834534861
H,6.9165449552,1.9692148291,-1.5892474576
H,-6.1334939658,-1.7389885784,0.0181542871
H,-5.9585743808,-3.3801070395,0.6531958168
H,-5.6927612954,-2.0019776335,1.7178053118
H,-2.6837280344,-0.7460122612,-3.094385685
H,-0.9589860552,-0.9004563935,-2.6629793196
H,-1.8294340918,-2.2694386949,-3.3465971437
H,-0.1975009737,-4.2230967824,1.4049418929
H,0.0053640214,-2.5865678089,2.0481355103
H,-1.1960643038,-3.6854171565,2.7658131965
C,0.2099213543,1.3121561566,4.4553041617
H,0.829725075,1.4355724553,5.3503673639
H,0.4841979304,2.09529227,3.7394892187
H,-0.8323569737,1.4670111585,4.7571155114
C,-0.0675659595,-1.1524310964,4.7904420189
H,-1.1182456777,-1.0235668089,5.0704130636
H,0.058833233,-2.1441375389,4.3429555548
H,0.5131747168,-1.1253177029,5.7193532145
H,-2.1143236073,-0.4922972486,3.3642610555

Ir(D)$_2$(PMe$_3$)(IMes)(PhCOMe)(Et$_2$O)

C,0.2974528126,0.0181325815,-0.3062894744
C,0.1199679053,0.0186176306,1.0774293
C,1.1998233477,-0.0281029721,1.9575887559
C,2.4814655616,-0.0591031124,1.4046866556
C,2.7073775369,-0.0916344889,0.0255139534
C,1.596964219,-0.041081508,-0.8133525577
N,3.6204658486,-0.064986027,2.2767470215
C,4.2141706132,-1.2383229252,2.7124972587
C,5.2866625033,-0.8800574201,3.4490532225
N,5.327025575,0.5084199241,3.4402840688
C,4.2974596122,1.0396515212,2.7170161016
C,6.3572062325,1.231531857,4.1259470625
C,7.5501928393,1.4996480856,3.4449169021
C,8.5496821437,2.1780316108,4.1385481598
C,8.3790518488,2.5853048339,5.4636183841
C,7.189019831,2.2640385537,6.1135571163
C,6.167043036,1.5681857425,5.4673529779
Ir,3.6942435714,3.0034890391,2.3725878723
O,4.4580469742,3.9217871708,4.3840763336
C,3.9899492417,4.162132875,5.5007077764
C,2.5772683656,3.8009799729,5.8503310009
C,7.7275977774,1.0835886913,2.0166415268
C,4.9260834722,1.1647604877,6.2029115801
C,9.4601716192,3.3467847183,6.1683502249
C,0.9919969896,-0.0469218858,3.4412997793

C,4.0978032637,-0.1872055372,-0.5242412946
C,-0.8815216872,0.0323466322,-1.2310028365
P,2.6113793384,5.0199121741,1.8761612934
C,1.0109644086,5.2304107541,2.7464961506
C,3.4404039619,6.6121793118,2.2669547266
C,2.0933640824,5.2512232673,0.1343733694
C,4.8435786667,4.8140971069,6.5135151784
C,6.0941538581,5.3219729633,6.1335883796
C,6.9280249107,5.9047732919,7.0750144588
C,6.5349978318,5.963923171,8.411343305
C,5.2982222365,5.45707239,8.8013696344
C,4.4512597963,4.8942828313,7.855957089
O,5.8416336024,3.7622313354,1.374885034
C,5.8007797598,4.315100474,0.0601169913
C,5.2868037258,3.3006338042,-0.9258632535
C,6.6031215884,4.5526342701,2.2972927653
C,8.0575630689,4.7330678221,1.9196842822
H,2.3185093015,2.5425779366,2.9399026958
H,3.8090714781,-2.2058462429,2.4509537296
H,6.0302952247,-1.4608640902,3.9767716305
H,3.141530376,2.4523098753,1.0224760979
H,2.7622441483,7.4584612022,2.1044838927
H,3.7694144472,6.6093191431,3.3133161529
H,4.3236880605,6.743579107,1.6323841884
H,1.5309707327,6.1845756321,0.0135057166
H,2.9646238708,5.2715046546,-0.5286792862
H,1.4611045375,4.405970258,-0.1588807636
H,1.178023354,5.2938019745,3.826918285
H,0.5025808625,6.1428310777,2.4131693405
H,0.3722342659,4.3640387253,2.5452062704
H,6.3966175919,5.2502378609,5.0911532614
H,7.8906555461,6.310132718,6.7725304689
H,7.1934597098,6.4125173038,9.1509240213
H,4.993001519,5.5049694559,9.843109704
H,3.4856203842,4.5044073682,8.1702294732
H,2.0813282769,3.3707911743,4.9758883547
H,2.5536229379,3.0679316189,6.6655885797
H,2.0257353801,4.6818055012,6.2009757833
H,6.1104023599,5.5330746241,2.4281871709
H,6.5288744983,4.012507201,3.2458999938
H,6.8150846945,4.619806294,-0.2291187579
H,5.1789386433,5.2291292288,0.0709140135
H,8.2208506681,5.4688925131,1.1262466612
H,8.6061214148,5.0836678581,2.8023939646
H,8.5001359858,3.7791262605,1.6094585695
H,4.2639963719,2.9869564873,-0.6915708971
H,5.2994457092,3.726557117,-1.9349553653
H,5.9283536559,2.4116630809,-0.9252705503
H,9.4887121531,2.4002242705,3.6293440242

H,7.0487141165,2.5647727111,7.1536128489
H,-0.8909992702,0.0455547002,1.4850171975
H,1.7493489478,-0.0595244011,-1.8929120698
H,4.5316847513,-1.1793855711,-0.3432511018
H,4.1056143718,-0.0134534339,-1.6047297049
H,4.7678962947,0.5438798813,-0.0538758866
H,-0.0740064143,-0.0409565885,3.686477215
H,1.4369457563,-0.9380907545,3.9018665338
H,1.4571682302,0.8244248089,3.9227312497
H,-0.6719970388,0.6023960208,-2.1422838443
H,-1.1461909377,-0.9858143119,-1.5425694411
H,-1.7652116369,0.4651569947,-0.7514968647
H,9.1153105201,3.7292828125,7.1347646386
H,10.3397708873,2.7179580724,6.3509761649
H,9.8001133049,4.2002377913,5.5676553769
H,4.7834553738,1.7847320399,7.095992429
H,4.0302388482,1.2335487601,5.5728986259
H,4.991981856,0.1227072309,6.5426207346
H,7.5111165808,0.0177901,1.8720568631
H,7.0403332794,1.6437259027,1.3676493225
H,8.7524164159,1.2674899866,1.6786738229

Ir(D)$_2$(PMe$_3$)(IMes)(PhCOMe)(2-MeTHF)

Ir,-0.6977034182,-0.5005280875,0.437059557
H,-1.5017698025,-1.2798690375,-0.6532137839
P,-0.7929104659,-2.454017811,1.7096888874
C,-2.1413227424,2.5290880555,-2.2336526777
C,-0.8522287046,2.9285782543,-2.2294472472
H,-3.0104890574,2.9002268617,-2.7584824634
H,-0.3421002906,3.7289414844,-2.7470611936
N,-2.2259575617,1.4467107231,-1.3725102773
N,-0.1777393743,2.0807455498,-1.3606007551
C,-1.0133298592,1.1426047197,-0.8153654226
H,-2.1190053421,-0.1930685338,1.0217858363
C,-0.9796104602,-2.2732103245,3.5231208047
H,-1.0778230643,-3.2560939708,3.9988979969
H,-0.1083799921,-1.757782695,3.94175681
H,-1.8709898424,-1.6768535613,3.7423691715
C,-2.2275288624,-3.5003196377,1.2708358508
H,-2.3045887501,-4.3786908794,1.9221096999
H,-3.1401106754,-2.8989399079,1.348609994
H,-2.1313265252,-3.8260594595,0.2290668569
C,0.6059412839,-3.6412677466,1.6095249404
H,1.5453847814,-3.1411610327,1.8721345636
H,0.4486881916,-4.4868296465,2.2893477746
H,0.6941723413,-4.0300636657,0.5893966064
C,3.3949722507,-2.0546833784,-1.0486419291
C,4.1879257227,-1.3180254112,-0.1563602978

C,5.5689590129,-1.4345508012,-0.188682392
C,6.1749613873,-2.2802591951,-1.1167820085
C,5.3977521636,-3.0130178152,-2.0097319472
C,4.0141671974,-2.9046412754,-1.9743345707
H,3.6994326208,-0.6471532253,0.5470397007
H,6.1792744769,-0.8624121592,0.5063187495
H,7.2581081245,-2.3693262805,-1.1430435796
H,5.8716090293,-3.670965152,-2.7329878387
H,3.4169303563,-3.4816161395,-2.6767659706
C,1.9292096504,-1.8912939241,-1.0083390616
C,1.0658415219,-2.7579513342,-1.8757885636
H,0.0125677346,-2.5866692181,-1.6341853588
H,1.2299664768,-2.5189879716,-2.9342649448
H,1.3124325421,-3.818509361,-1.748869101
O,1.4411367156,-1.0344611705,-0.2651866192
C,-0.0780835639,1.7175981832,2.9195867348
O,0.4321534348,0.5639114068,2.2070848336
C,1.8366823816,0.4099436418,2.4253745761
C,2.0938330902,1.1264894213,3.7333669514
C,1.1448467416,2.3153810592,3.6136918486
H,-0.4929735217,2.3997263355,2.1644890428
H,2.0550164928,-0.6658521646,2.4415591095
H,2.3915968461,0.8686063202,1.5898258297
H,1.8182719328,0.488477719,4.5836019388
H,3.140200222,1.4211162414,3.8572055009
H,0.8893637798,2.7697109595,4.5763167881
H,1.6031116744,3.0891895033,2.9841404235
C,1.2189616801,2.2233144709,-1.0765019048
C,2.136848596,1.4594976706,-1.8013165324
C,1.6208735509,3.1655015987,-0.1219660829
C,3.485118544,1.5717921551,-1.4658128281
C,2.9783077964,3.2324502824,0.1894889346
C,3.919535409,2.4246148591,-0.452450295
H,4.2156132888,0.9707426232,-2.0090980015
H,3.3128130979,3.946190008,0.9445605566
C,-3.4573231311,0.756251899,-1.1151919224
C,-4.2442766138,1.1750182664,-0.038507123
C,-3.8154434373,-0.3161778316,-1.9356595808
C,-5.4057483586,0.4561529079,0.2324630028
C,-4.9842892129,-1.0071842014,-1.6211173966
C,-5.7882708217,-0.6401357779,-0.5420059659
H,-6.0342706013,0.764572888,1.0685175494
H,-5.2811871183,-1.8503993278,-2.245428951
C,-2.9719364049,-0.7152291575,-3.1082196703
H,-3.4120412611,-1.5685640488,-3.6326011697
H,-2.8681382152,0.1025856145,-3.8324701858
H,-1.9558552857,-0.9938572788,-2.7959806174
C,-3.8389897613,2.3404320262,0.8114197082
H,-4.6122222467,2.573360353,1.549099571

H,-2.9065230253,2.1283098831,1.3531201944
H,-3.6617558712,3.2433250634,0.213424619
C,-7.0603031146,-1.3753152237,-0.2478112058
H,-7.2505660878,-1.4371869635,0.8289015227
H,-7.9208885609,-0.8636475469,-0.6966685085
H,-7.0410417399,-2.392760734,-0.6509765378
C,0.6459186074,4.1345253015,0.4787467299
H,0.9848253176,4.4919118201,1.4572121721
H,0.5448875797,5.0195328561,-0.1635919338
H,-0.359854454,3.7119964109,0.5872535734
C,1.6957214964,0.5959402315,-2.942359274
H,1.454951624,1.2062438305,-3.8228184122
H,2.4923024472,-0.0967588712,-3.2377749309
H,0.7939631292,0.0213826975,-2.6996262317
C,5.3631355953,2.4717938682,-0.0533003332
H,5.4975644109,2.1040767184,0.9731250095
H,5.9820423836,1.8541309679,-0.7123374802
H,5.7579386509,3.4938612379,-0.0768186829
C,-1.1718396379,1.2810105412,3.8650376432
H,-1.6447422328,2.156799972,4.3239794705
H,-1.941897416,0.7190389757,3.3234179322
H,-0.7716581766,0.647344519,4.6667310145

Ir(D)$_2$(PMe$_3$)(IMes)(PhCOMe)(acetone)

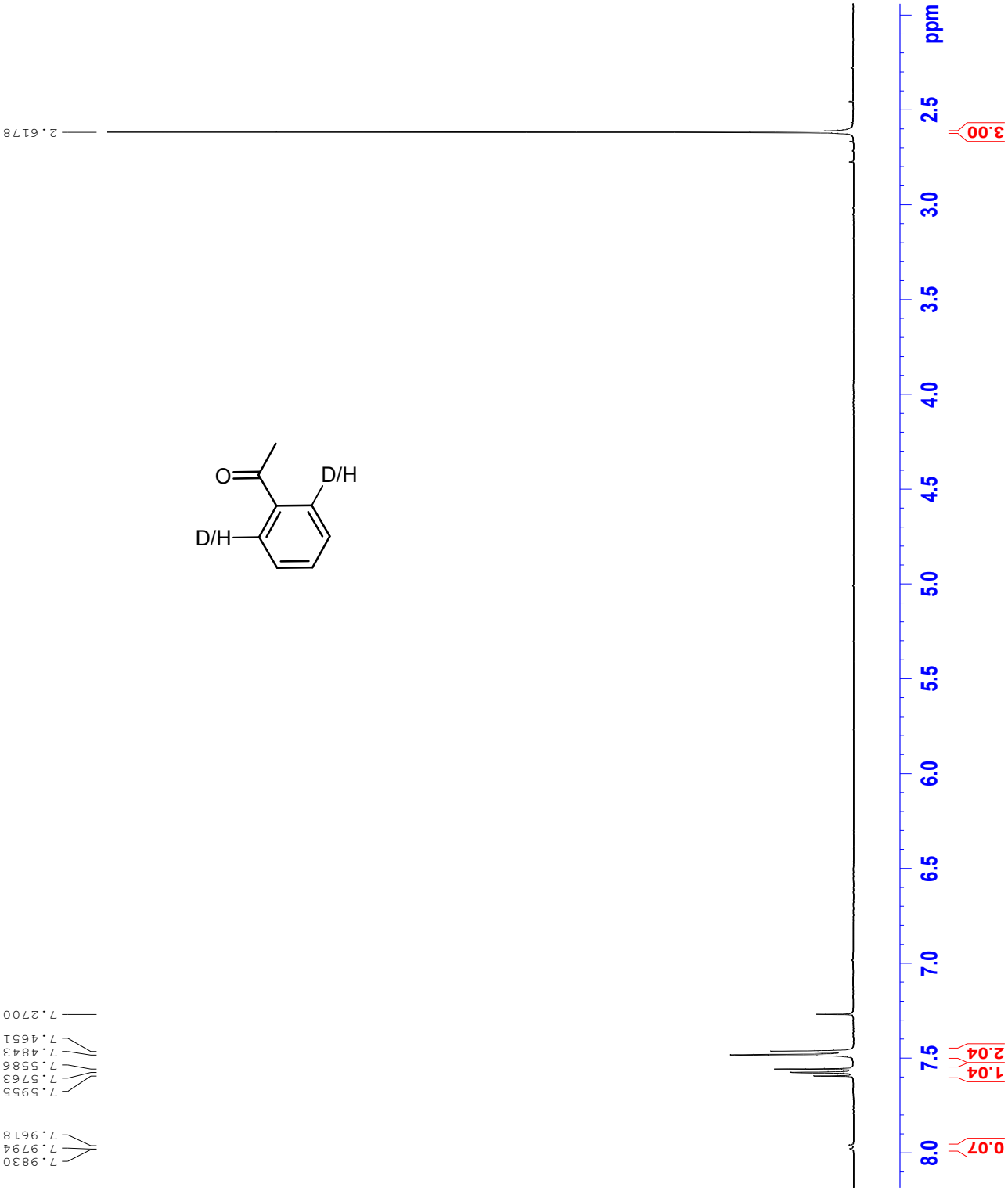
Ir,-0.7614955834,-0.2744292977,0.4865134313
H,-1.5849519796,-1.4453735059,-0.1524318953
P,-0.5448734608,-1.628364416,2.3761718871
C,-2.4420981024,1.6497597592,-2.9615834837
C,-1.2209934888,2.2232208933,-3.0089259757
H,-3.3136573228,1.7557200709,-3.5923270669
H,-0.7843772677,2.9413102684,-3.6889607145
N,-2.4427965054,0.8005476863,-1.8650152838
N,-0.5020943737,1.7104494791,-1.9378691987
C,-1.2422979339,0.8203673654,-1.2125877108
H,-2.1848680434,0.1298557841,0.9976430505
C,0.6769679172,-1.1143715224,3.647216154
H,0.7864895653,-1.8825730601,4.4217044609
H,1.6470014707,-0.9414089455,3.1656687795
H,0.3534641463,-0.1849589161,4.1294316098
C,-2.0759470449,-1.853762237,3.3487959499
H,-1.9202250224,-2.5355083987,4.192960565
H,-2.4132836002,-0.8818430931,3.7245467779
H,-2.8577461918,-2.2516045418,2.6931512484
C,-0.0200029556,-3.3541728605,2.0563484369
H,0.9821184638,-3.3541923975,1.6133399222
H,0.0060938791,-3.9357936828,2.9853585004
H,-0.7149103159,-3.8258218365,1.3540094094
C,3.4898503251,-1.6290675275,-0.7391946865

C,4.1290948787,-0.6438914822,0.0279800435
C,5.5114130738,-0.5414110434,0.0146093761
C,6.2663333668,-1.4058074458,-0.7774178175
C,5.6395013249,-2.3803899849,-1.5494126859
C,4.2559928033,-2.4976667595,-1.5256044618
H,3.5140046034,0.0362798725,0.6161347099
H,6.0081370553,0.2138601567,0.6189763448
H,7.3501572805,-1.3211602718,-0.7906843342
H,6.2308513288,-3.0526662434,-2.165105178
H,3.7741204383,-3.2660486084,-2.1265076274
C,2.0166235373,-1.6994655981,-0.7089492146
C,1.3011216981,-2.8227537317,-1.3949661066
H,0.2251324868,-2.7196261581,-1.228500681
H,1.5019000135,-2.8136866468,-2.4729873956
H,1.6437870551,-3.7928986226,-1.0153435055
O,1.3981288592,-0.8200982403,-0.1056211011
C,0.4225443484,2.139950833,2.3853055077
O,0.5883764186,1.3338243873,1.4761045735
C,-0.9140668589,2.4102937617,2.9994646965
H,-1.2295298658,3.4303751511,2.7417777778
H,-1.6608608516,1.6987244266,2.633576903
H,-0.848989993,2.3772144078,4.0941203236
C,1.6006737678,2.8808866555,2.935046141
H,1.3665172364,3.9382535621,3.1041099972
H,1.8608267437,2.4564797713,3.9145864785
H,2.4558606114,2.7780993398,2.2614194908
C,-3.5857768748,0.0138481467,-1.4985833124
C,-4.5150025503,0.5536491684,-0.6058809235
C,-3.7297839803,-1.2594483524,-2.0554705971
C,-5.6010420993,-0.2406420134,-0.2444012118
C,-4.8322789176,-2.0152961154,-1.6636723102
C,-5.7742457979,-1.5265387559,-0.7580002525
H,-6.3373159689,0.1585535413,0.4537828252
H,-4.9620471543,-3.0137828084,-2.0820505678
C,0.8524386279,2.0865277885,-1.6635617095
C,1.8856913233,1.3698441318,-2.2676763762
C,1.0875042059,3.1834192716,-0.8291149226
C,3.1961055814,1.7336377339,-1.9571757694
C,2.4103061158,3.5137987621,-0.5525640374
C,3.4756197578,2.7882333613,-1.0911121925
H,4.0196135971,1.1710230591,-2.4001231856
H,2.6199404172,4.3653797599,0.0977107278
C,-2.7300215852,-1.7949254481,-3.0344767347
H,-1.7214637201,-1.8184631738,-2.6009105057
H,-2.9921377549,-2.8105187395,-3.3450034789
H,-2.6722073842,-1.1749699271,-3.9382581048
C,-4.3453865729,1.935273458,-0.0508450197
H,-5.1776187726,2.1954194822,0.6095899715
H,-3.4125588933,2.0223882785,0.523648881

H,-4.3003618028,2.69091645,-0.8455967851
C,-6.9673054562,-2.3494823042,-0.3778358791
H,-7.314527209,-2.1136892172,0.6333999607
H,-7.8067614488,-2.1630351917,-1.0593450026
H,-6.747050714,-3.4210915736,-0.4226249728
C,-0.0538685314,3.978877667,-0.2729849049
H,-0.5627178889,4.5527402501,-1.0582363712
H,-0.8152157094,3.3293605817,0.1793508993
H,0.2926788395,4.6968427252,0.4789966378
C,4.8866532231,3.139826767,-0.7288435304
H,5.6103707199,2.5335421752,-1.2830073602
H,5.103880397,4.1948171916,-0.9320592958
H,5.0671472254,2.9792740808,0.342748312
C,1.6027791227,0.2727448528,-3.2478590344
H,2.4685538706,-0.3917255545,-3.3518177955
H,0.7254680106,-0.3212743633,-2.9613378535
H,1.3911849067,0.6814754677,-4.2448558995

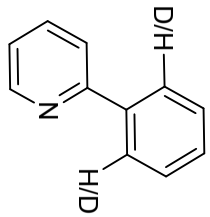
Scanned spectra

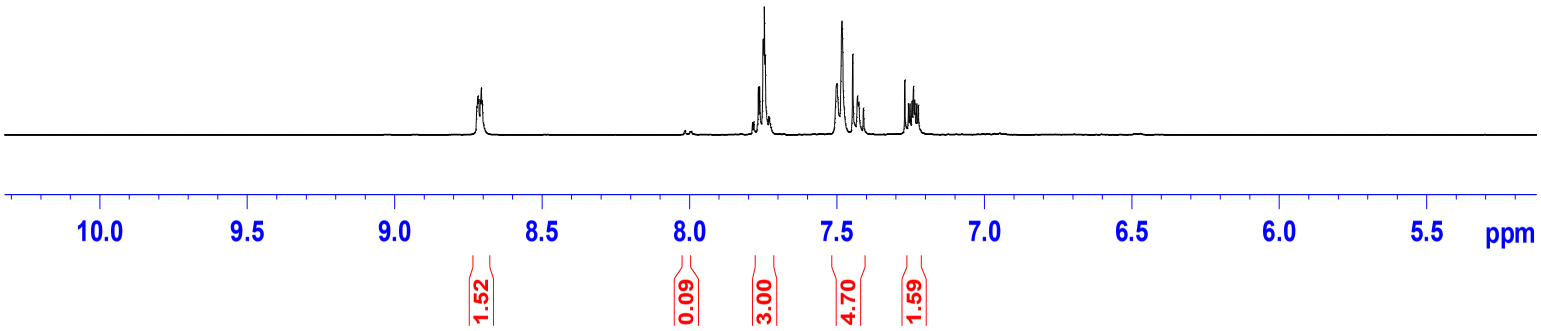
Acetophenone, **1**



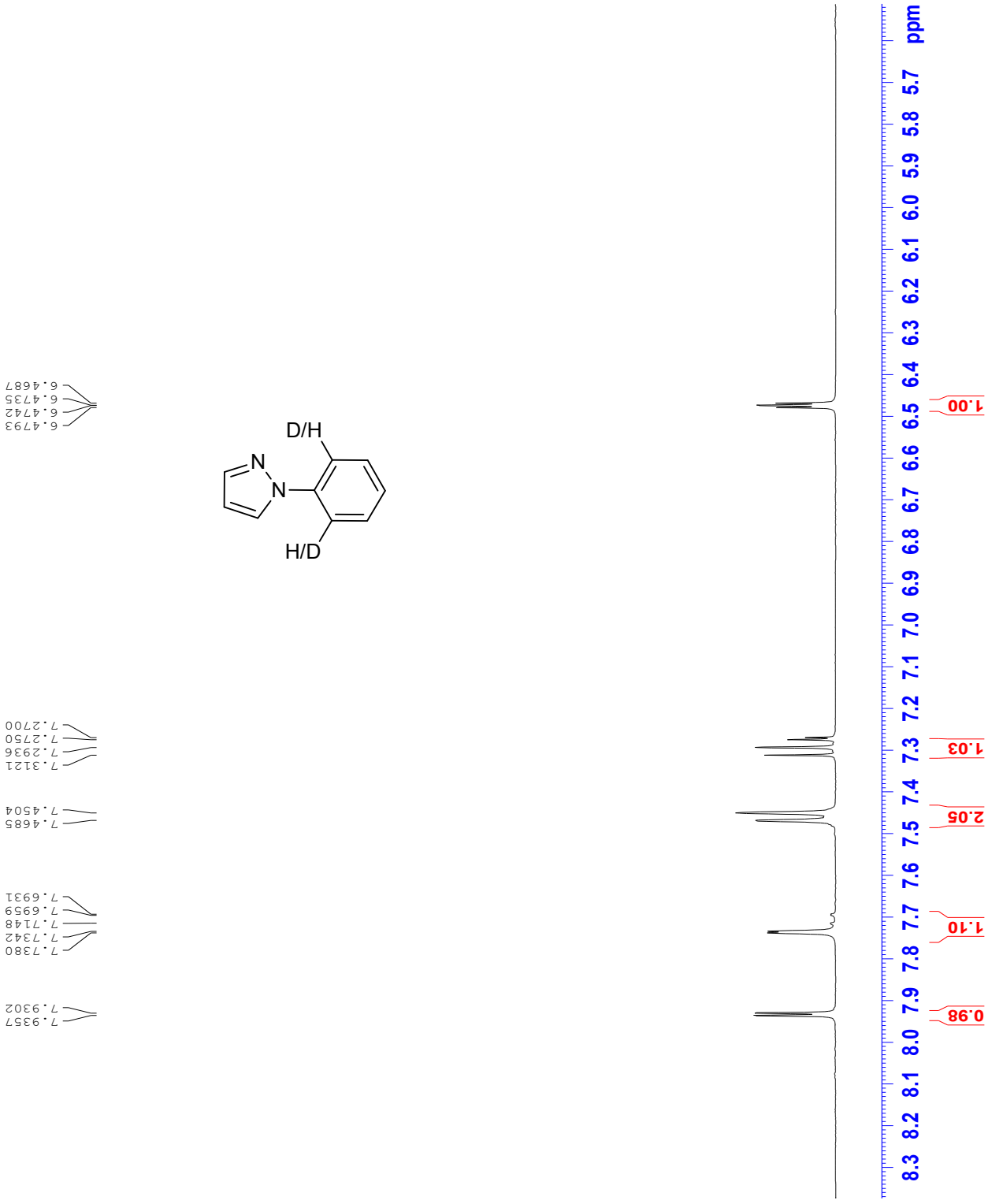
2-Phenylpyridine, **11**

8.0154
7.9978
7.9943
7.7867
7.7823
7.7667
7.7623
7.7504
7.7491
7.7463
7.7434
7.7313
7.7288
7.5010
7.4831
7.4466
7.4306
7.4264
7.4103
7.2576
7.2525
7.2455
7.2406
7.2361
7.2294
7.2240

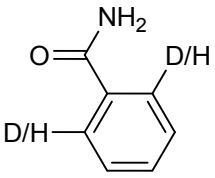


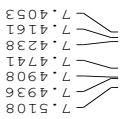


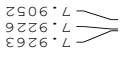
N-Phenylpyrazole, **12**

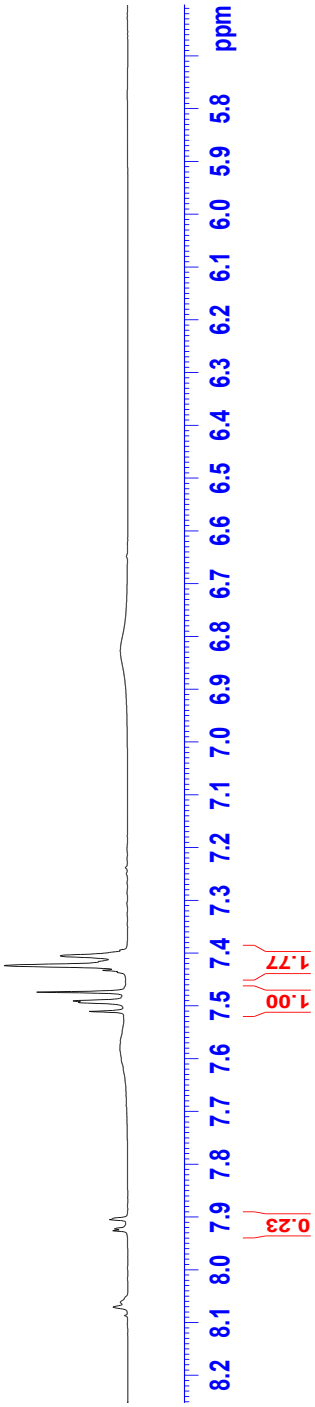


Benzamide, **13**

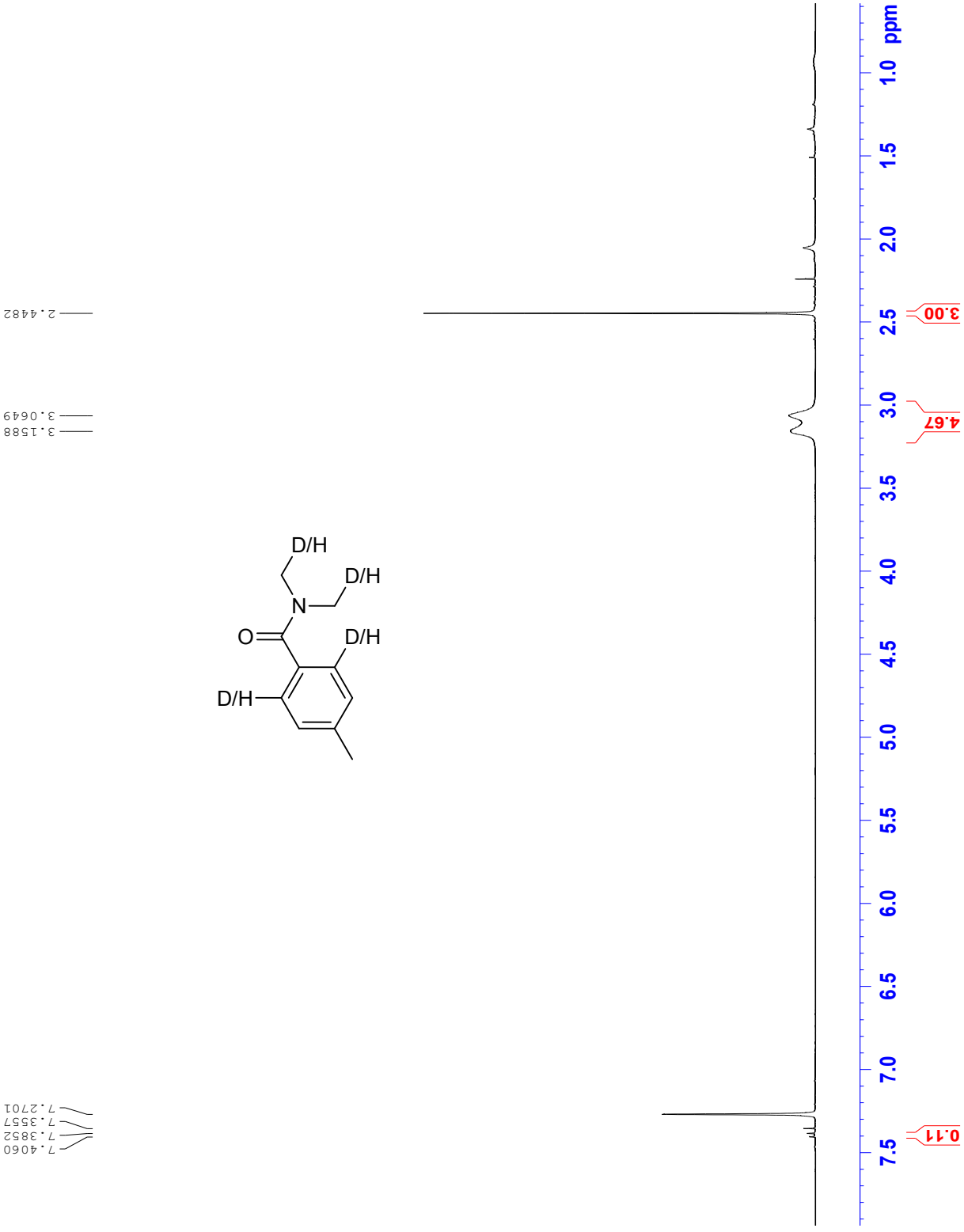






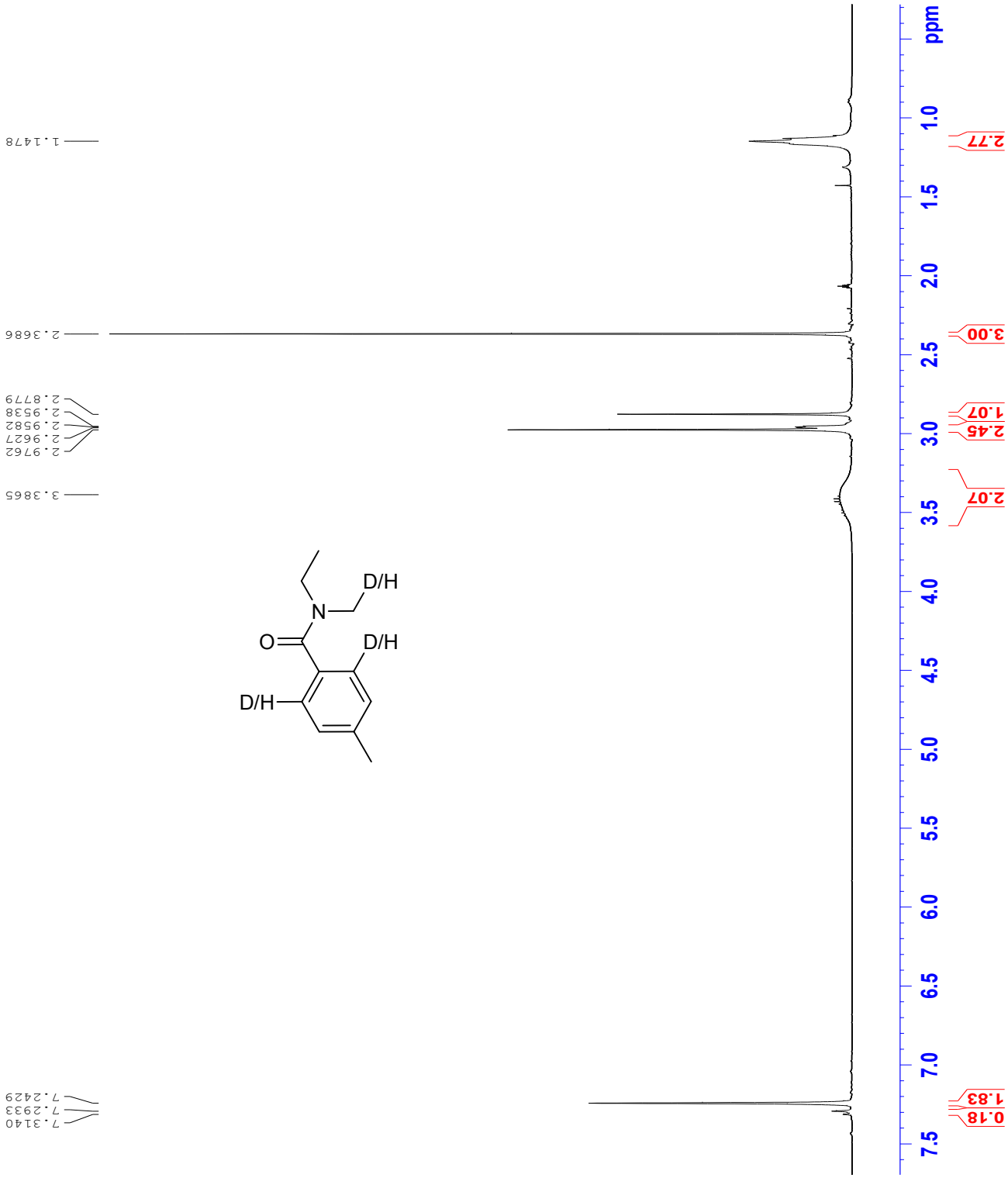


N,*N*-4-Trimethylbenzamide, **14**

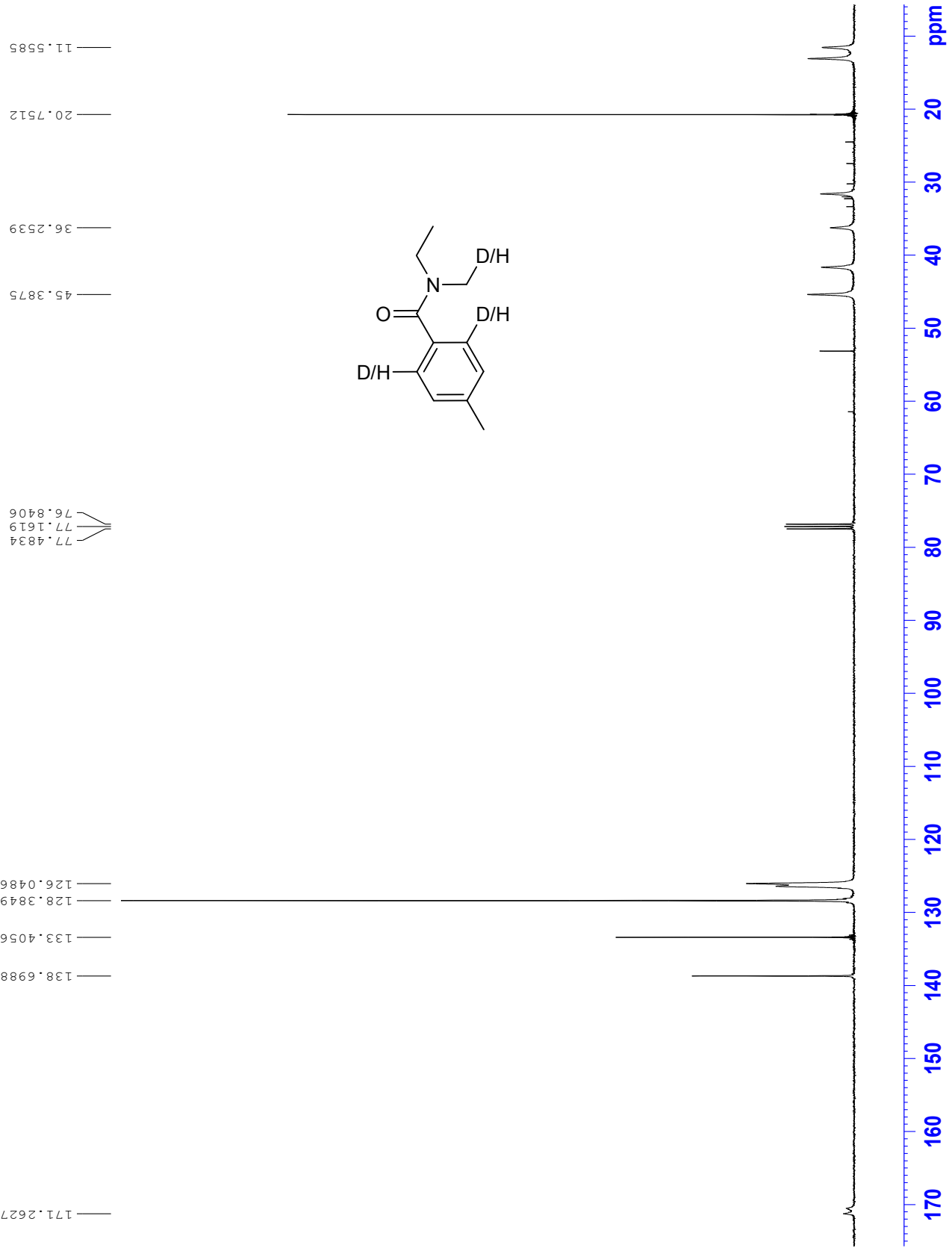


N-Ethyl-*N*, 4-dimethylbenzamide, **15**

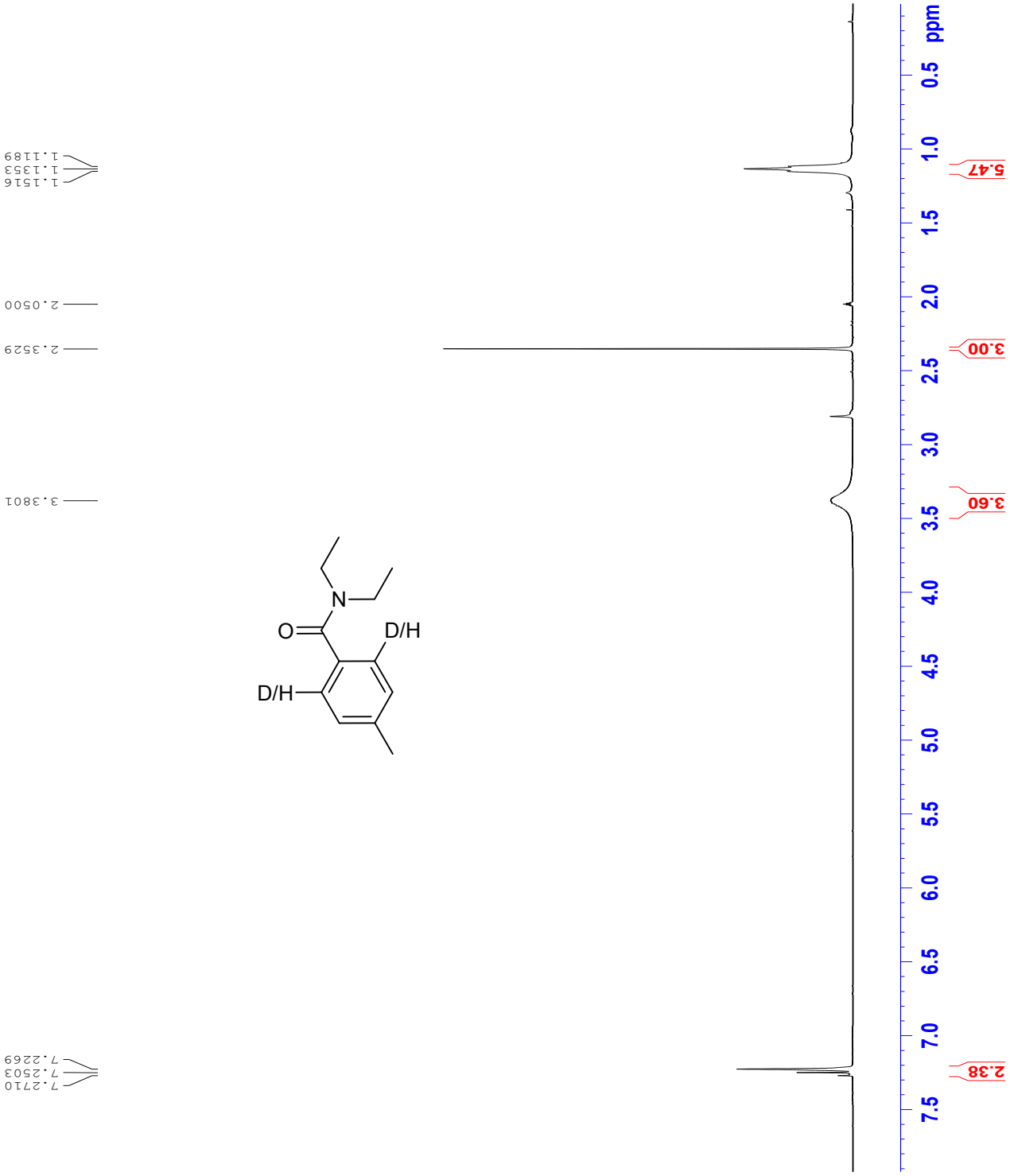
^{1}H:



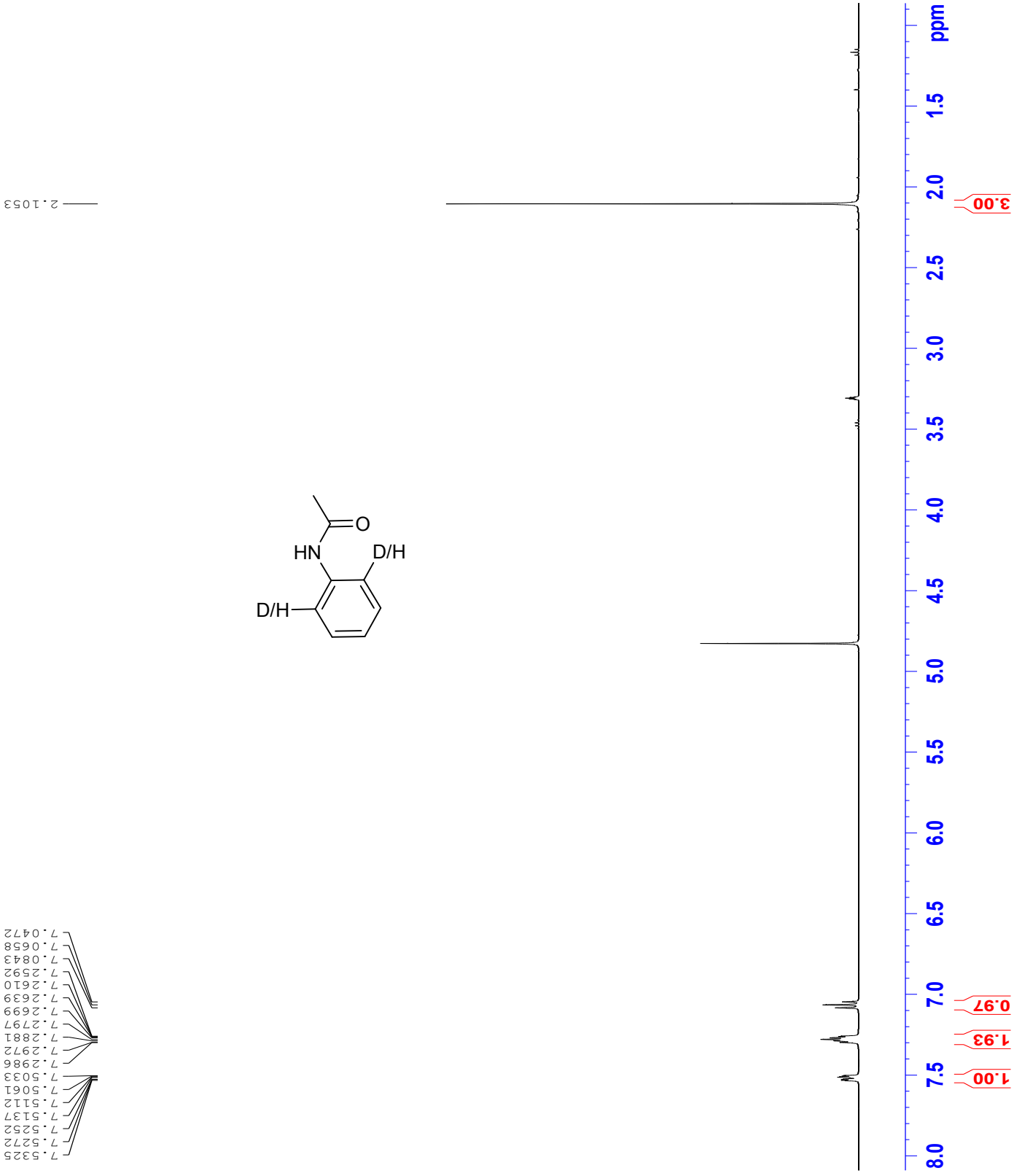
^{13}C:


11.5585
20.7512
36.2539
45.3875
77.4834
77.1619
76.8406
126.0486
128.3849
133.4056
138.6988
171.2627
D/H
N
O
D/H
D/H
ppm
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170

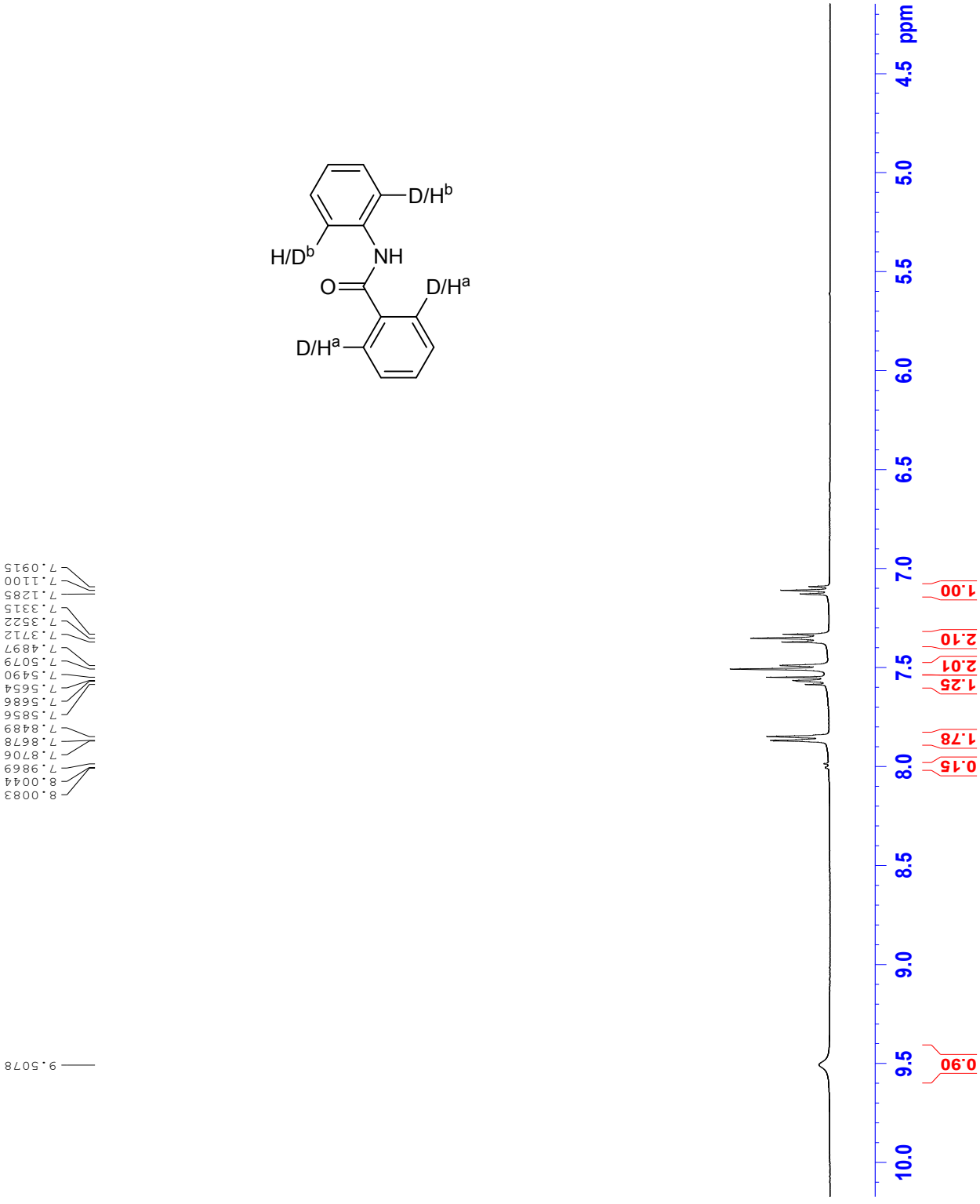
N,*N*-Diethyl-4-methylbenzamide, **16**



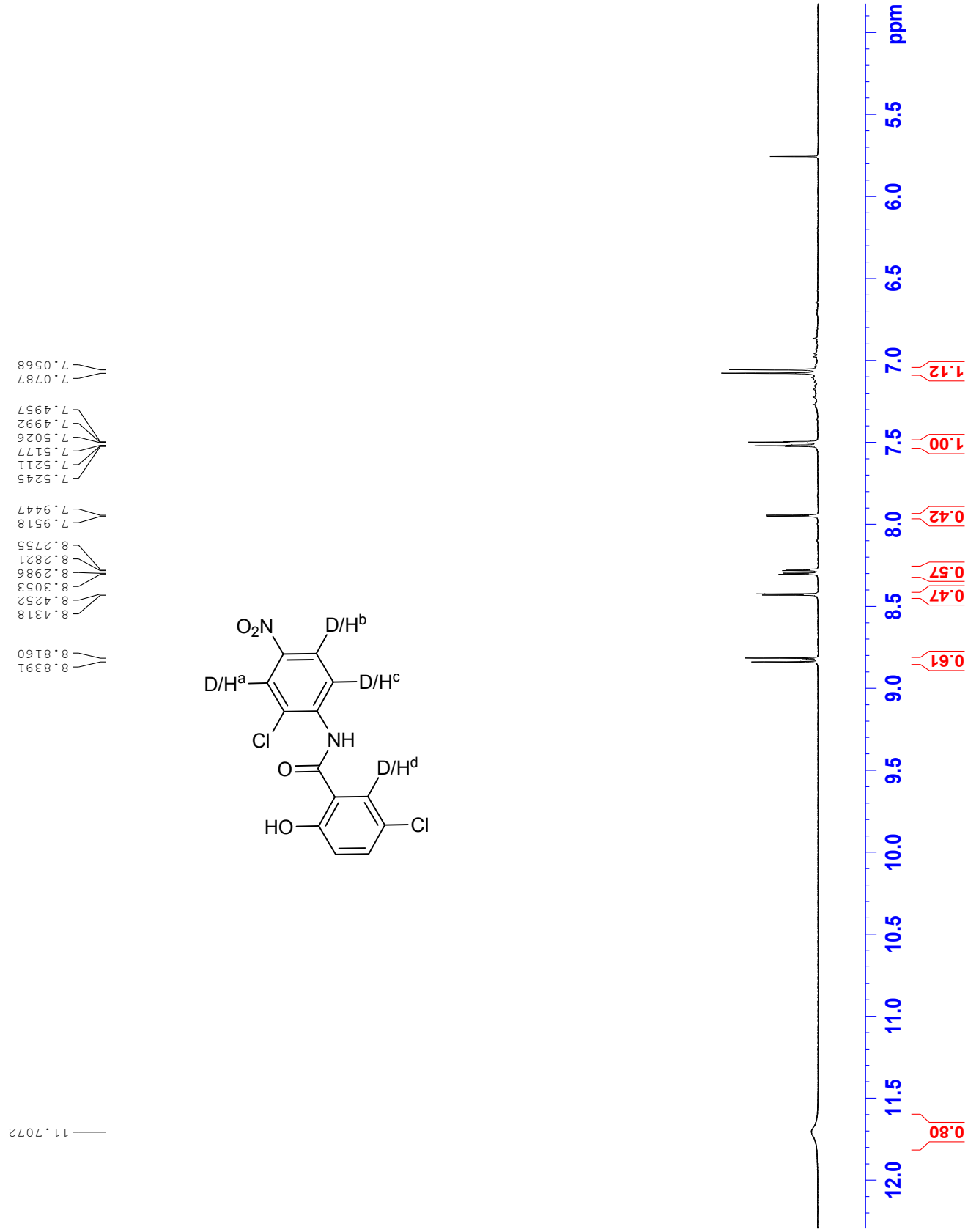
Acetanilide, **17**



Benzanilide, **18**



Niclosamide, **20**



References

[1] Z. Liu, Z.-C. Chen, Q.-G. Zheng, *Org. Lett*. **2003**, *5*, 3321-3323.

[2] Q. Dai, W. Gao, D. Lui, L. M. Kapes, X. Zhang, *J. Org. Chem.* **2006**, *71*, 3928-3934.

[3] L. Xu, D. Zhu, F. Wu, R. Wang, B. Wan, *Tetrahedron* **2005**, *61*, 6553-6560.

[4] R. Das, D. Chakraborty, *Org. Lett*. **2011**, *13*, 2976-2976.

[5] K. Hosoi, K. Nozaki, T. Hiyama, *Org. Lett.* **2002**, *4*, 2849-2851.

[6] J. McNulty, J. J. Nair, A. Robertson, *Org. Lett.* **2007**, *9*, 4575-4578.

[7] Y. Furuya, K. Ishihara, H. Yamamoto, *J. Am. Chem. Soc.* **2005**, *127*, 11240-11241.

[8] T. Yuzuri, H. Suezawa, M. Hirota, *Bull. Chem. Soc. Jpn.* **1994**, *67*, 1664-1673.

[9] a) M. Navab, *International Patent Application WO 2008021088 A2*, **2008**; b) A. M. Fogelman, M. Navab, *International Patent Application WO 2009032749 A2*, **2009**.

[10] Y. Zhao, D. G. Truhlar, *Theor. Chem. Account* **2008**, *120*, 215-241.

[11] a) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257-2261; b) M. M. Francl, W. J. Petro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees, J. A. Pople, *J. Chem. Phys.* **1982**, *77*, 3654-3665.

[12] a) D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, *77*, 123-141; b) A. Bergner, M. Dolg, W. Küchle, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *80*, 1431-1441.

[13] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09*, revision A.02; Gaussian, Inc.: Wallingford, CT, **2009**.