Azobenzene-functionalized iridium(III) tris-cyclometalated complexes

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2-(*o*-phenylazobenzene)pyridine, **1**

SYNTHESIS:

B-[2-[(1E)-2-phenyldiazenyl]phenyl]-Boronic acid (1 g, 4.424 mmol) was dissolved in 15 mL of degassed THF. To this mixture, 2-bromopyridine (0.762 g, 0.462 mL, 4.822 mmol), $Pd(PPh_3)_4$ (2 mol %, 0.102 g, 0.088 mmol), Na_2CO_3 (1M aq., 7.5 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water was added. The resulting mixture was extracted with ethyl acetate (5 x 10 mL), dried ($MgSO_4$), filtered and evaporated in *vacuo*. The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as red oil (0.917 g, 80%).

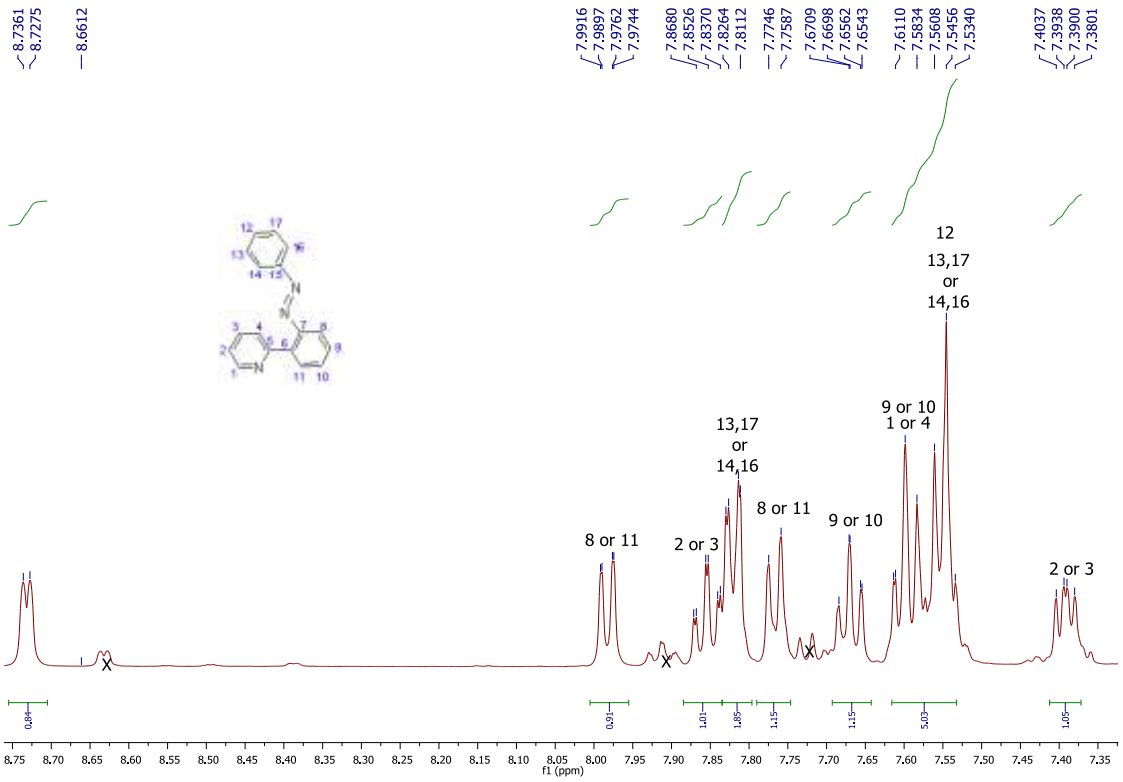
Elemental Analysis: calculated for $C_{17}H_{13}N_3 \cdot 0.1CH_2Cl_2$: C, 76.47; H, 4.96; N, 15.64. Found: C, 77.00; H, 4.80; N, 15.06.

Exact mass (MALDI) - m/z: 260.1178 for $[M + H]^+$.

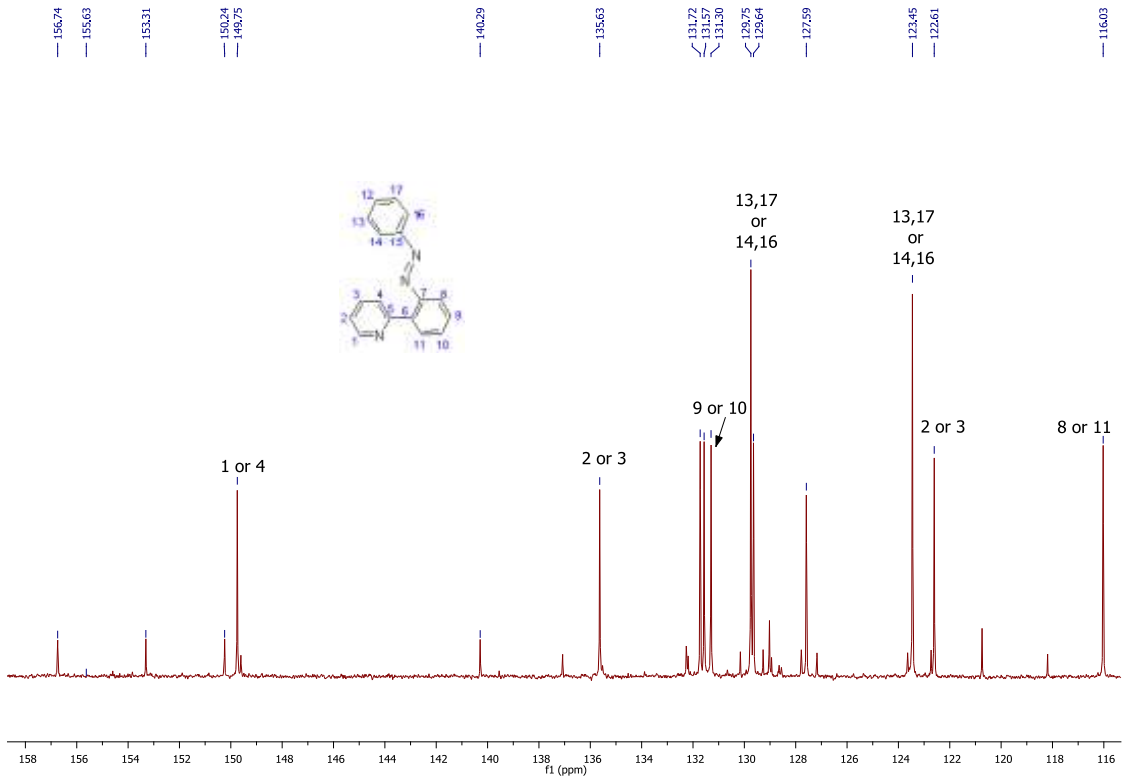
^{1}H NMR (500 MHz, Acetone): δ 8.73 (d, J = 4.3, 1H, C_5H_4N), 7.98 (dd, J = 7.7, 0.9, 1H, C_6H_4), 7.85 (td, J = 7.8, 1.7, 1H, C_5H_4N), 7.82 (dd, J = 7.8, 1.5, 2H, C_6H_5), 7.77 (d, J = 8.0, 1H, C_6H_4), 7.67 (td, J = 7.8, 1.0, 1H, C_6H_4), 7.62–7.53 (m, 5H), 7.39 (ddd, J = 6.9, 5.0, 0.9, 1H, C_5H_4N).

^{13}C NMR (126 MHz, Acetone): δ 157.13 (1C, $C_{quat.}$), 153.70 (1C, $C_{quat.}$), 150.63 (1C, $C_{quat.}$), 150.13 (1C, CH, C_5H_4N), 140.68 (1C, $C_{quat.}$), 136.02 (1C, CH, C_5H_4N), 132.11, 131.96, 131.69 (1C, CH, C_6H_4), 130.13 (2C, CH, C_6H_5), 130.03, 127.97, 123.84 (2C, CH, C_6H_5), 122.99 (1C, CH, C_5H_4N), 116.41 (1C, CH, C_6H_4).

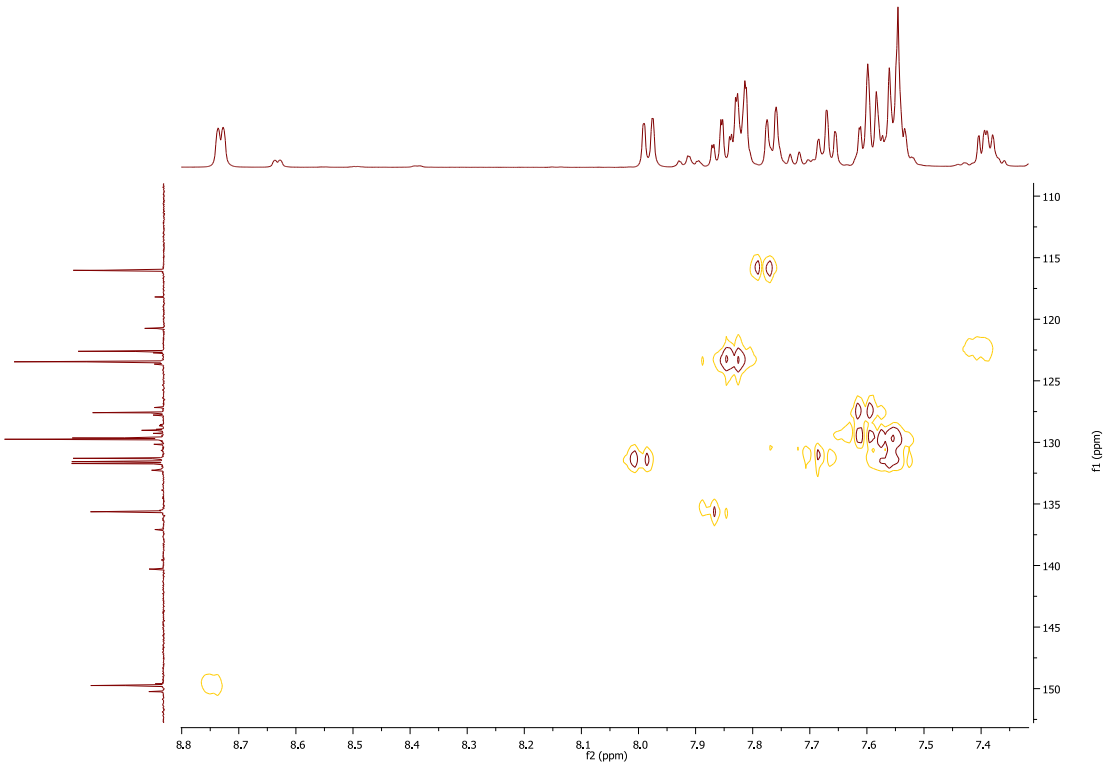
^{1}H NMR (500 MHz, Acetone):



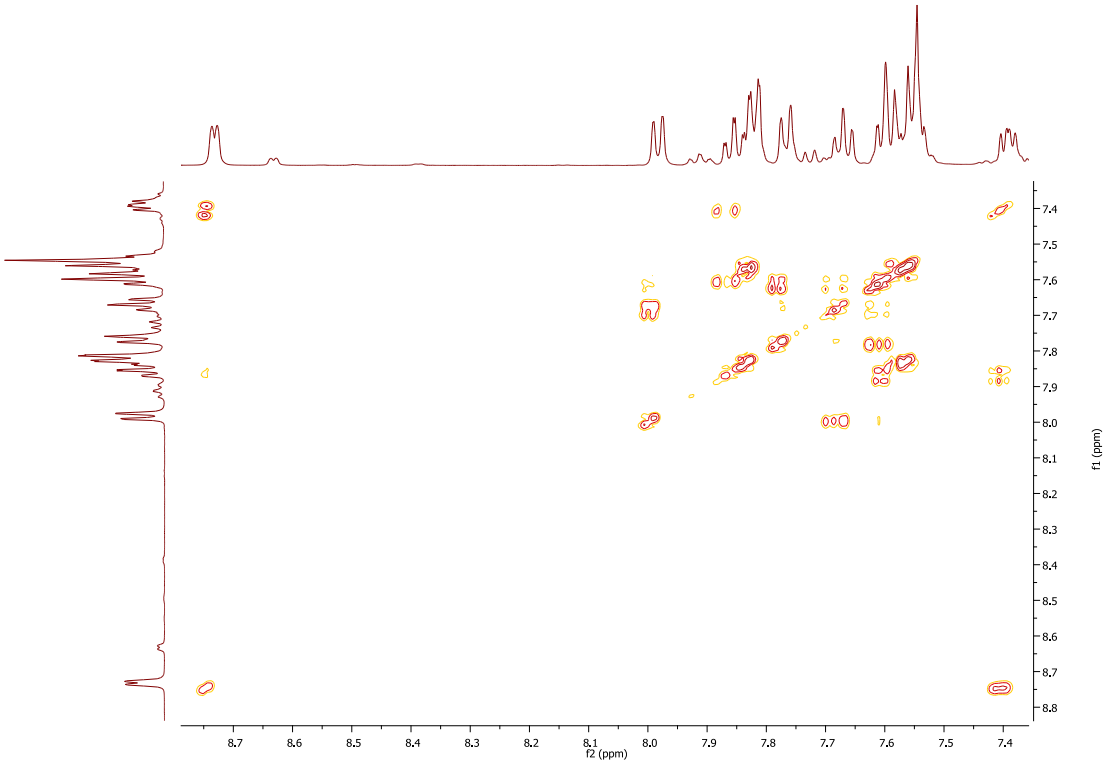
^{13}C NMR (126 MHz, Acetone):



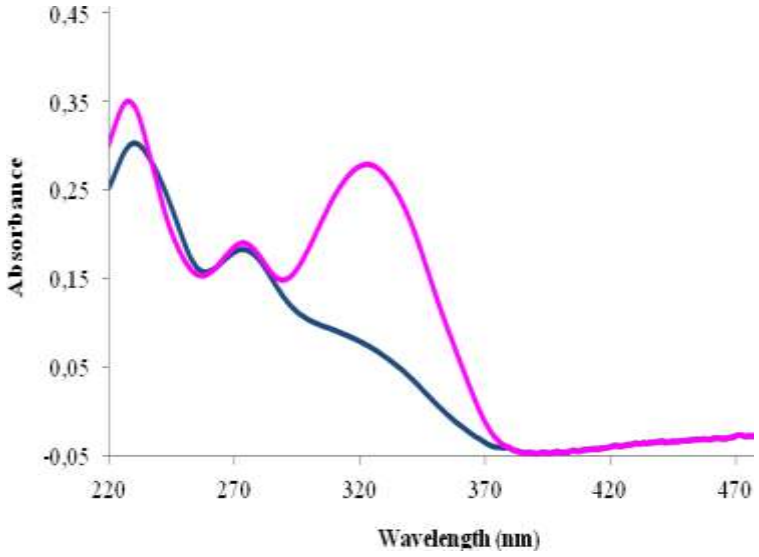
HSQC-NMR:



COSY.NMR:

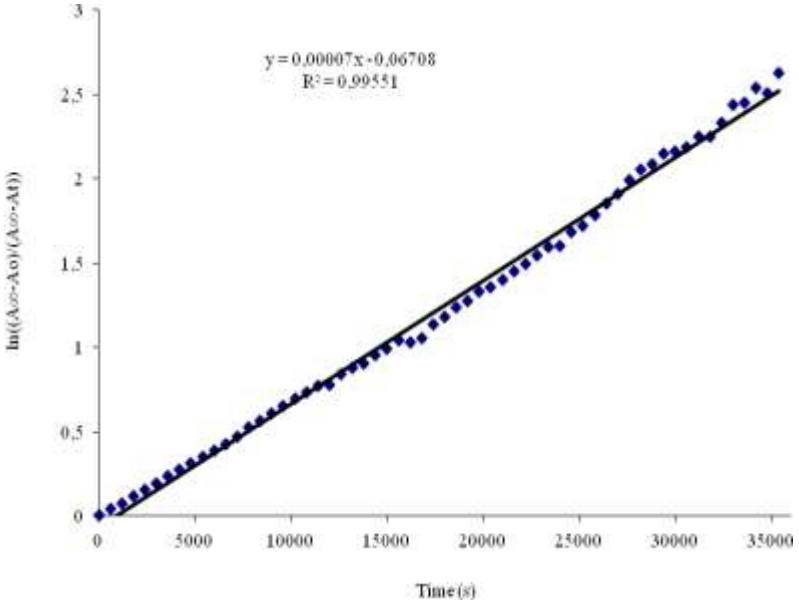


UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 327 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
323 ($1.6 \cdot 10^4$), 454 ($0.4 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 327 nm ($2.5 \cdot 10^{-5}$M). Cis to trans thermal isomerization of this complex is slow, and the A∞ (0.299) value obtained in the kinetic measure doesn't correspond to A∞ value (0.332) obtained as maximum of absorbance before the photoisomerization. We have used A∞ = 0.332 as maximum of absorbance corresponding to trans isomer.



K (s^{-1})	**$0.7 \cdot 10^{-4}$**
Half-life (s)	**9500**

2-(*m*-phenylazobenzene)pyridine, **2**

SYNTHESIS:

B-[3-[(1E)-2-phenyldiazenyl]phenyl]-Boronic acid (1 g, 4.424 mmol) was dissolved in 15 mL of degassed THF. To this mixture, 2-bromopyridine (0.762 g, 0.462 mL, 4.822 mmol), $Pd(PPh_3)_4$ (2 mol %, 0.102 g, 0.088 mmol), Na_2CO_3 (1M aq., 7.5 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water was added. The resulting mixture was extracted with ethyl acetate (5 x 10 mL), dried ($MgSO_4$), filtered and evaporated in *vacuo*. The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as red oil (0.906 g, 79%).

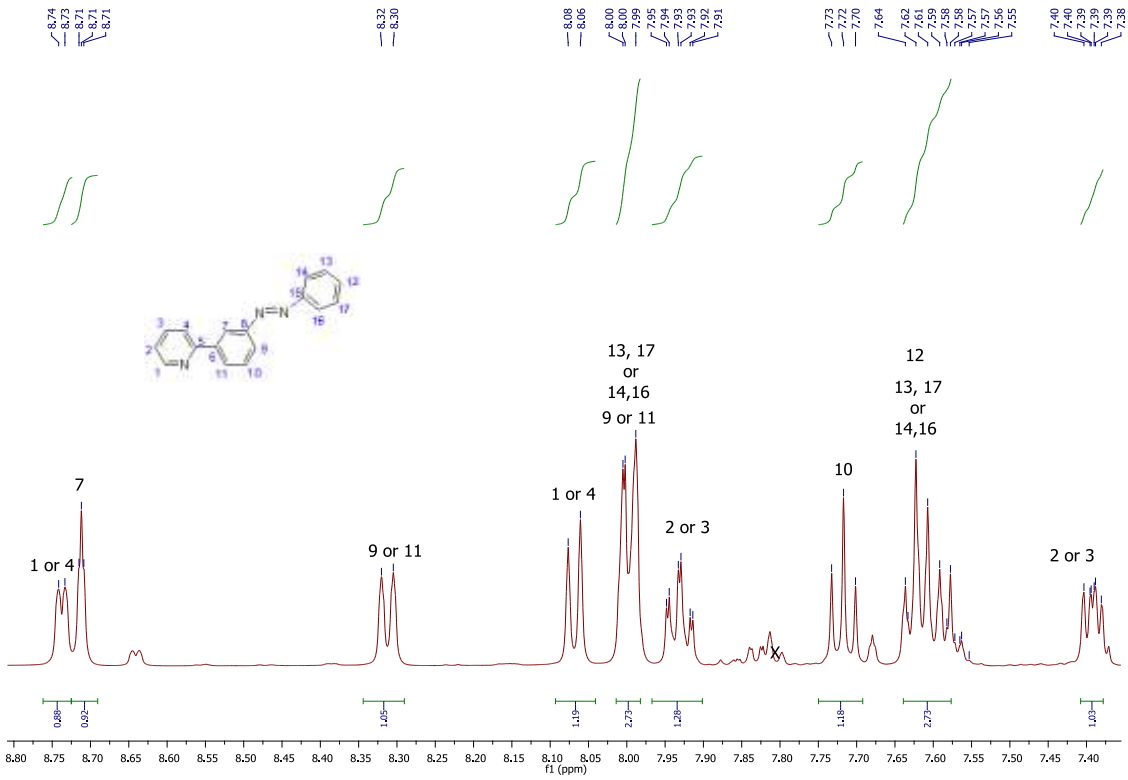
Elemental Analysis: calculated for $C_{17}H_{13}N_3 \cdot 0.7CH_2Cl_2$: C, 67.16; H, 4.57; N, 13.30. Found: C, 67.41; H, 4.15; N, 13.79.

Exact mass (MALDI) - m/z: 260.1175 for $[M + H]^+$.

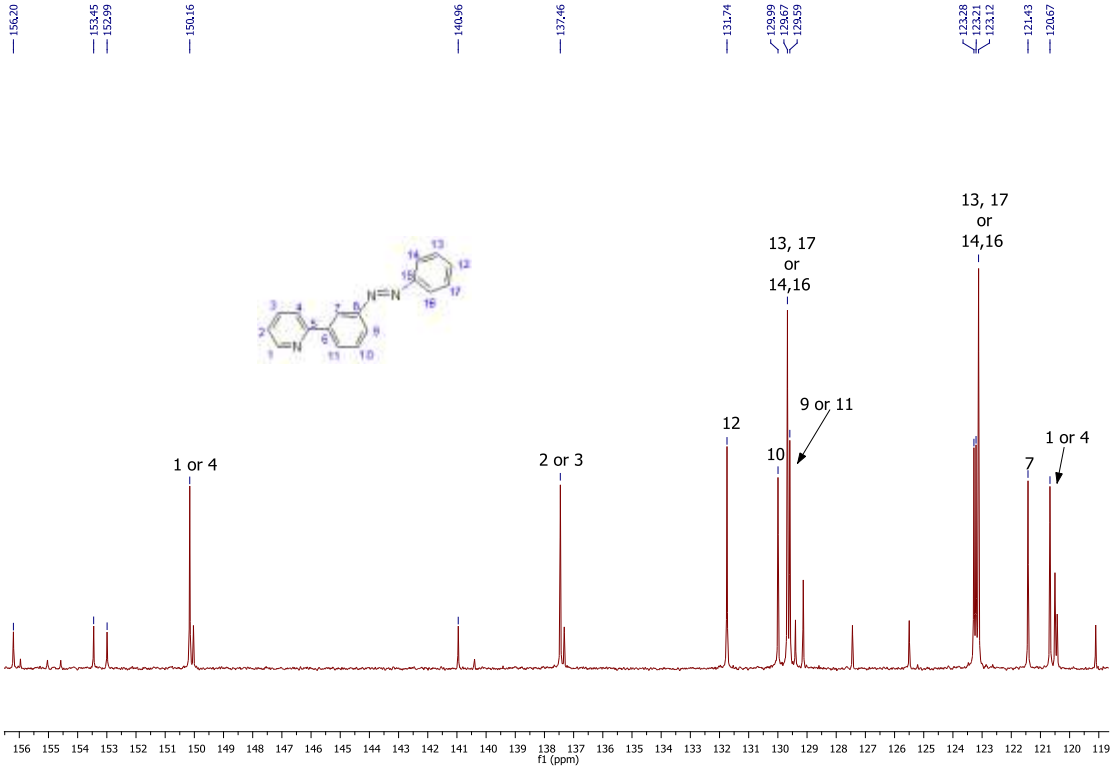
^{1}H NMR (500 MHz, Acetone): δ 8.74 (d, J = 4.1, 1H, C_5H_4N), 8.71 (t, J = 1.6, 1H, C_6H_4), 8.31 (d, J = 7.7, 1H, C_6H_4), 8.07 (d, J = 8.0, 1H, C_5H_4N), 8.01–7.98 (m, 3H), 7.93 (td, J = 7.7, 1.8, 1H, C_5H_4N), 7.72 (t, J = 7.8, 1H, C_6H_4), 7.64–7.58 (m, 3H, C_6H_5), 7.39 (ddd, J = 7.6, 4.7, 0.9, 1H, C_5H_4N).

^{13}C NMR (126 MHz, Acetone): δ 156.20 (1C, $C_{quat.}$), 153.45 (1C, $C_{quat.}$), 152.99 (1C, $C_{quat.}$), 150.16 (1C, CH, C_5H_4N), 140.96 (1C, $C_{quat.}$), 137.46 (1C, CH, C_5H_4N), 131.74 (1C, CH, C_6H_5), 129.99 (1C, CH, C_6H_4), 129.67 (2C, CH, C_6H_5), 129.59 (1C, CH, C_6H_4), 123.28 (1C, CH), 123.21 (1C, CH), 123.12 (2C, CH, C_6H_5), 121.43 (1C, CH, C_6H_4), 120.67 (1C, CH, C_5H_4N).

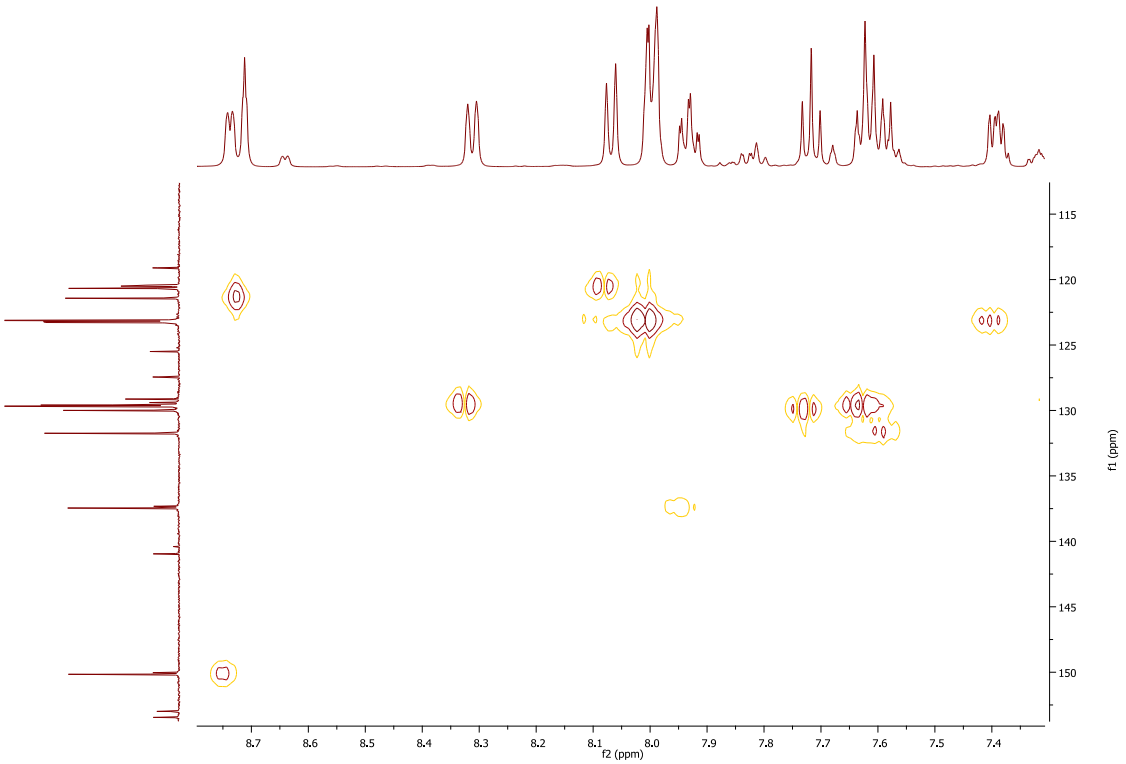
^{1}H NMR (500 MHz, Acetone):



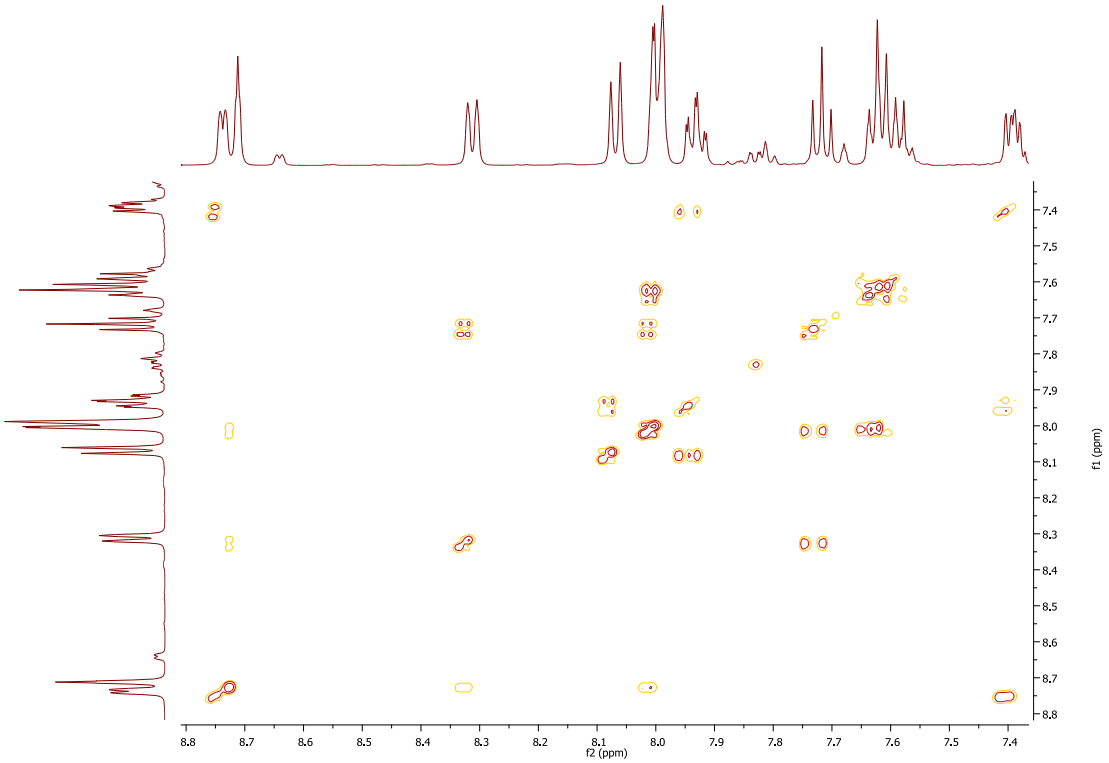
^{13}C NMR (126 MHz, Acetone):



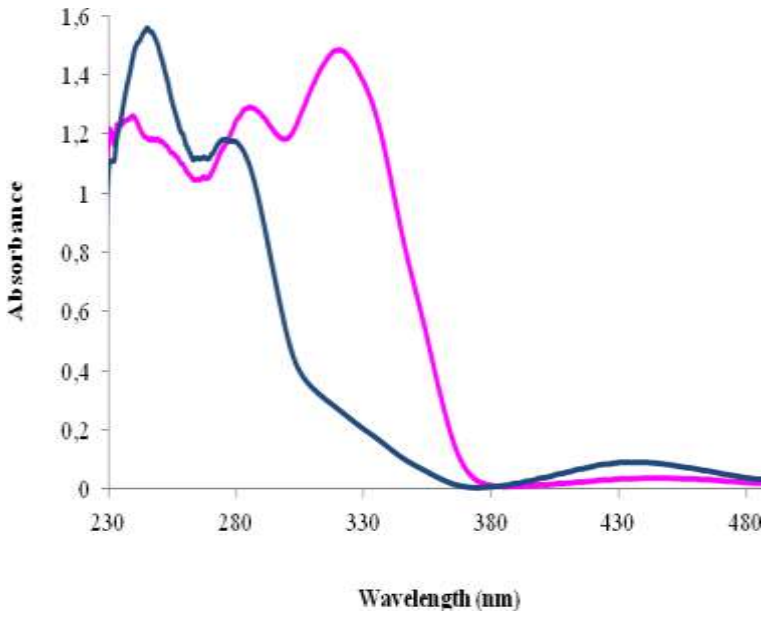
HSQC-NMR:



COSY.NMR:

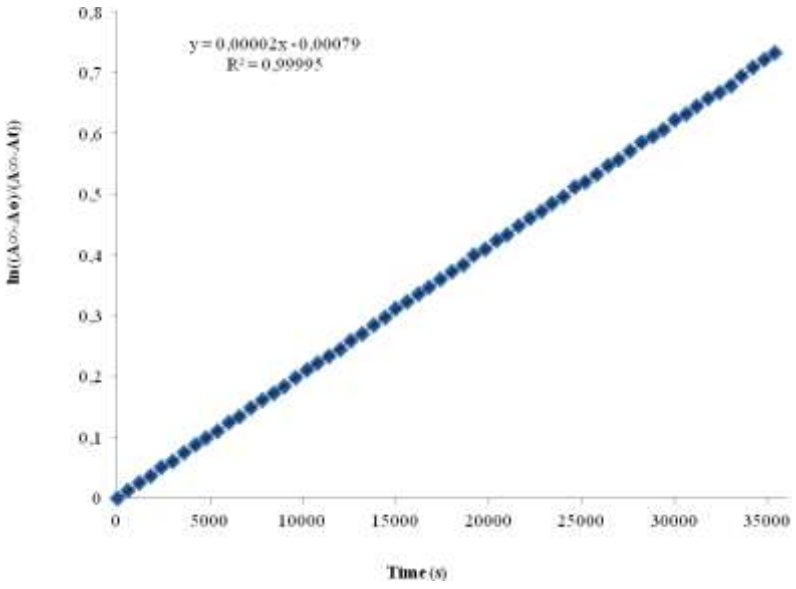


UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 321 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
319 ($1.8 \cdot 10^4$), 429 ($0.4 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 321 nm ($2.5 \cdot 10^{-5}$M). Cis to trans thermal isomerization of this complex is slow, and the A∞ (1.354) value obtained in the kinetic measure doesn't correspond to A∞ value (1.954) obtained as maximum of absorbance before the photoisomerization. We have used A∞ = 1.954 as maximum of absorbance corresponding to trans isomer.



K (s^{-1})	**$0.2 \cdot 10^{-4}$**
Half-life (s)	**33000**

2-(*p*-phenylazobenzene)pyridine, **3**

SYNTHESIS:

1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (1 g, 3.245 mmol) was dissolved in 15 mL of degassed THF. To this mixture, 2-bromopyridine (0.559 g, 0.339 mL, 3.537 mmol), $Pd(PPh_3)_4$ (2 mol %, 0.075 g, 0.065 mmol), Na_2CO_3 (1M aq., 7.5 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water was added. The resulting mixture was extracted with ethyl acetate (5 x 10 mL), dried ($MgSO_4$), filtered and evaporated in *vacuo*. The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as orange powder (0.589 g, 70%).

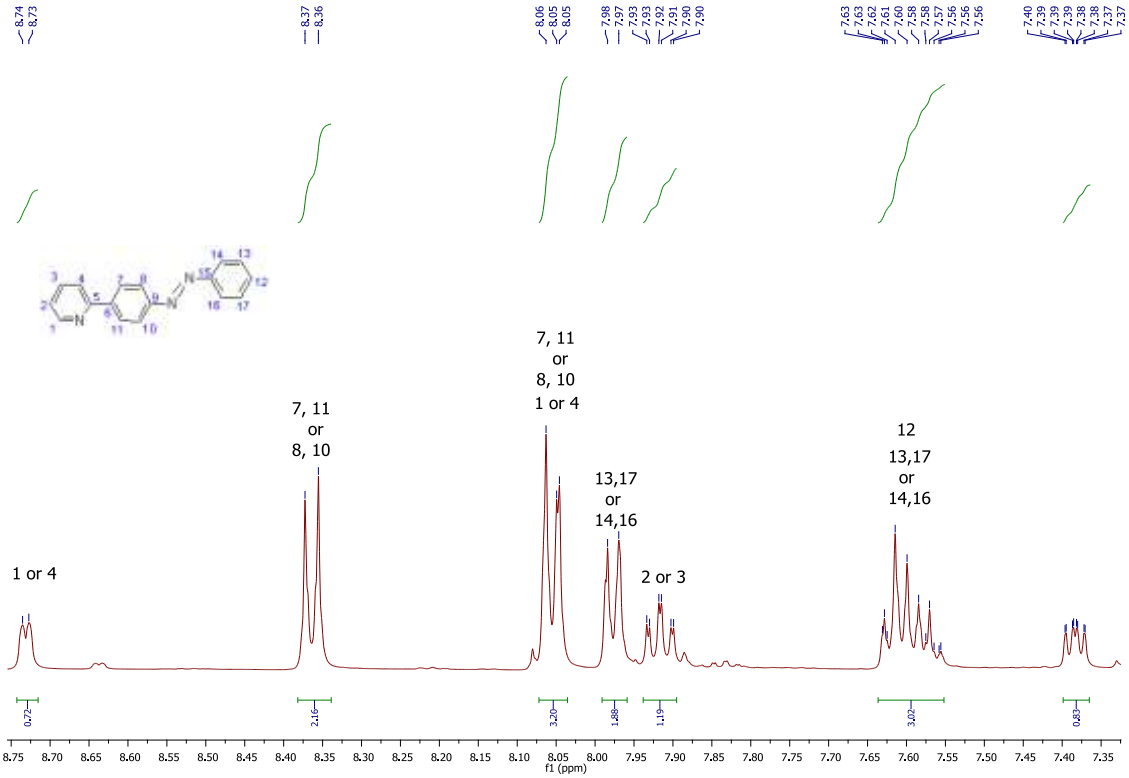
Elemental Analysis: calculated for $C_{17}H_{13}N_3$: C, 78.74; H, 5.05; N, 16.20. Found: C, 78.78; H, 5.04; N, 15.94.

Exact mass (MALDI) - m/z: 260.1178 for $[M + H]^+$

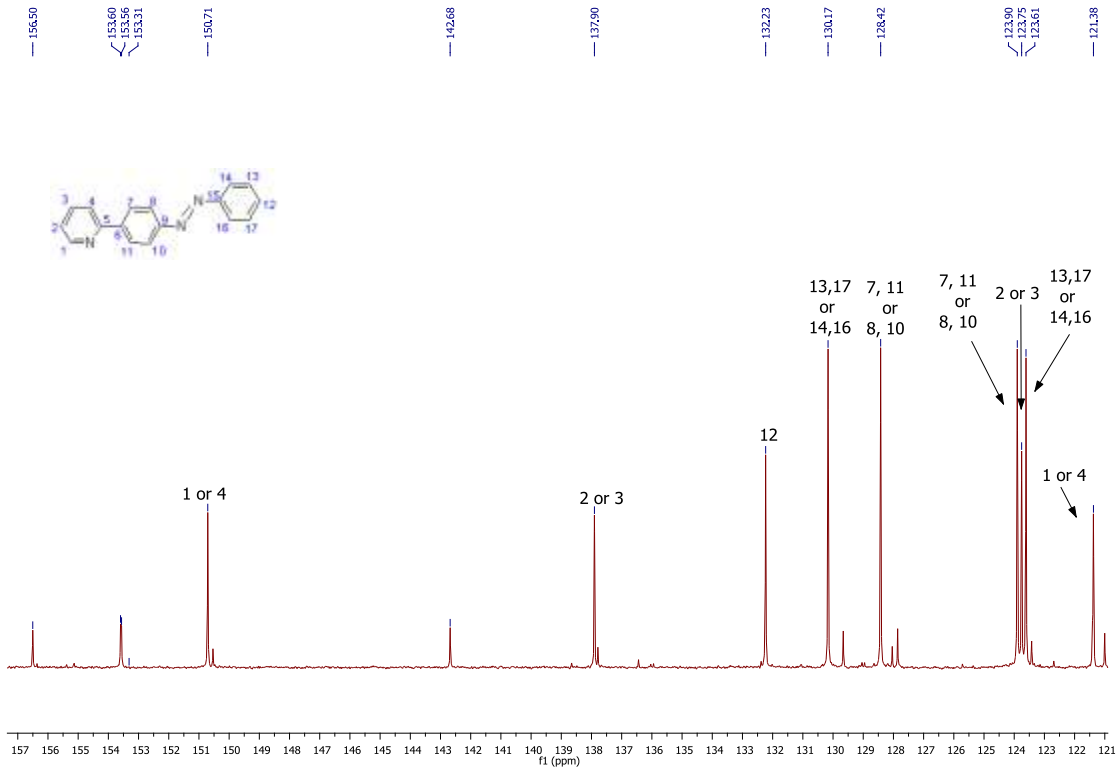
^{1}H NMR (500 MHz, Acetone): δ 8.73 (d, J = 4.0, 1H, C_5H_4N), 8.36 (d, J = 8.6, 2H, C_6H_4), 8.07–8.04 (m, 3H), 7.98 (d, J = 7.2, 2H, C_6H_5), 7.92 (td, J = 7.8, 1.7, 1H, C_5H_4N), 7.64–7.55 (m, 3H, C_6H_5), 7.38 (ddd, J = 7.4, 4.8, 0.7, 1H, C_5H_4N).

^{13}C NMR (126 MHz, Acetone): δ 156.50 (1C, $C_{quat.}$), 153.60 (1C, $C_{quat.}$), 153.56 (1C, $C_{quat.}$), 150.71 (1C, CH, C_5H_4N), 142.68 (1C, $C_{quat.}$), 137.90 (1C, CH, C_5H_4N), 132.23 (1C, CH, C_6H_5), 130.17 (2C, CH, C_6H_5), 128.42 (2C, CH, C_6H_4), 123.90 (2C, CH, C_6H_4), 123.75 (1C, CH, C_5H_4N), 123.61 (2C, CH, C_6H_5), 121.38 (1C, CH, C_5H_4N).

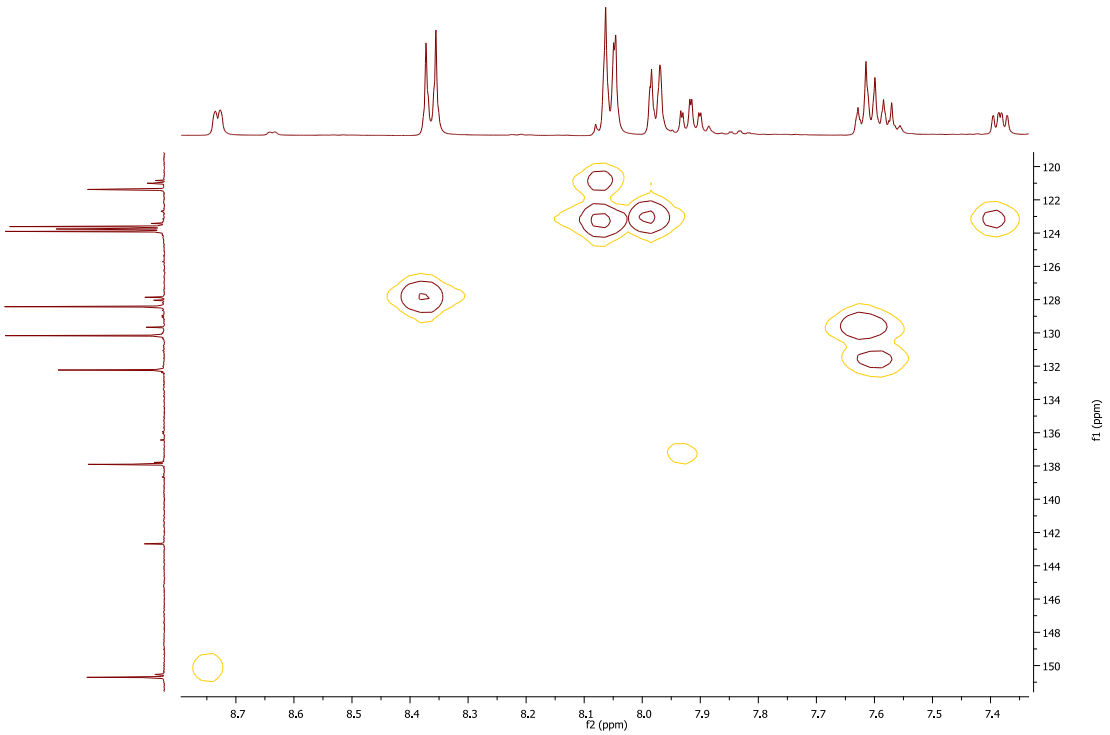
^{1}H NMR (500 MHz, Acetone):



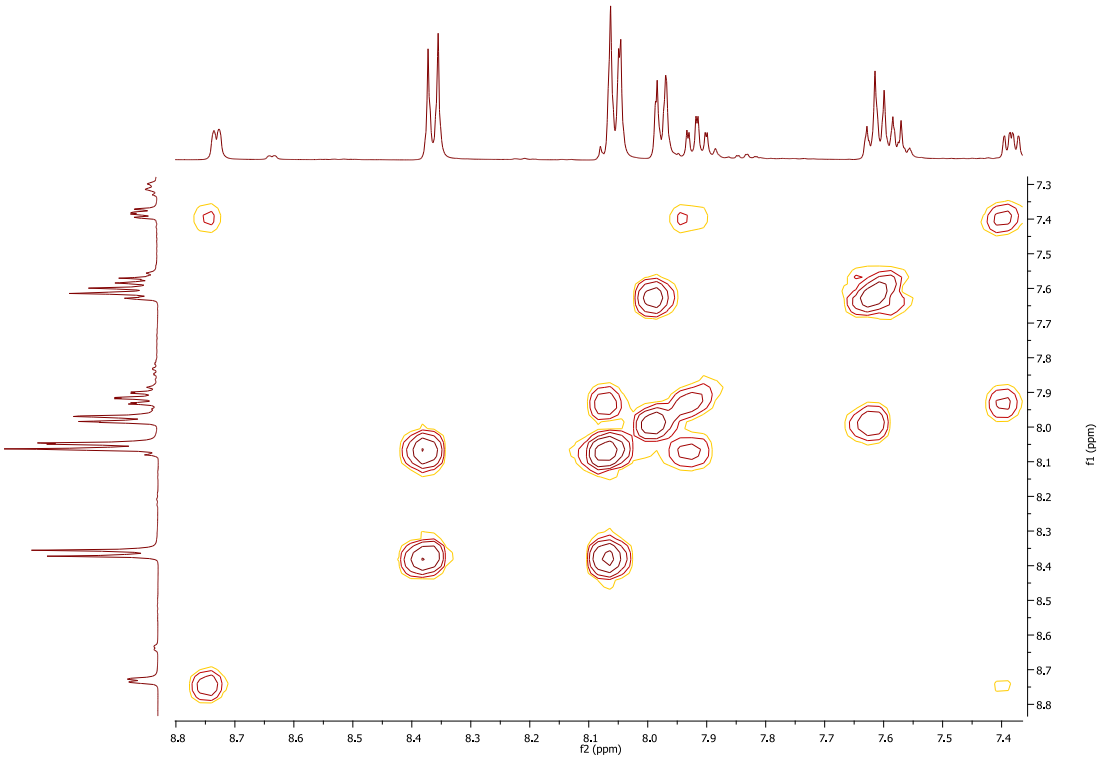
^{13}C NMR (126 MHz, Acetone):



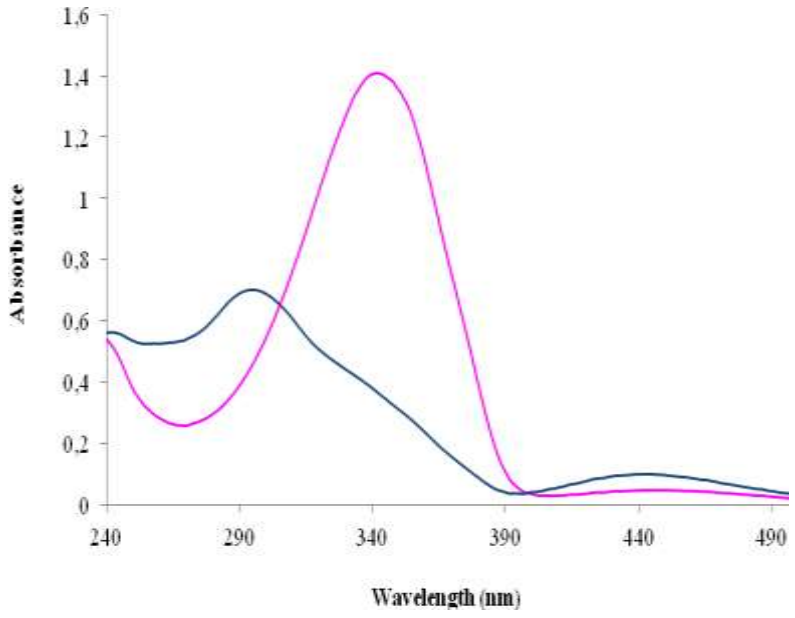
HSQC-NMR:



COSY.NMR:

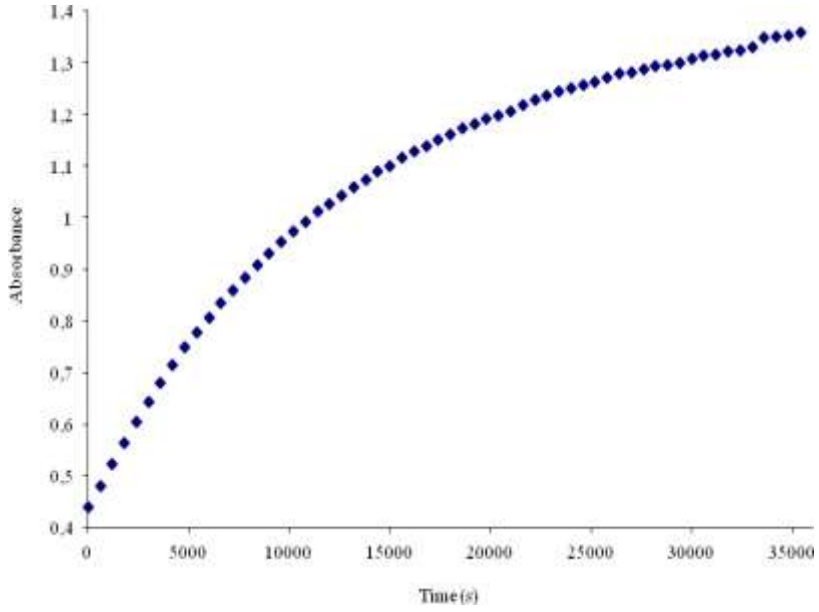


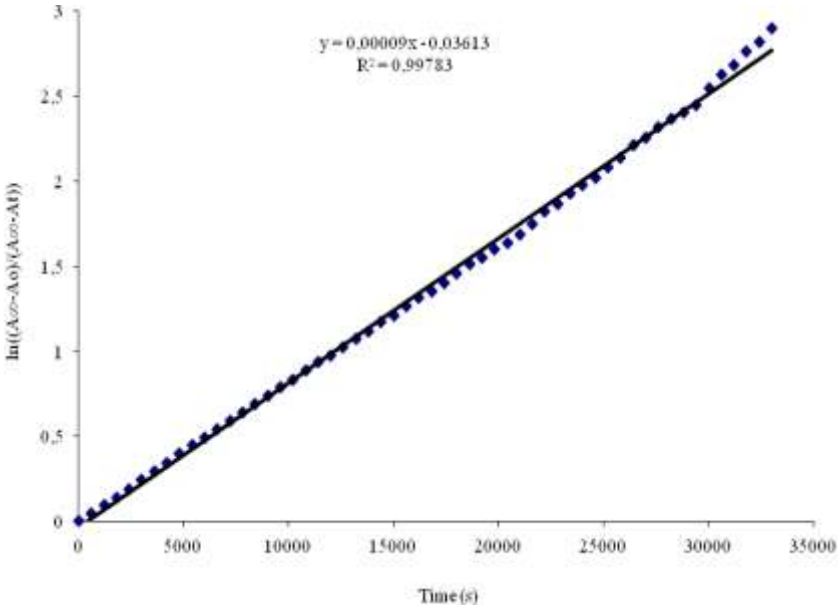
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 343 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
339 ($2.8 \cdot 10^4$), 439 ($0.9 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 343 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$0.9 \cdot 10^{-4}$**
Half-life (s)	**8100**

(2-phenyl(4-azophenyl)pyridine)**, 4**

SYNTHESIS:

2-(4-bromophenyl)pyridine (0.300g, 0.128mmol) was dissolved in 4 mL of degassed THF. To this mixture, 4-azophenylboronic acid pinacol ester , f, (0.434mg, 0.141mmol), $Pd(PPh_3)_4$ (2 mol %, 2.958mg, 0.003mmol), and Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50ml of water was added. The resulting mixture was extracted with ethyl acetate (5 x 10 mL). The organic phase was dried ($MgSO_4$), and filtered. After evaporation of the solvent from the filtrate, the resulting solid was purified by column chromatography eluting with dichloromethane. The product was obtained as a light orange powder (0.260g, 60%).

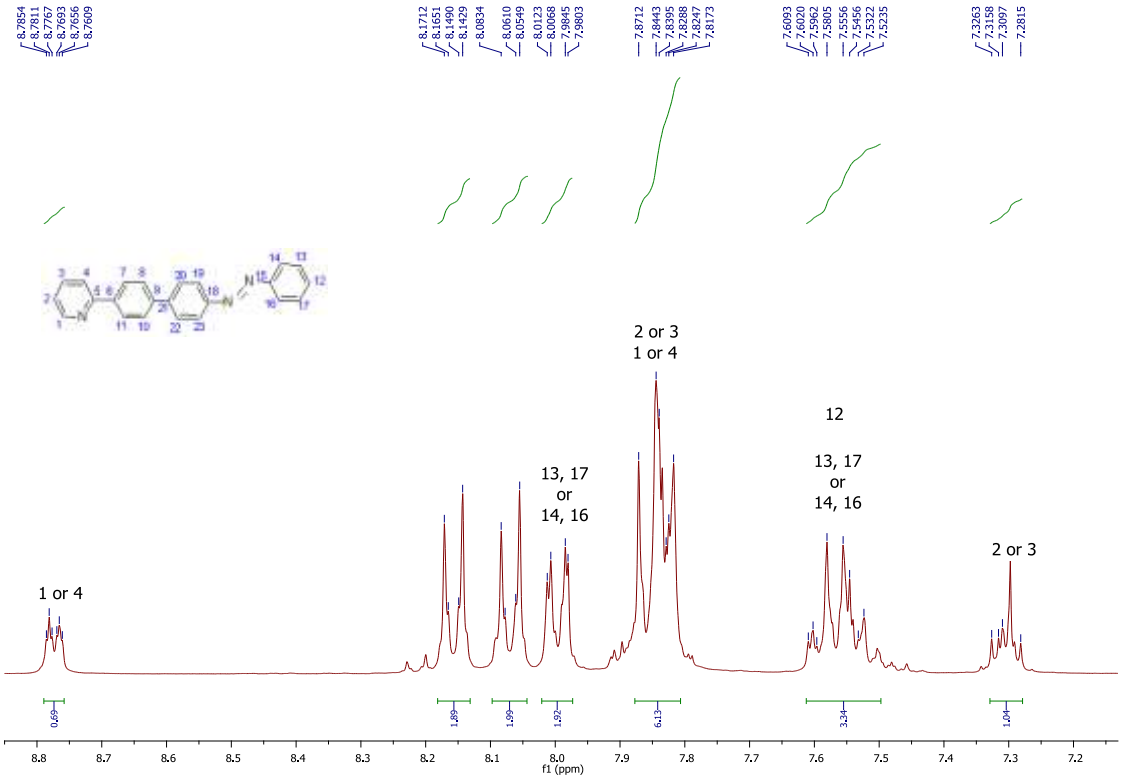
Elemental Analysis: calculated for $C_{23}H_{17}N_3$: C, 82.36; H, 5.11; N, 12.53. Found: C, 82.17; H, 5.03; N, 12.53.

Exact mass (MALDI) - m/z: 336.1485 for $[M + H]^+$.

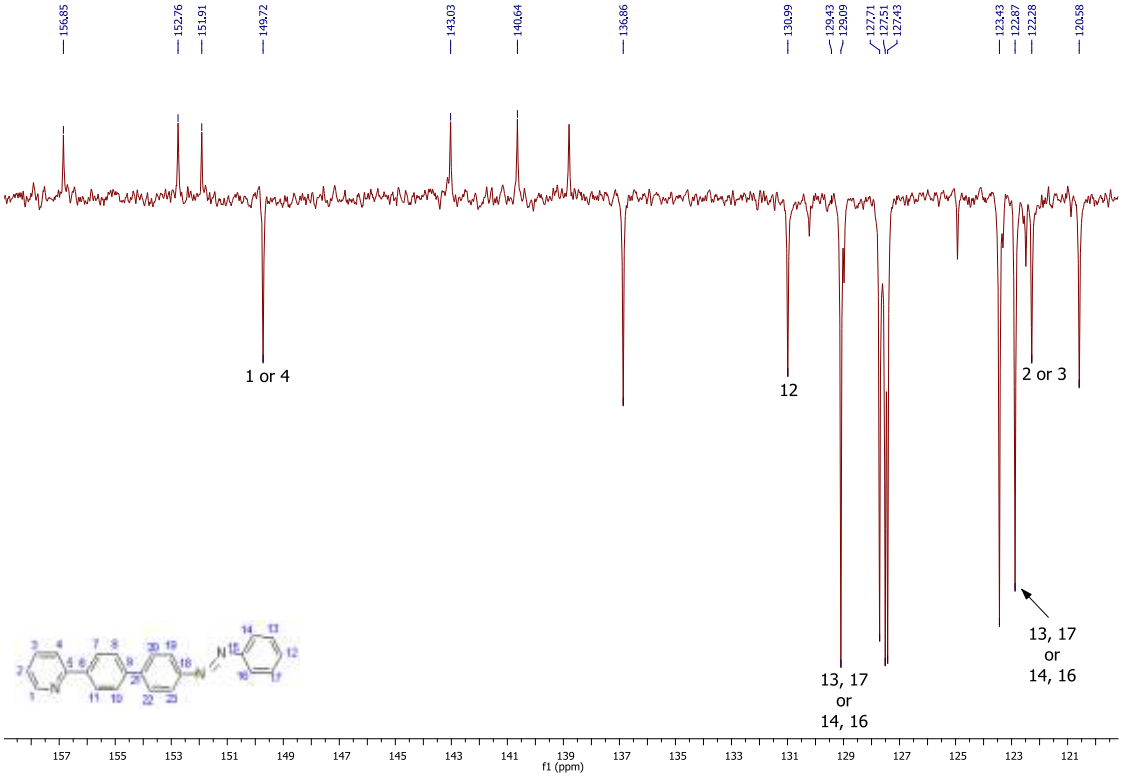
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.77 (ddd, *J* = 4.8, 1.3, 1.3, 1H, C_5H_4N), 8.16 (d, *J* = 8.5, 2H, C_6H_4), 8.07 (d, *J* = 8.6, 2H, C_6H_4), 8.00 (dd, *J* = 8.2, 1.5, 2H, C_6H_5), 7.88 – 7.81 (m, 6H), 7.61 – 7.50 (m, 3H, C_6H_5), 7.33 – 7.28 (ddd, *J* = 5.0, 5.0, 3.2, 1H, C_5H_4N).

^{13}C NMR (75 MHz, $CDCl_3$): δ 156.85 (1C, $C_{quat.}$), 152.76 (1C, $C_{quat.}$), 151.91 (1C, $C_{quat.}$), 149.72 (1C, CH, C_5H_4N), 143.03 (1C, $C_{quat.}$), 140.64 (1C, $C_{quat.}$), 138.80 (1C, $C_{quat.}$), 136.86 (1C, CH, C_5H_4N), 130.99 (1C, CH, C_6H_5), 129.09 (2C, CH, C_6H_5), 127.71 (2C, CH, C_6H_4), 127.51 (2C, CH, C_6H_4), 127.43 (2C, CH, C_6H_4), 123.43 (2C, CH, C_6H_4), 122.87 (2C, CH, C_6H_5), 122.28 (1C, CH, C_5H_4N), 120.58 (1C, CH, C_5H_4N).

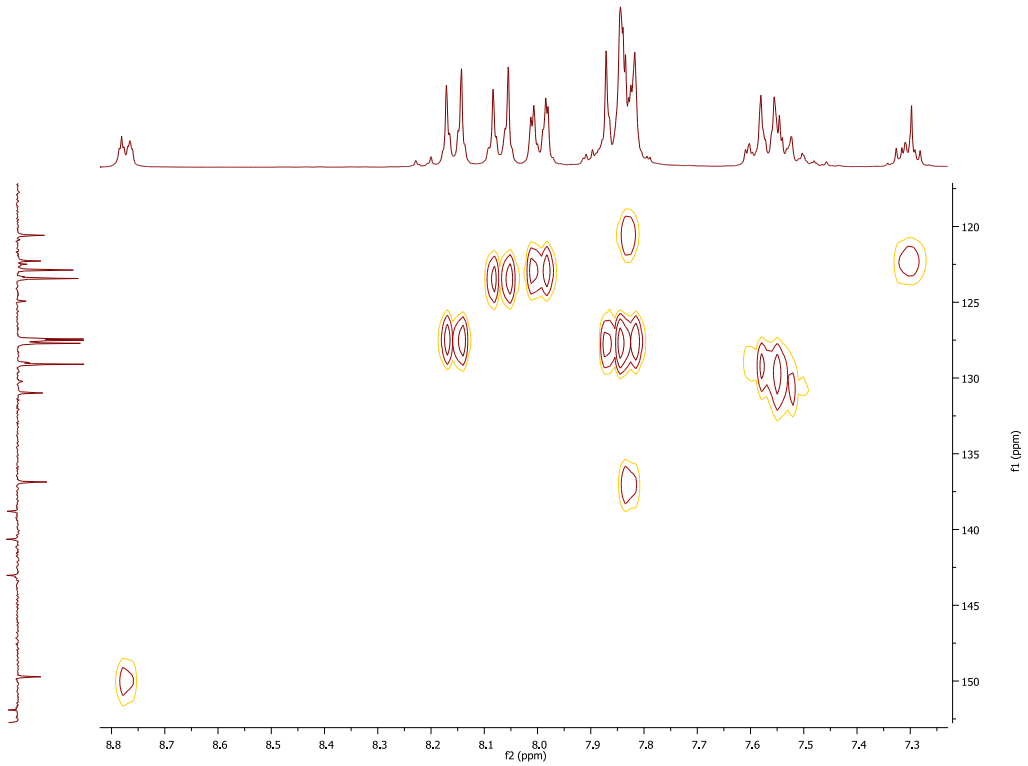
^{1}H NMR (300 MHz, $CDCl_3$):



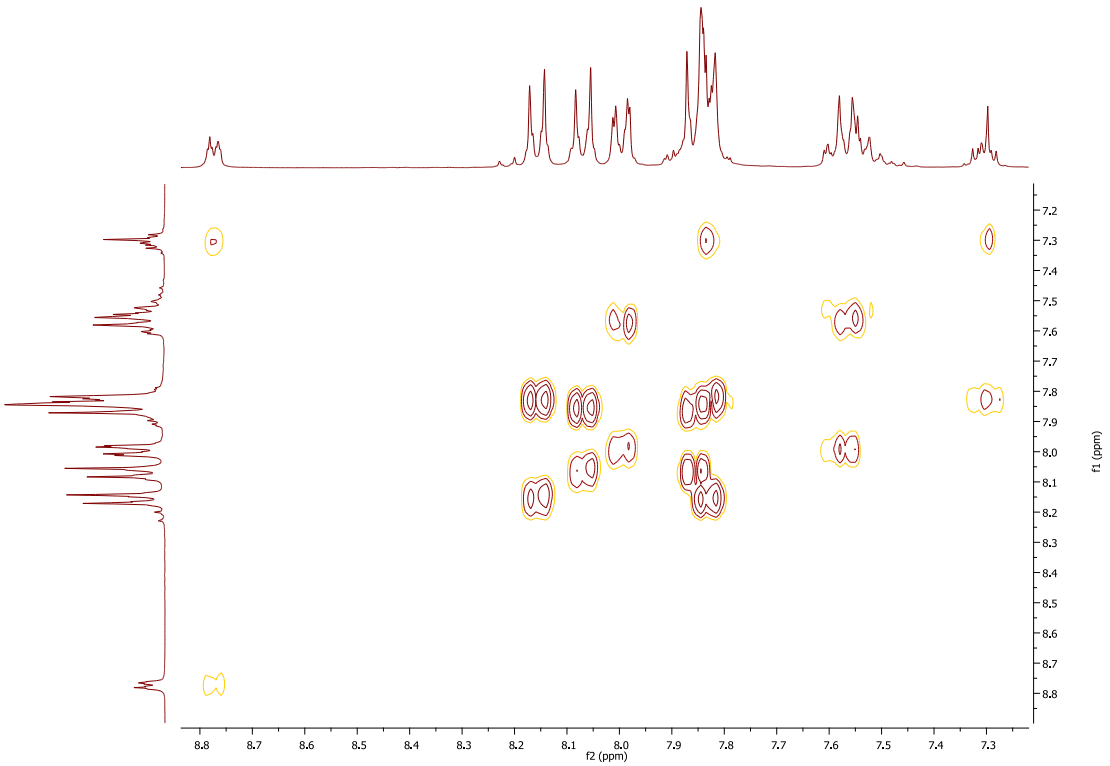
^{13}C APT NMR (75 MHz, $CDCl_3$):



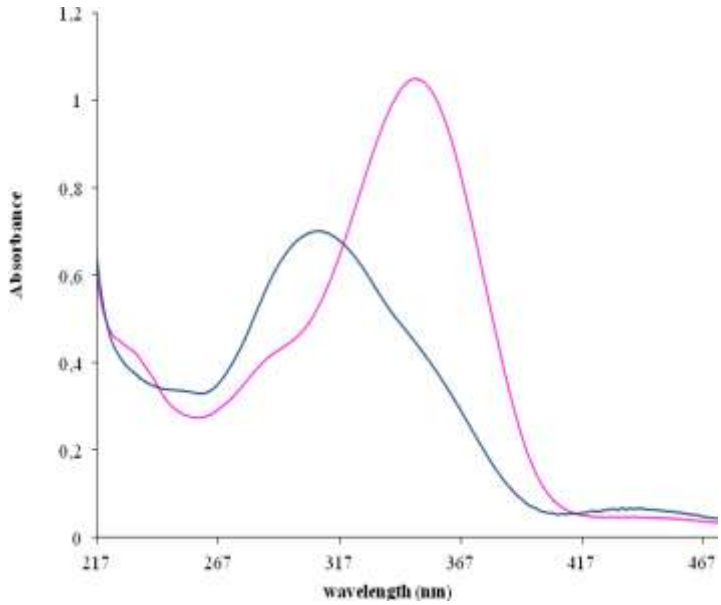
HSQC-NMR:



COSY.NMR:

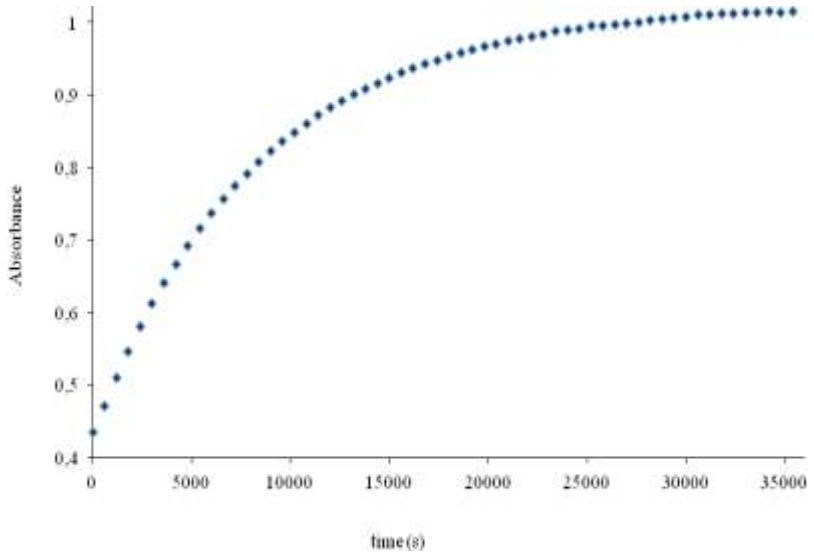


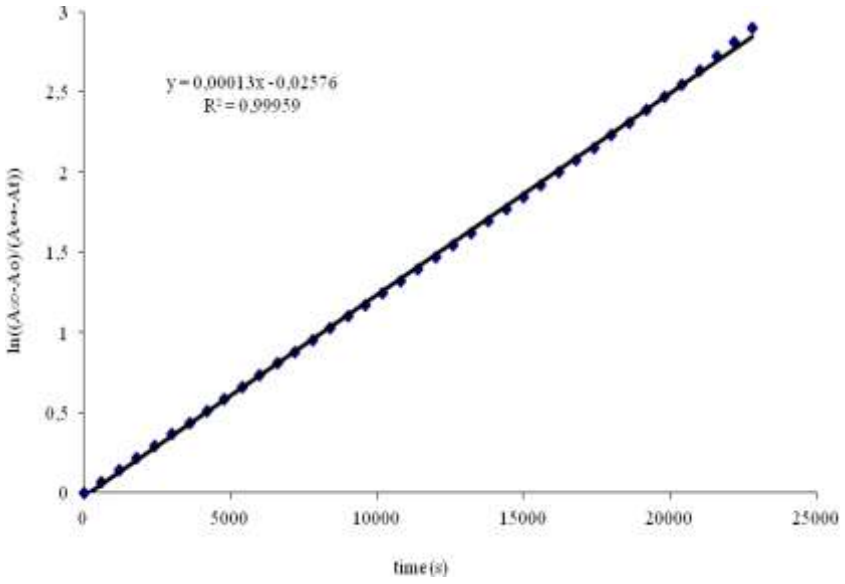
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 354 nm.



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
348 ($3.8 \cdot 10^4$), 441 ($1.4 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 354 nm ($2{,}5 \cdot 10^{-5}$M).



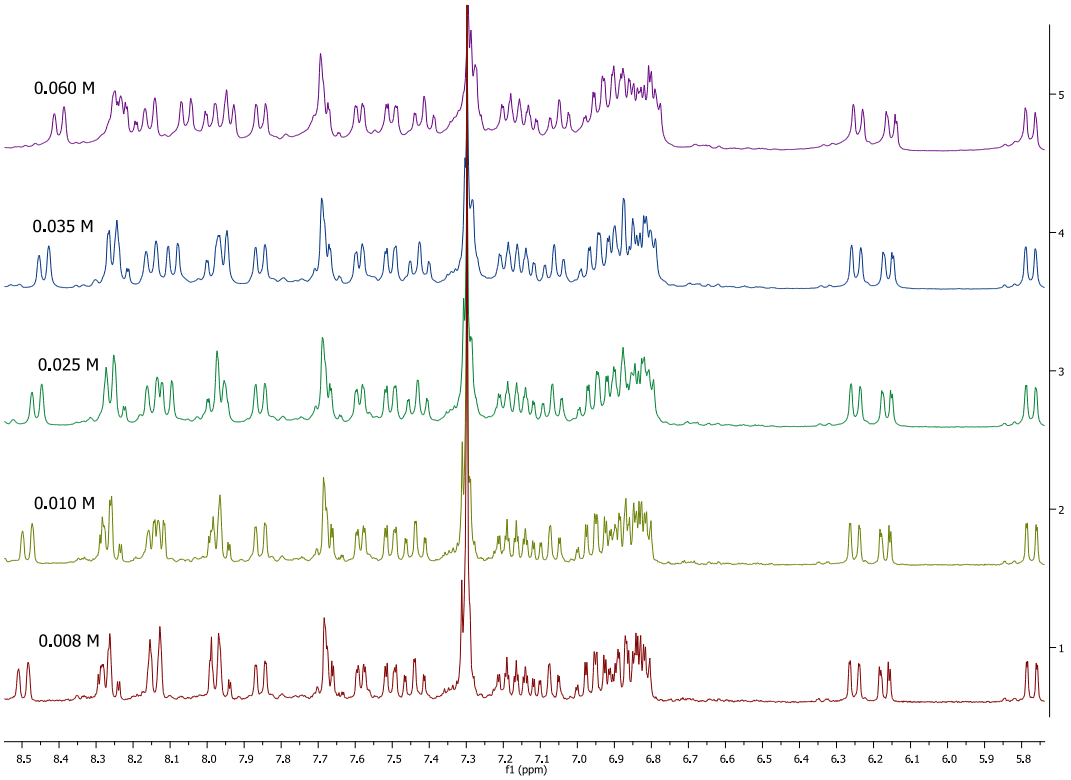


K (s^{-1})	**$1.3 \cdot 10^{-4}$**
Half-life (s)	**5500**

[Ir(ppy)$_2$1][OTf], **A1'**

SYNTHESIS:

[Ir(ppy)$_2$Cl]$_2$ (0.150 g, 0.140 mmol) and silver triflate (0.108 g, 0.420 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **1** (0.146 g, 0.560 mmol) and triethylamine (0.147 mL, 1.054 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with ethyl acetate; when the ligand is extracted, we add acetone for the extraction of the complex (the complex degrades with solvent). The product was obtained as dark-red crystalline solid (0.178 g, 70%). The NMR-spectra of the complex varies with the concentration.



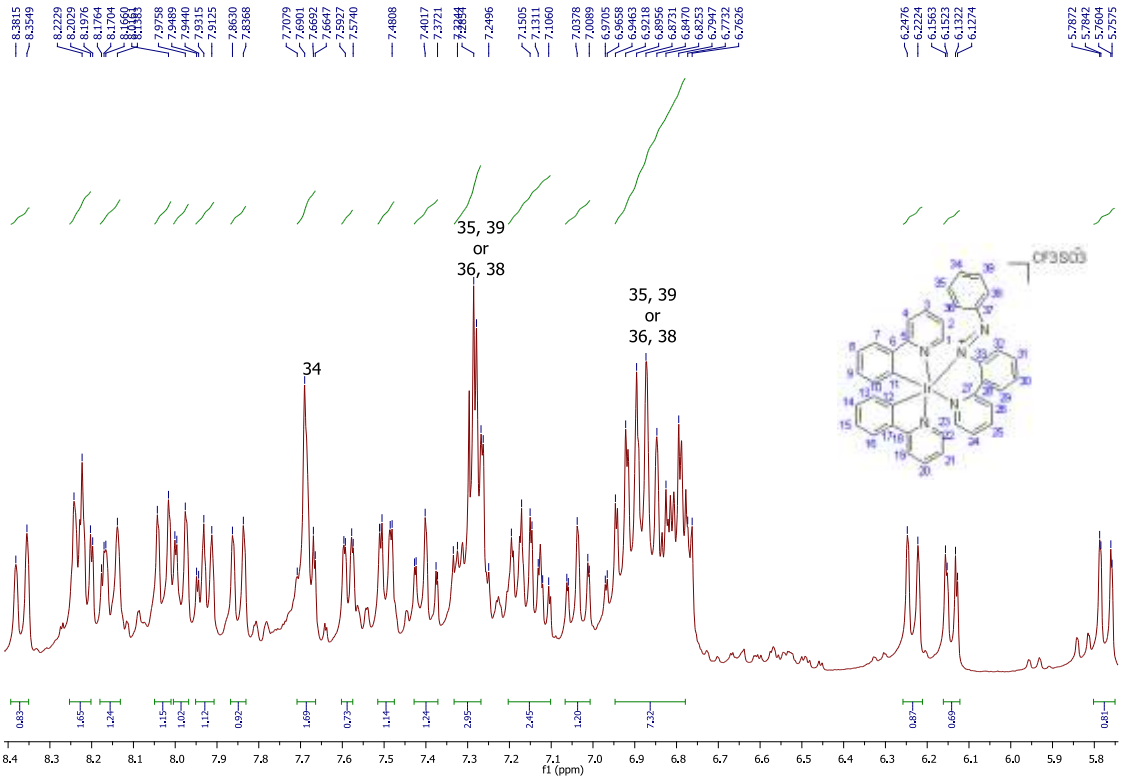
Elemental Analysis: calculated for $C_{40}H_{29}F_3IrN_5O_3S$: C, 52.85; H, 3.22; N, 7.70; S, 3.53. Found: C, 52.47; H, 3.62; N, 7.69; S, 3.54.

Exact mass (EI) - m/z: 760.2070 for $[M]^+$ with (^{193}Ir).

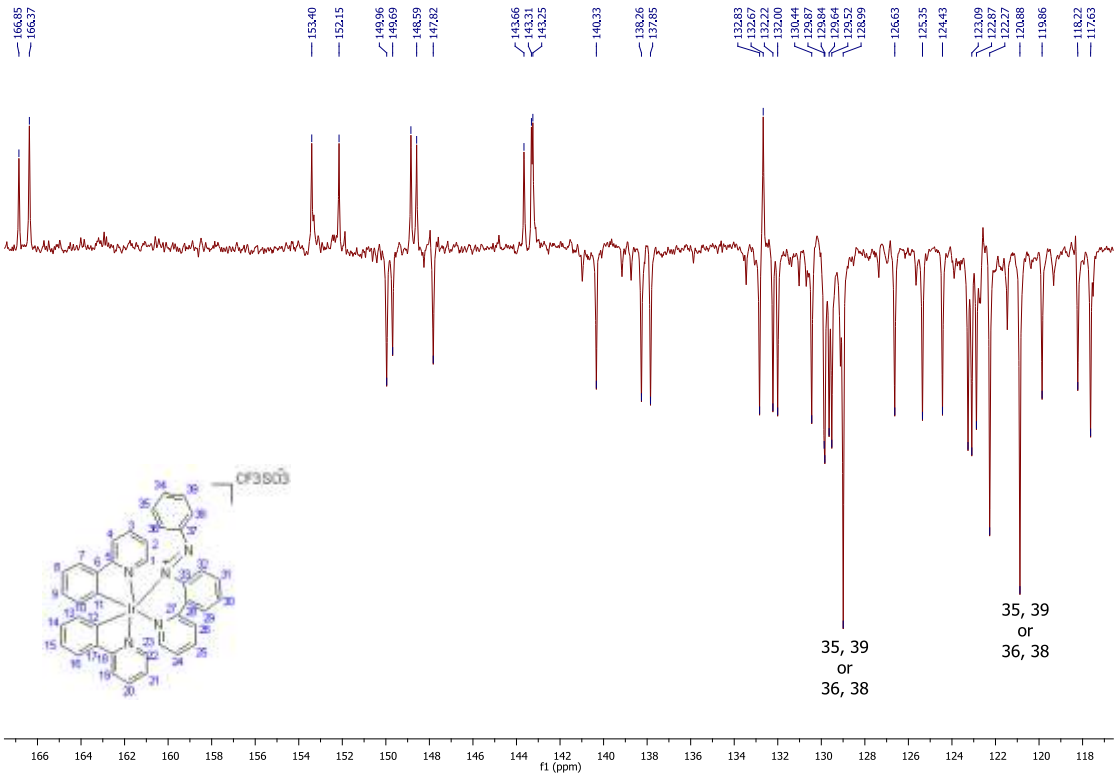
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.37 (d, J = 8.0, 1H), 8.25–8.20 (m, 2H), 8.16 (d, J = 8.3, 1H), 8.03 (d, J = 8.0, 1H), 8.00–7.97 (td, J = 7.5, 1.4, 1H), 7.93 (d, J = 5.7, 1H), 7.85 (d, J = 7.8, 1H), 7.71–7.66 (m, 2H), 7.59 (dd, J = 5.6, 1.1, 1H), 7.50 (dd, J = 7.6, 1.7, 1H), 7.40 (td, J = 7.6, 1.1 1H), 7.33–7.25 (m, 3H), 7.20–7.10 (m, 2H), 7.04 (td, J = 7.4, 1.1, 1H), 6.95–6.78 (m, 7H), 6.23 (d, J = 7.6, 1H), 6.14 (dd, J = 7.3, 1.3, 1H), 5.77 (dd, J = 8.0, 0.9, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 166.85 (1C, $C_{quat.}$), 166.37 (1C, $C_{quat.}$), 153.40 (1C, $C_{quat.}$), 152.15 (1C, $C_{quat.}$), 149.96 (1C, CH), 149.69 (1C, CH), 148.85 (1C, $C_{quat.}$), 148.59 (1C, $C_{quat.}$), 147.82 (1C, CH), 143.66 (1C, $C_{quat.}$), 143.31 (1C, $C_{quat.}$), 143.25 (1C, $C_{quat.}$), 140.33 (1C, CH), 138.26 (1C, CH), 137.85 (1C, CH), 132.83 (1C, CH), 132.67 (1C, $C_{quat.}$), 132.22 (1C, CH), 132.00 (1C, CH), 130.44 (1C, CH), 129.87 (1C, CH), 129.84 (1C, CH), 129.64 (1C, CH), 129.52 (1C, CH), 128.99 (2C, CH, C_6H_5), 126.63 (1C, CH), 125.35 (1C, CH), 124.43 (1C, CH), 123.26 (1C, CH), 123.09 (1C, CH), 122.87 (1C, CH), 122.27 (2C, CH), 120.88 (2C, CH, C_6H_5), 119.86 (1C, CH), 118.22 (1C, CH), 117.63 (1C, CH).

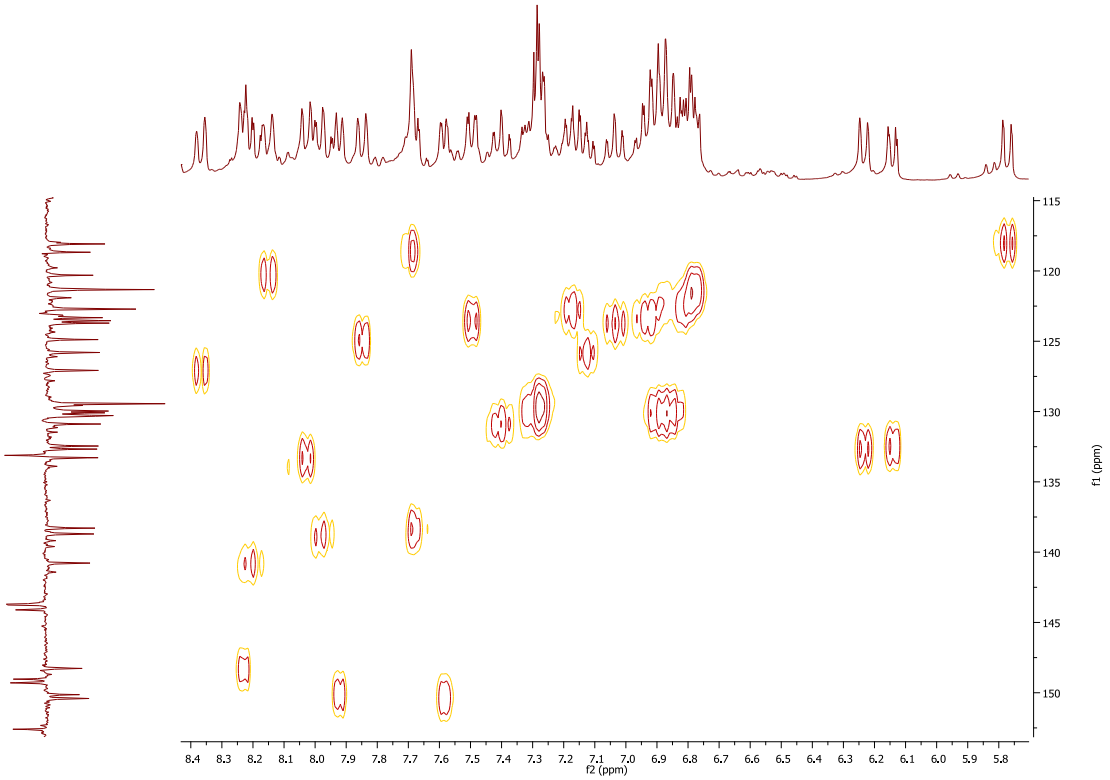
^{1}H NMR (300 MHz, $CDCl_3$) 0.075M:



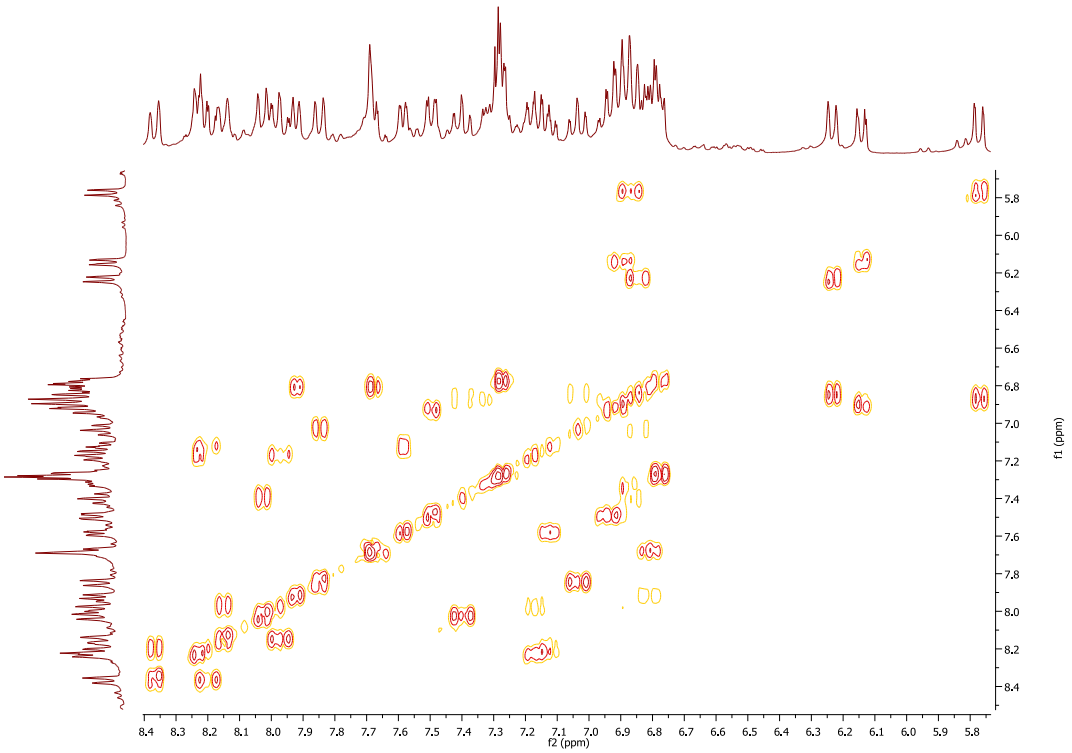
^{13}C APT NMR (75 MHz, $CDCl_3$) 0.075M:



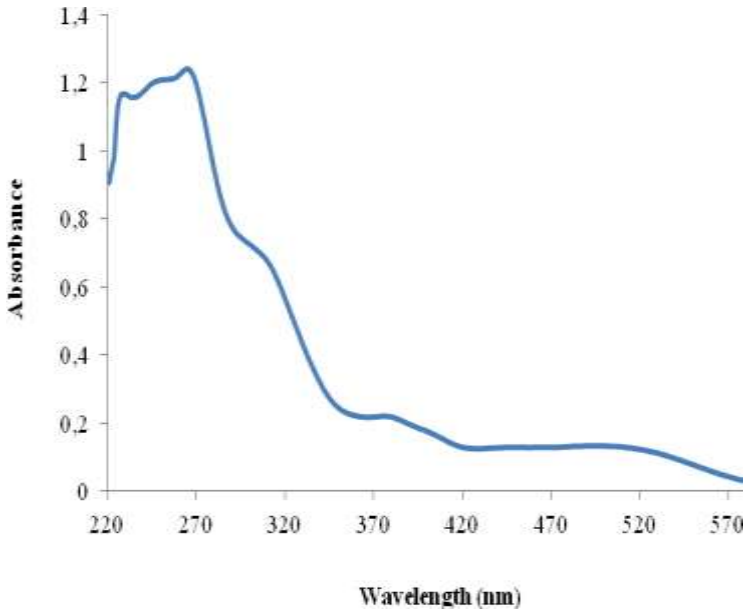
HMQC-NMR, 0.075 M:



COSY.NMR, 0.075M:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
230 ($4.1 \cdot 10^4$), 249 ($4.2 \cdot 10^4$), 265 ($4.3 \cdot 10^4$), 304 ($2.2 \cdot 10^4$), 376 ($8.3 \cdot 10^3$), 458 ($4.6 \cdot 10^3$), 495 ($4.3 \cdot 10^3$)

[Ir(ppy)$_2$**2**], **A2**

SYNTHESIS:

[Ir(ppy)$_2$Cl]$_2$ (0.150 g, 0.140 mmol) and silver triflate (0.108 g, 0.420 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **2** (0.146 g, 0560 mmol) and triethylamine (0.147 mL, 1.054 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as light-orange solid (0.042 g, 20%).

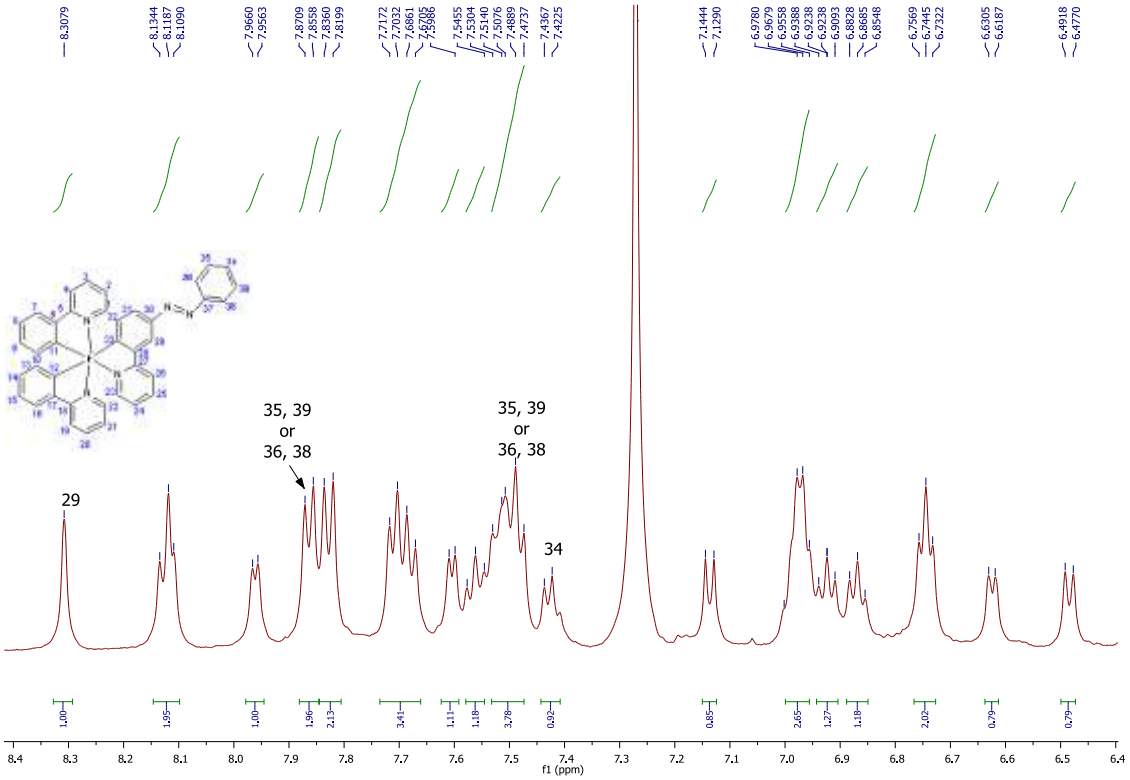
Elemental Analysis: calculated for $C_{39}H_{28}IrN_5$: C, 61.72; H, 3.72; N, 9.23. Found: C, 61.57; H, 3.59; N, 8.94.

Exact mass (MALDI) - m/z: 759.1978 for $[M]^+$ with (^{193}Ir).

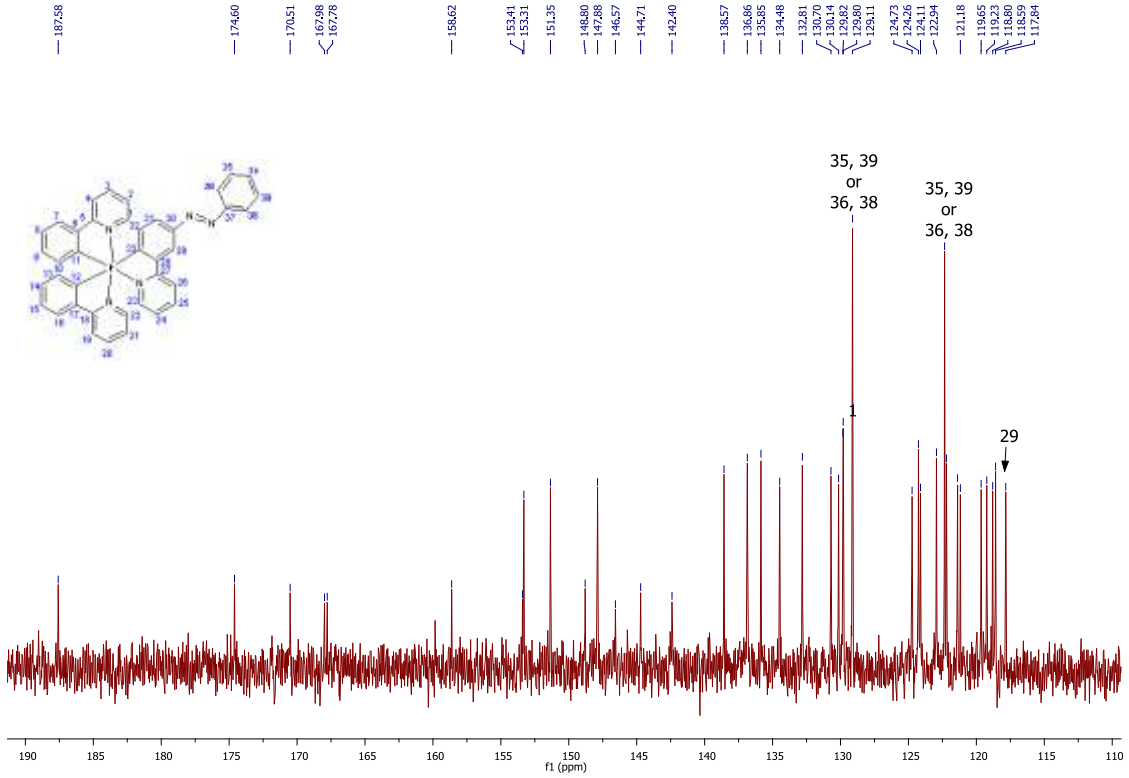
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (s, 1H, C_6H_3), 8.12 (m, 2H), 7.96 (d, J = 4.8, 1H), 7.86 (d, J = 7.5, 2H, C_6H_5), 7.83 (d, J = 8.1, 2H), 7.72–7.67 (m, 3H), 7.60 (d, J = 5.4, 1H), 7.56 (t, J =7.9, 1H), 7.53–7.47 (m, 4H), 7.43 (d, J = 7.1, 1H, C_6H_5), 7.14 (d, J = 7.7, 1H), 6.99–6.95 (m, 3H), 6.92 (t, J =7.5, 1H), 6.87 (t, J =7.0, 1H), 6.74 (t, J = 6.2, 2H), 6.62 (d, J = 5.9, 1H), 6.48 (d, J = 7.4, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 187.58 (1C, $C_{quat.}$), 174.60 (1C, $C_{quat.}$), 170.51 (1C, $C_{quat.}$), 167.98 (1C, $C_{quat.}$), 167.78 (1C, $C_{quat.}$), 158.62 (1C, $C_{quat.}$), 153.41 (1C, $C_{quat.}$), 153.31 (1C, CH), 151.35 (1C, CH), 148.80 (1C, $C_{quat.}$), 147.88 (1C, CH), 146.57 (1C, $C_{quat.}$), 144.71 (1C, $C_{quat.}$), 142.40 (1C, $C_{quat.}$), 138.57 (1C, CH), 136.86 (1C, CH), 135.85 (1C, CH), 134.48 (1C, CH), 132.81 (1C, CH), 130.70 (1C, CH), 130.14 (1C, CH), 129.82 (1C, CH), 129.80 (1C, CH), 129.11 (2C, CH, C_6H_5), 124.73 (1C, CH), 124.26 (1C, CH), 124.11 (1C, CH), 122.94 (1C, CH), 122.34 (2C, CH, C_6H_5), 122.20 (1C, CH), 121.38 (1C, CH), 121.18 (1C, CH), 119.65 (1C, CH), 119.23 (1C, CH), 118.80 (1C, CH), 118.59 (1C, CH), 117.84 (1C, CH, C_6H_3).

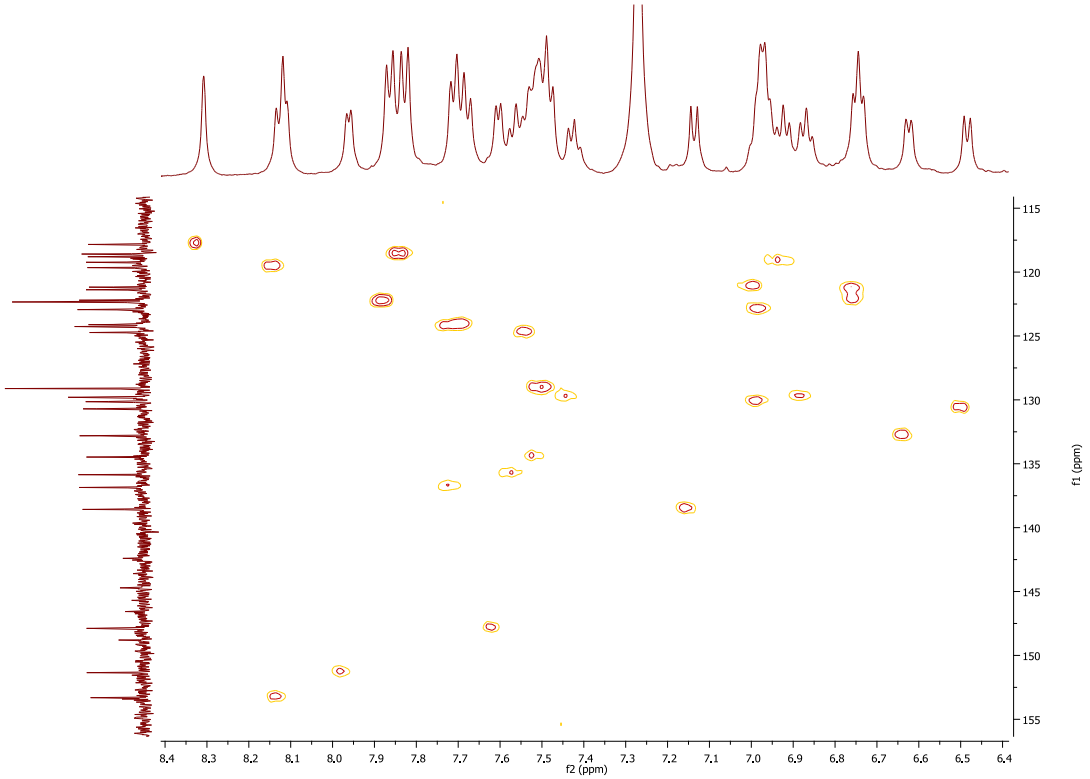
^{1}H NMR (500 MHz, $CDCl_3$):



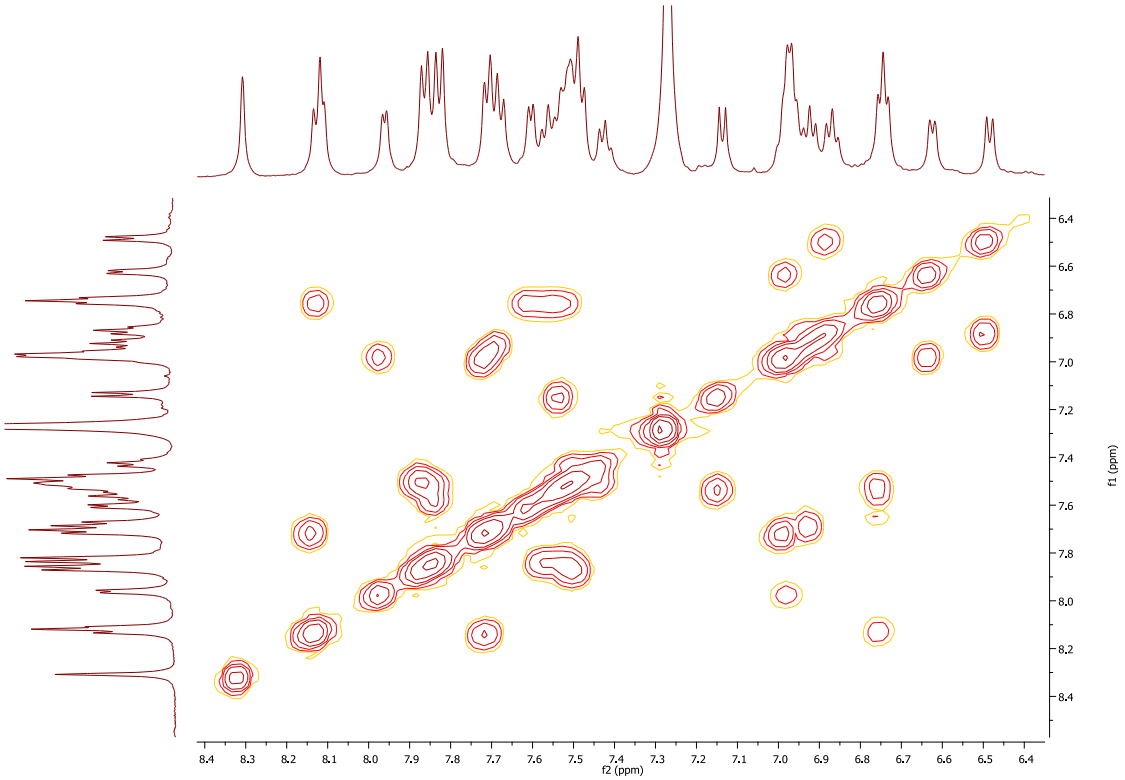
^{13}C NMR (126 MHz, $CDCl_3$):



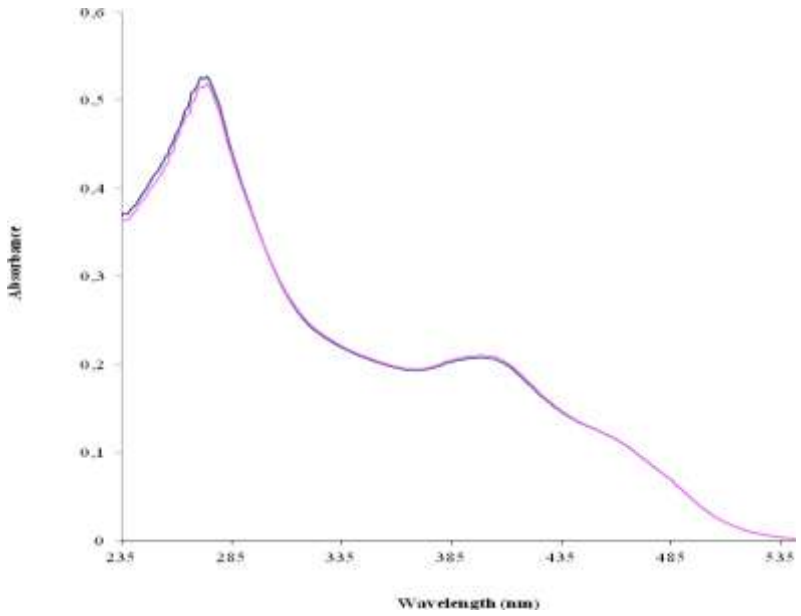
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 409 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
398 ($1.9 \cdot 10^4$), 466 ($9.5 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 409 nm. ($2.5 \cdot 10^{-5}$M).

Due to its low photoisomerization, it has been impossible to calculate k value.

[Ir(ppy)$_2$**3**], **A3**

SYNTHESIS:

$[Ir(ppy)_2Cl]_2$ (0.150 g, 0.140 mmol) and silver triflate (0.108 g, 0.420 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **3** (0.146 g, 0.560 mmol) and triethylamine (0.147 mL, 1.054 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as dark-orange solid (0.119 g, 56%).

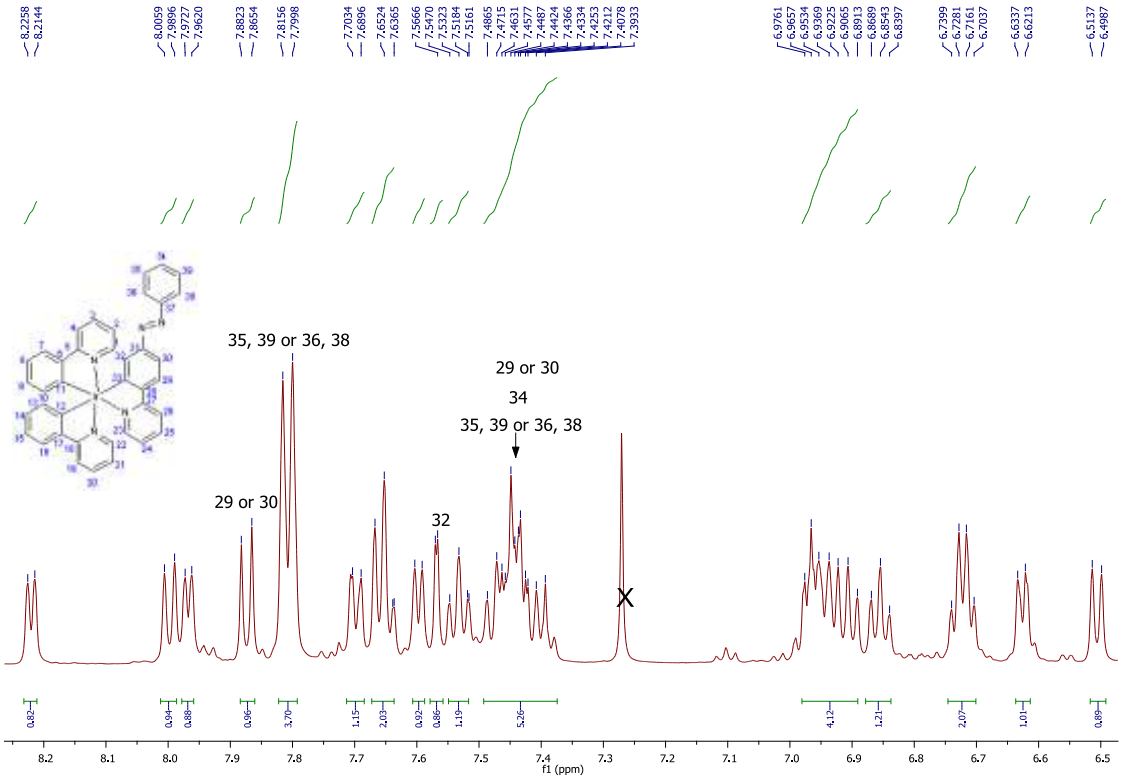
Elemental Analysis: calculated for $C_{39}H_{28}IrN_5$: C, 61.72; H, 3.72; N, 9.23. Found: C, 61.43; H, 3.33; N, 9.61.

Exact mass (MALDI) - m/z: 759.1971 for $[M]^+$ with (^{193}Ir)

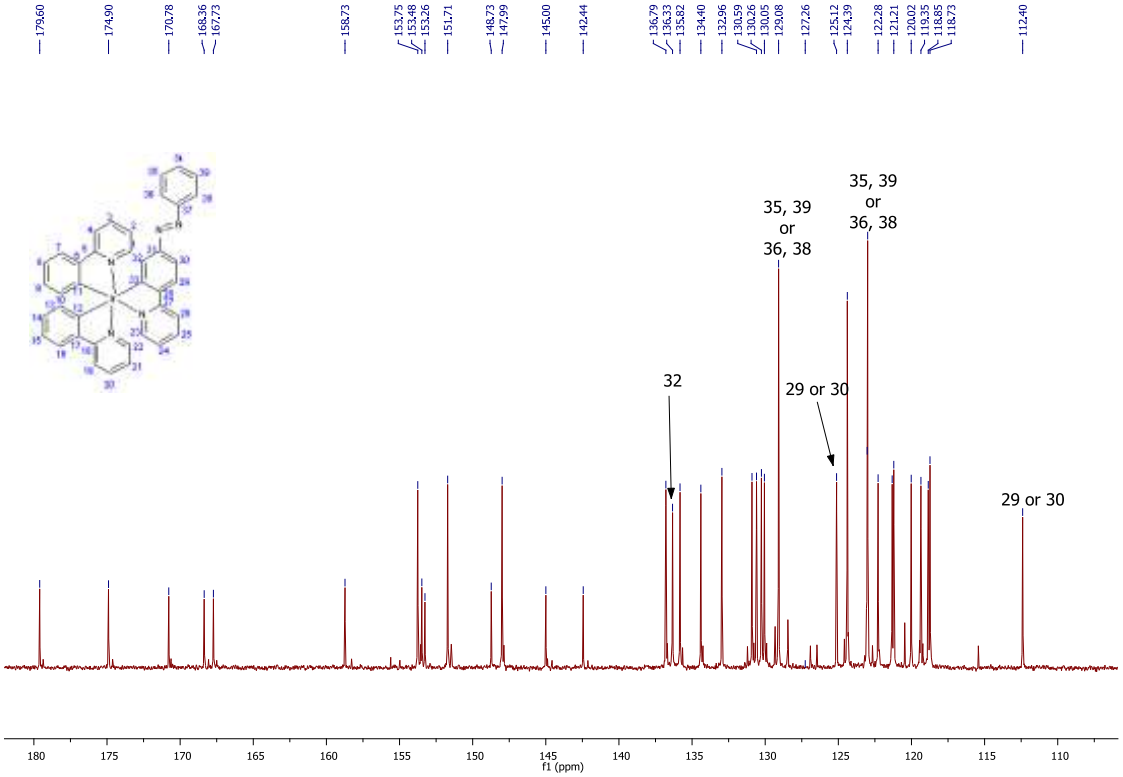
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.22 (d, J = 5.7, 1H), 8.00 (d, J = 8.1, 1H), 7.97 (d, J = 5.3, 1H), 7.87 (d, J = 8.4, 1H, C_6H_3), 7.81 (d, J = 7.9, 4H), 7.70 (d, J = 6.9, 1H), 7.65 (t, J = 7.2, 2H), 7.60 (d, J = 5.9, 1H), 7.57 (d, J = 1.8, 1H, C_6H_3), 7.53 (t, J = 7.2, 1H), 7.49–7.37 (m, 5H), 6.98–6.89 (m, 4H), 6.85 (t, J = 7.3, 1H), 6.73 (t, J = 6.1, 1H), 6.72 (t, J = 6.1, 1H), 6.63 (d, J = 6.2, 1H), 6.51 (d, J = 7.5, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 179.60 (1C, $C_{quat.}$), 174.90 (1C, $C_{quat.}$), 170.78 (1C, $C_{quat.}$), 168.36 (1C, $C_{quat.}$), 167.73 (1C, $C_{quat.}$), 158.73 (1C, $C_{quat.}$), 153.75 (1C, CH), 153.48 (1C, $C_{quat.}$), 153.26 (1C, $C_{quat.}$), 151.71 (1C, CH), 148.73 (1C, $C_{quat.}$), 147.99 (1C, CH), 145.00 (1C, $C_{quat.}$), 142.44 (1C, $C_{quat.}$), 136.79 (1C, CH), 136.33 (1C, CH, C_6H_3), 135.82 (1C, CH), 134.40 (1C, CH), 132.96 (1C, CH), 130.90 (1C, CH), 130.59 (1C, CH), 130.26 (1C, CH), 130.05 (1C, CH), 129.08 (2C, CH, C_6H_5), 125.12 (1C, CH, C_6H_3), 124.39 (2C, CH), 123.03 (1C, CH), 122.99 (2C, CH, C_6H_5), 122.28 (1C, CH), 121.32 (1C, CH), 121.21 (1C, CH), 120.02 (1C, CH), 119.35 (1C, CH), 118.85 (1C, CH), 118.73 (1C, CH), 112.40 (1C, CH, C_6H_3).

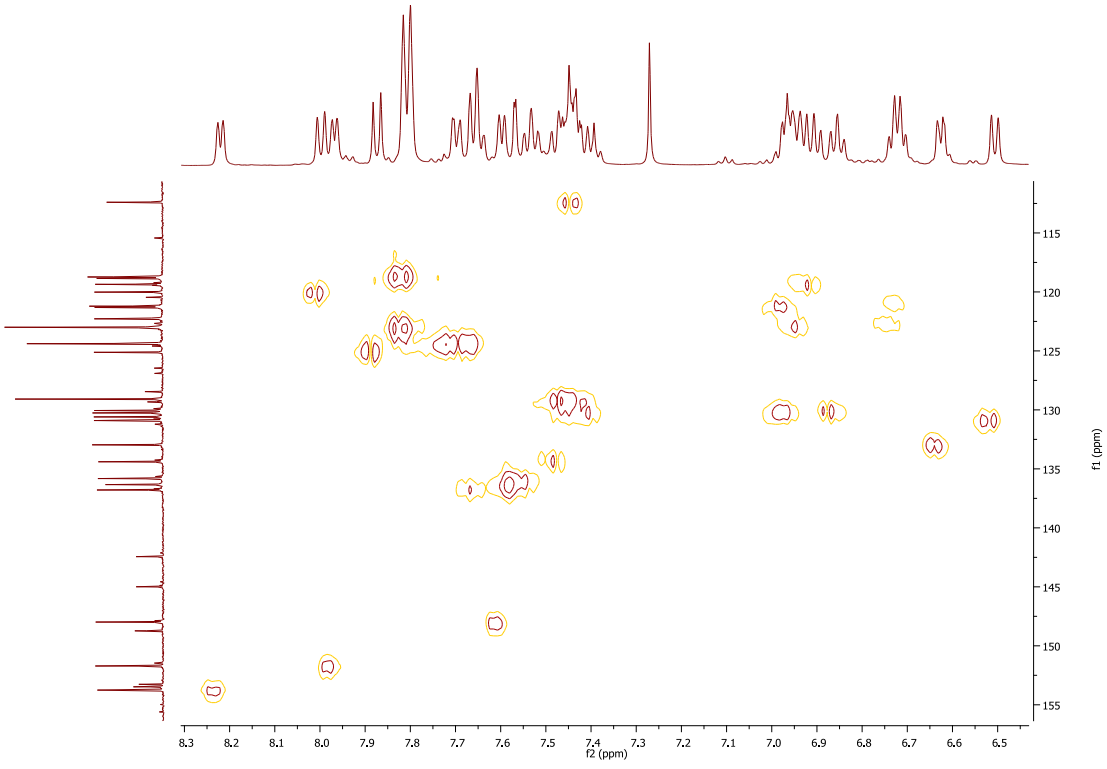
^{1}H NMR (500 MHz, $CDCl_3$):



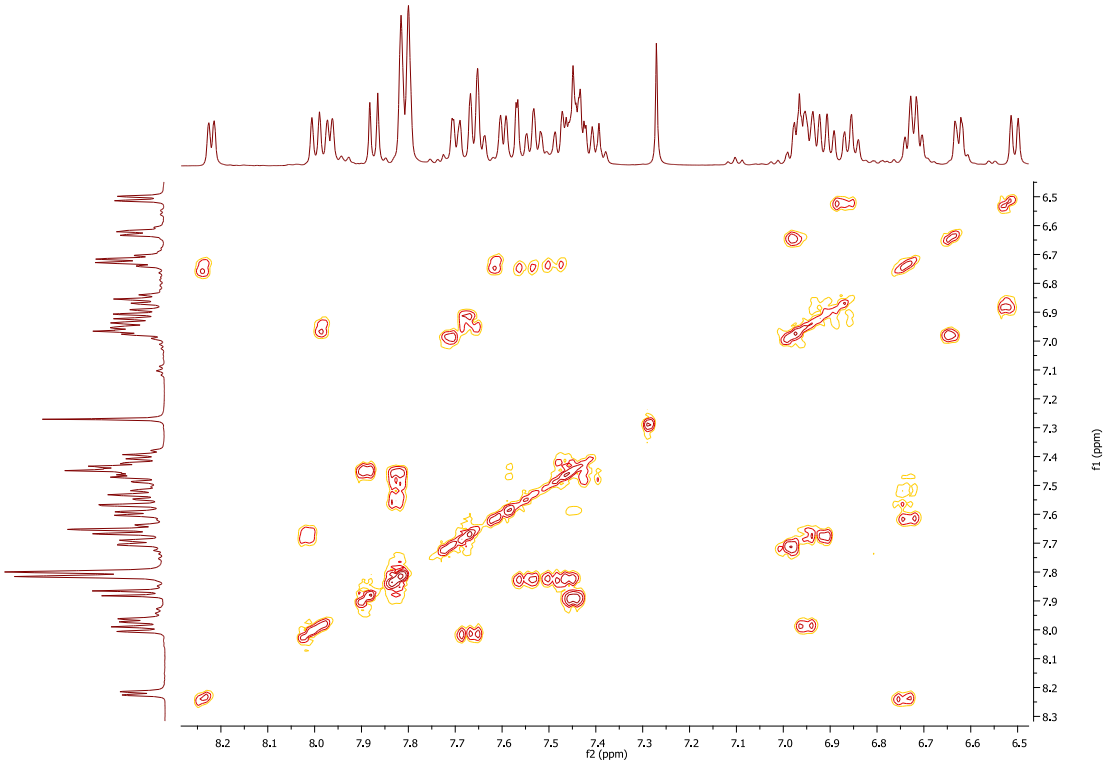
^{13}C NMR (126 MHz, $CDCl_3$):



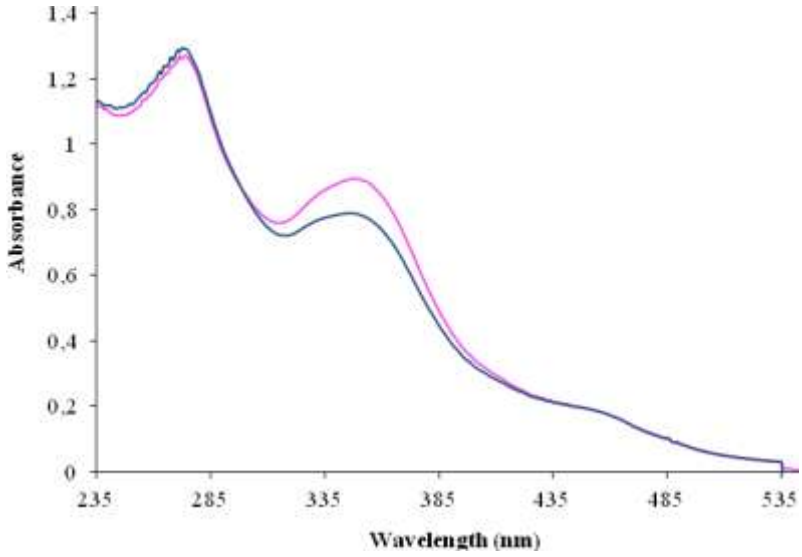
HSQC-NMR:



COSY.NMR:

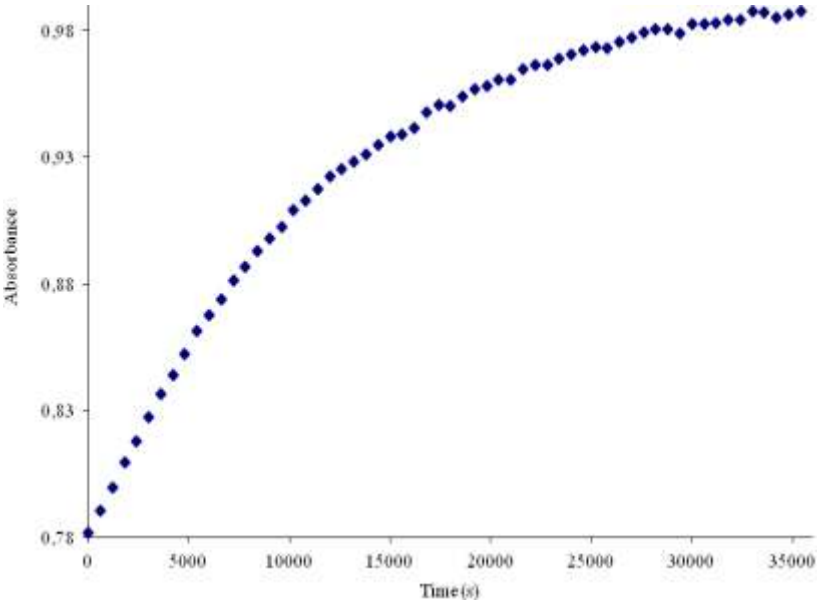


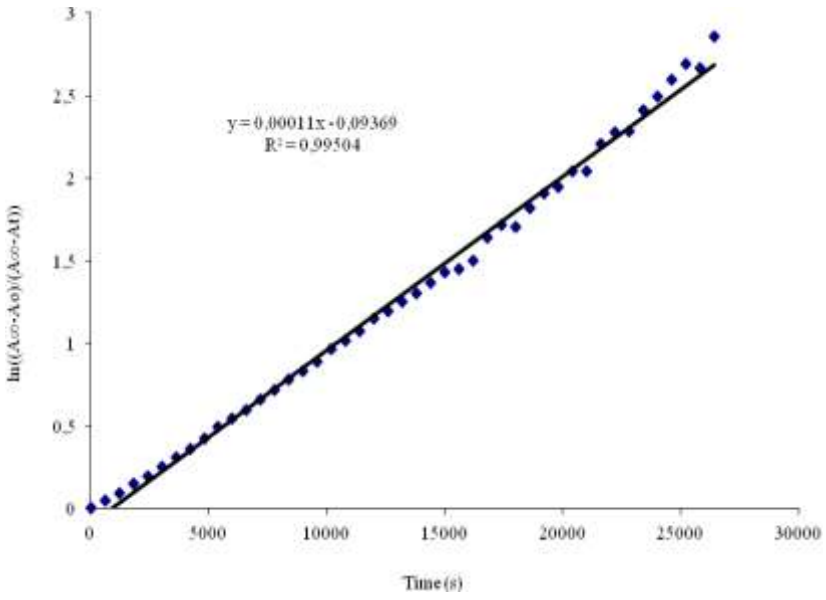
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 351 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
346 ($2.9 \cdot 10^4$), 454 ($6.0 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 351 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$1.1 \cdot 10^{-4}$**
Half-life (s)	**6600**

[Ir(ppy)$_2$((5-bromo-2-pyridyl)phenyl)], **C**

SYNTHESIS:

$[Ir(ppy)_2Cl]_2$ (0.150 g, 0.140 mmol) and silver triflate (0.108 g, 0.420 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of 2-(4-bromophenyl)pyridine) (0.131 g, 0.560 mmol) and triethylamine (0.130 mL, 0.932 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane:hexane (5:1). The product was obtained as yellow powder (0.082 g, 40%).

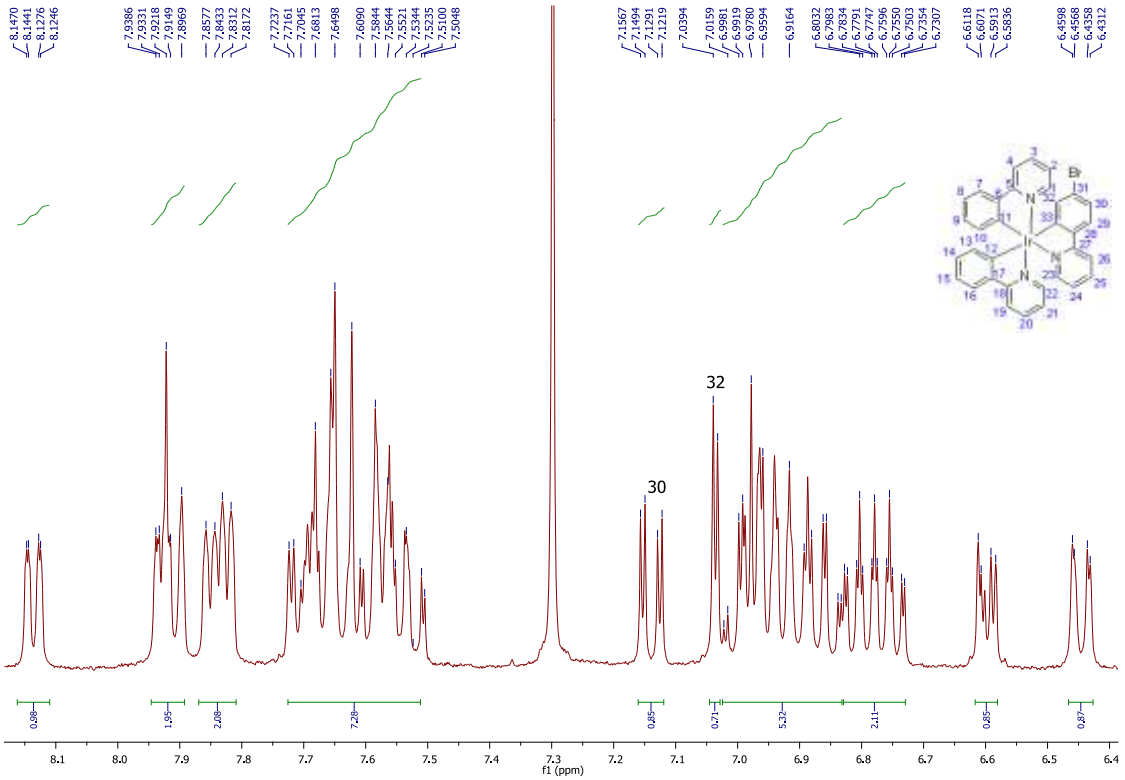
Elemental Analysis: calculated for $C_{33}H_{23}BrIrN_3 \cdot C_6H_{14}$: C, 57.13; H, 4.55; N, 5.13. Found: C, 57.02; H, 4.50; N, 5.20.

Exact mass (MALDI) - m/z: 733.0684 for $[M]^+$ with (^{193}Ir)(^{79}Br).

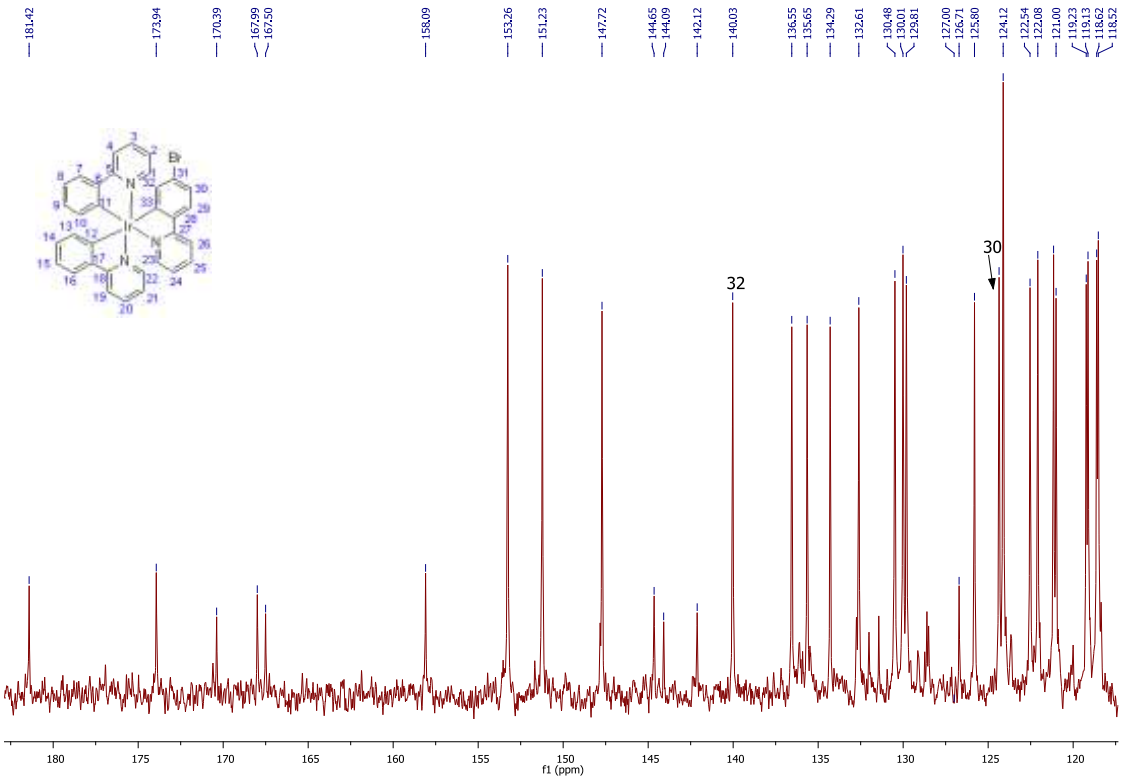
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.14 (dd, J = 5.8, 0.9, 1H), 7.95–7.89 (m, 2H), 7.86–7.82 (m, 2H), 7.73–7.51 (m, 7H), 7.14 (dd, J = 8.3, 2.2, 1H, C_6H_3Br), 7.04 (d, J = 2.1, 1H, C_6H_3Br), 7.02–6.83 (m, 5H), 6.80 (ddd, J = 7.3, 5.9, 1.4, 2H), 6.76 (ddd, J = 7.3, 5.9, 1.4, 2H), 6.62–6.58 (m, 1H), 6.45 (dd, J = 7.4, 1.1, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 181.42 (1C, $C_{quat.}$), 173.94 (1C, $C_{quat.}$), 170.39 (1C, $C_{quat.}$), 167.99 (1C, $C_{quat.}$), 167.50 (1C, $C_{quat.}$), 158.09 (1C, $C_{quat.}$), 153.26 (1C, CH), 151.23 (1C, CH), 147.72 (1C, CH), 144.65 (1C, $C_{quat.}$), 144.09 (1C, $C_{quat.}$), 142.12 (1C, $C_{quat.}$), 140.03 (1C, CH, C_6H_3Br), 136.55 (1C, CH), 135.65 (1C, CH), 134.29 (1C, CH), 132.61 (1C, CH), 130.48 (1C, CH), 130.01 (1C, CH), 129.81 (1C, CH), 126.71 (1C, $C_{quat.}$), 125.80 (1C, CH), 124.36 (1C, CH, C_6H_3Br), 124.12 (2C, CH), 122.54 (1C, CH), 122.08 (1C, CH), 121.15 (1C, CH), 121.00 (1C, CH), 119.23 (1C, CH), 119.13 (1C, CH), 118.62 (1C, CH), 118.52 (1C, CH).

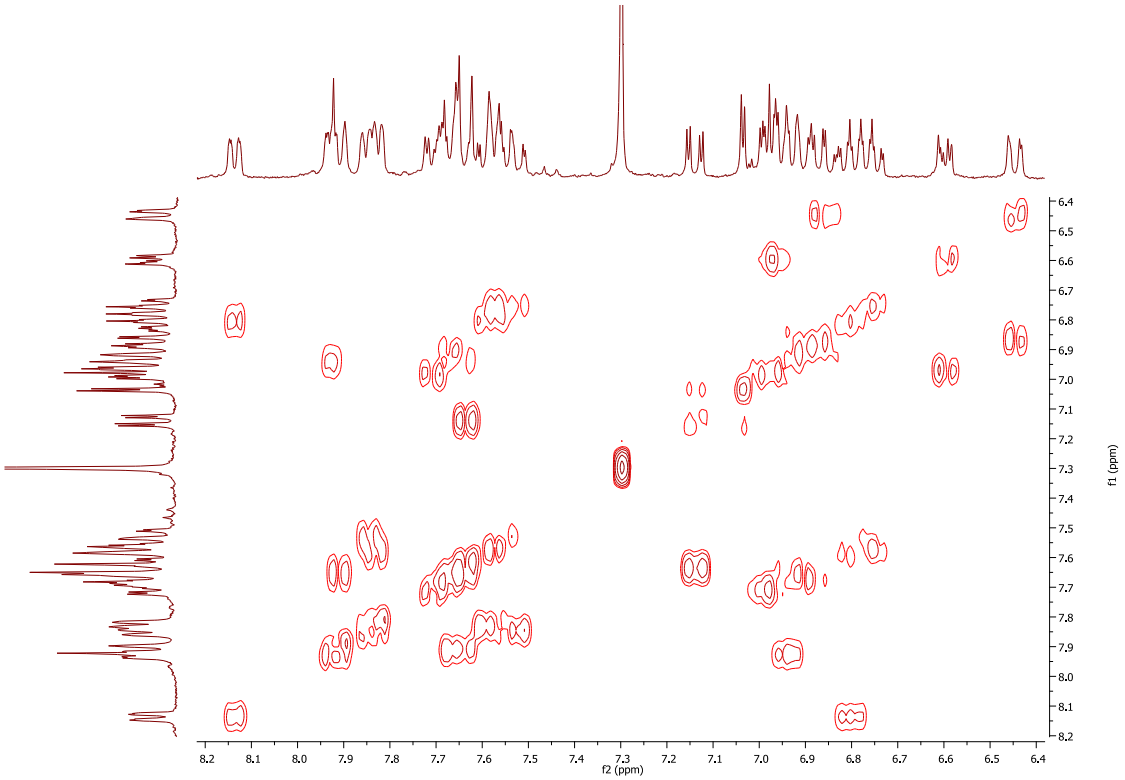
^{1}H NMR (300 MHz, $CDCl_3$):



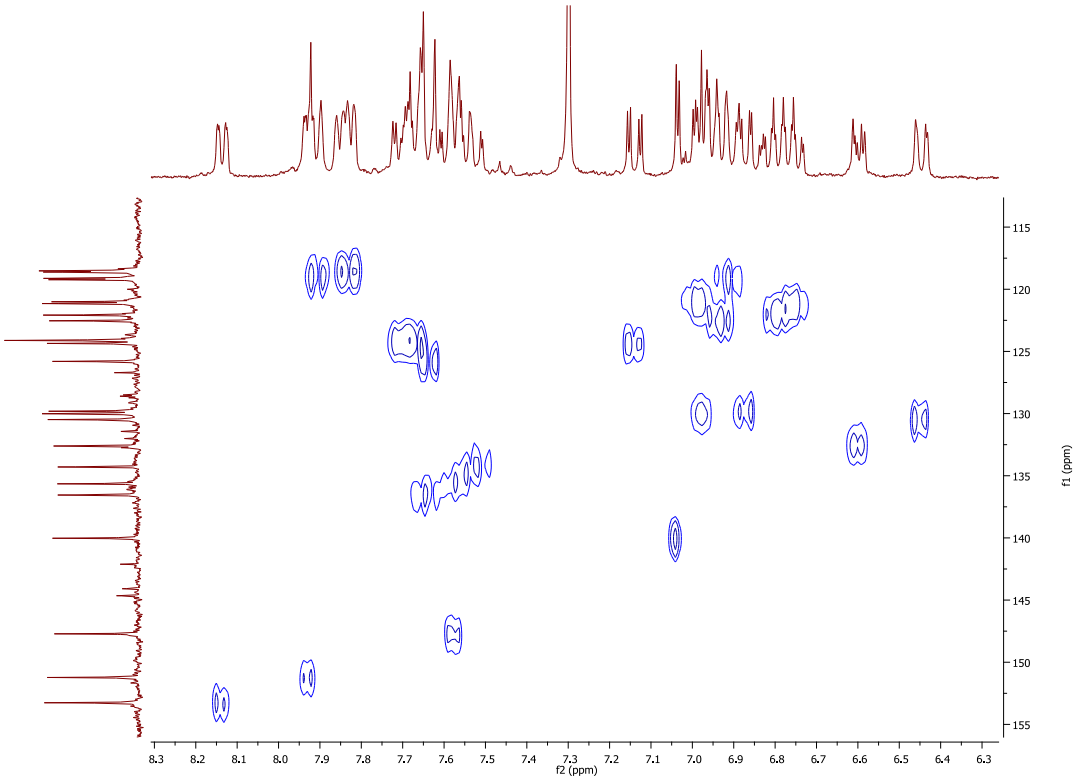
^{13}C APT NMR (75 MHz, $CDCl_3$):



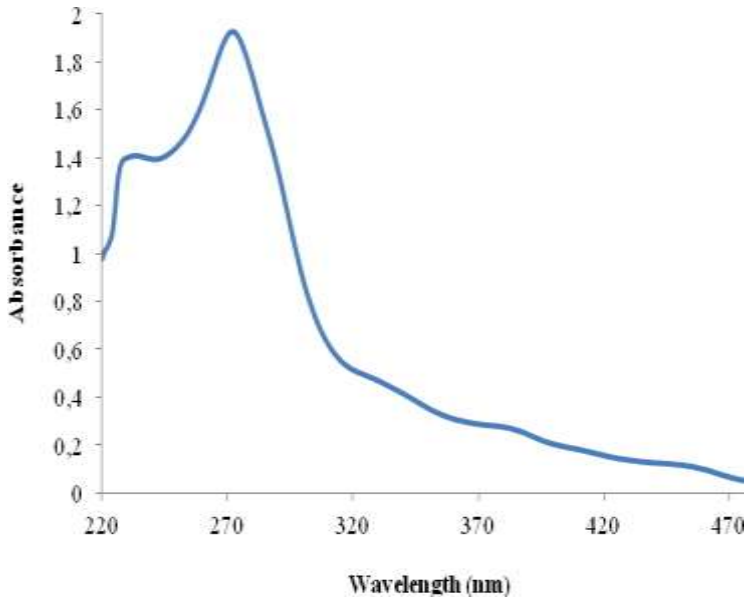
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN):

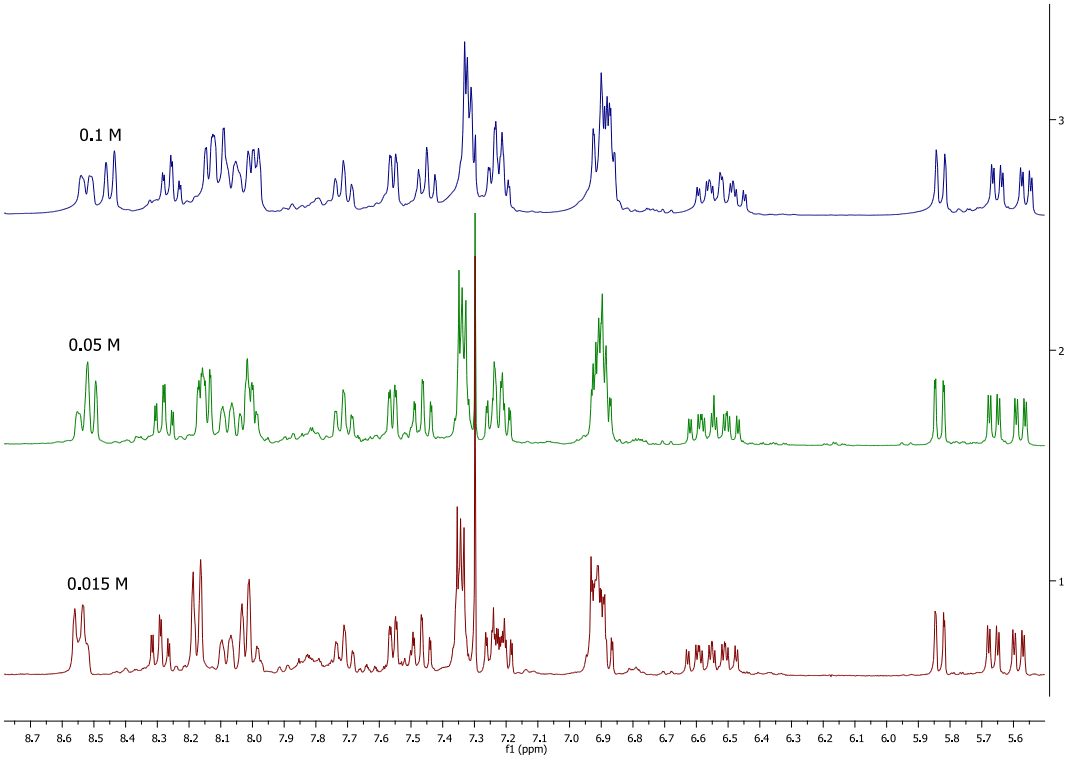


λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
235 ($3.7 \cdot 10^4$), 269 ($4.8 \cdot 10^4$), 327 ($1.2 \cdot 10^4$), 379 ($6.7 \cdot 10^3$), 408 ($4.5 \cdot 10^3$), 452 ($2.6 \cdot 10^3$), 482 ($0.8 \cdot 10^3$)

[Ir(Fppy)$_2$1][OTf], **B1'**

SYNTHESIS:

$[Ir(Fppy)_2Cl]_2$ (0.150 g, 0.123 mmol) and silver triflate (0.095 g, 0.37 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **1** (0.128 g, 0.492 mmol) and triethylamine (0.130 mL, 0.932 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with ethyl acetate; when the ligand is extracted, we add acetone for the extraction of the complex (the complex degrades with solvent). The product was obtained as red crystalline solid (0.190 g, 79%). The NMR-spectra of the complex varies with the concentration.



Elemental Analysis: calculated for $C_{40}H_{25}F_7IrN_5O_3S$: C, 48.98; H, 2.57; N, 7.14; S, 3.27. Found: C, 49.40; H, 2.62; N, 6.99; S, 3.41.

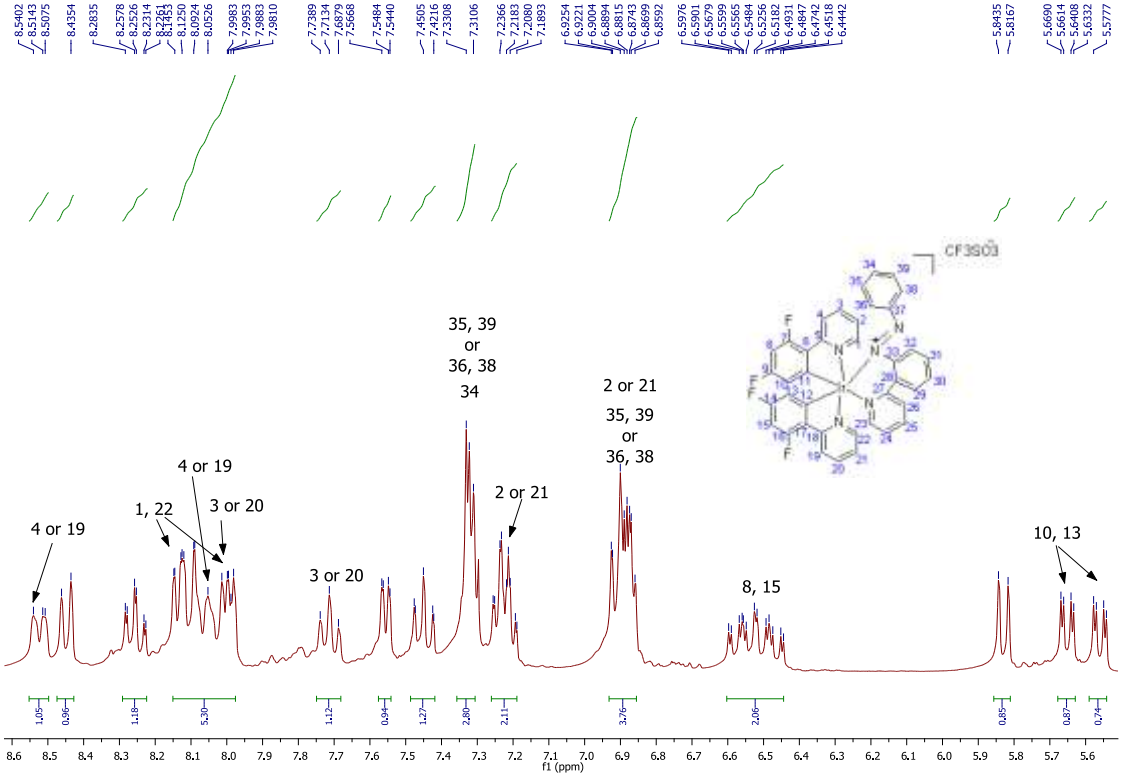
Exact mass (EI) - m/z: 832.1677 for $[M]^+$ with (^{193}Ir)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.52 (dd, J = 7.8, 2.2, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 8.45 (d, J = 7.9, 1H, $C_{17}H_{13}N_3$), 8.25 (td, J = 7.8, 1.6, 1H, $C_{17}H_{13}N_3$), 8.15–7.98 (m, 5H), 7.71 (t, J = 7.7, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 7.56 (dd, J = 5.6, 1.3, 1H, $C_{17}H_{13}N_3$), 7.45 (td, J = 7.7, 0.9, 1H, $C_{17}H_{13}N_3$), 7.36–7.31 (m, 3H, C_6H_5 ($C_{17}H_{13}N_3$)), 7.26–7.19 (m, 2H), 6.93–6.86 (m, 4H), 6.60–6.44 (m, 2H, $C_6H_2F_2$), 5.83 (d, J = 8.0, 1H, $C_{17}H_{13}N_3$), 5.65 (dd, J = 8.5, 2.3, 1H, $C_6H_2F_2$), 5.56 (dd, J = 8.4, 2.3, 1H, $C_6H_2F_2$).

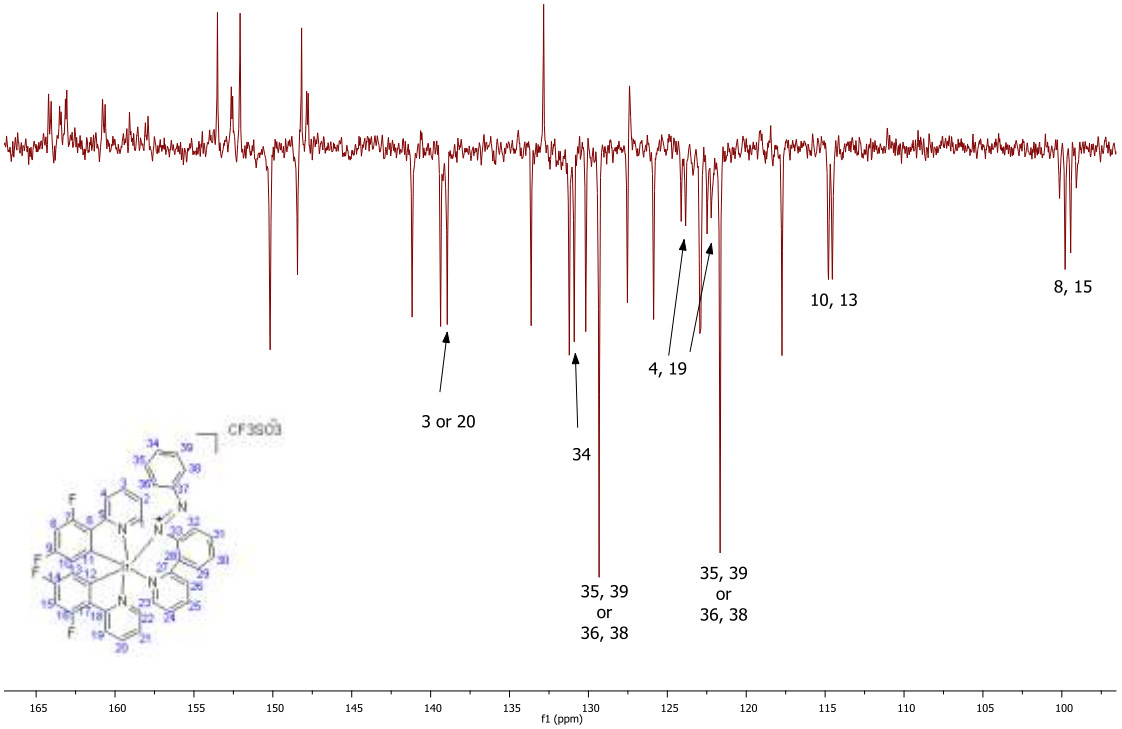
^{13}C NMR (75 MHz, $CDCl_3$): δ 163.25 (d, J =7.2, 1C, $C_{quat.\ C11H6NF2}$), 162.89 (d, J =6.6, 1C, $C_{quat.\ C11H6NF2}$), 162.22 (dd, J =257, 12.4, 2C, $C_{quat.\ C\text{-}F}$), 160.70 (dd, J =260, 12.4, 1C, $C_{quat.\ C\text{-}F}$), 159.51 (dd, J =259, 12.5, 1C, $C_{quat.\ C\text{-}F}$), 153.30 (1C, $C_{quat.\ C17H13N3}$), 152.38 (d, J =6.5, 1C, $C_{quat.\ C11H6NF2}$), 151.87 (1C, $C_{quat.\ C17H13N3.}$), 149.96 (2C, CH), 148.23 (1C, CH), 147.97 (1C, $C_{quat.\ C17H13N3.}$), 147.60 (d, J =7.3, 1C, $C_{quat.\ C11H6NF2}$), 140.97 (1C, CH, $C_{17}H_{13}N_3$), 139.16 (1C, CH), 138.74 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 133.42 (1C, CH), 132.63 (1C, $C_{quat.\ C17H13N3}$), 131.00 (1C, CH), 130.69 (1C, CH, C_6H_5), 129.96 (1C, CH), 129.12 (2C, CH, C_6H_5), 127.32 (1C, CH, $C_{17}H_{13}N_3$), 127.19 (1C, $C_{quat.\ C11H6NF2}$), 127.16 (1C, $C_{quat.\ C11H6NF2}$), 125.66 (1C, CH), 123.77 (d, J =21.1, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)) ,

122.73 (1C, CH), 122.66 (1C, CH), 122.14 (d, J =19.6, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 121.45 (2C, CH, C_6H_5), 117.53 (1C, CH, $C_{17}H_{13}N_3$), 114.45 (d, J =18.4, 2C, CH, $C_6H_2F_2$), 99.58 (pst, J =27.0, 1C, CH, $C_6H_2F_2$), 99.23 (pst, J =27.0, 1C, CH, $C_6H_2F_2$).

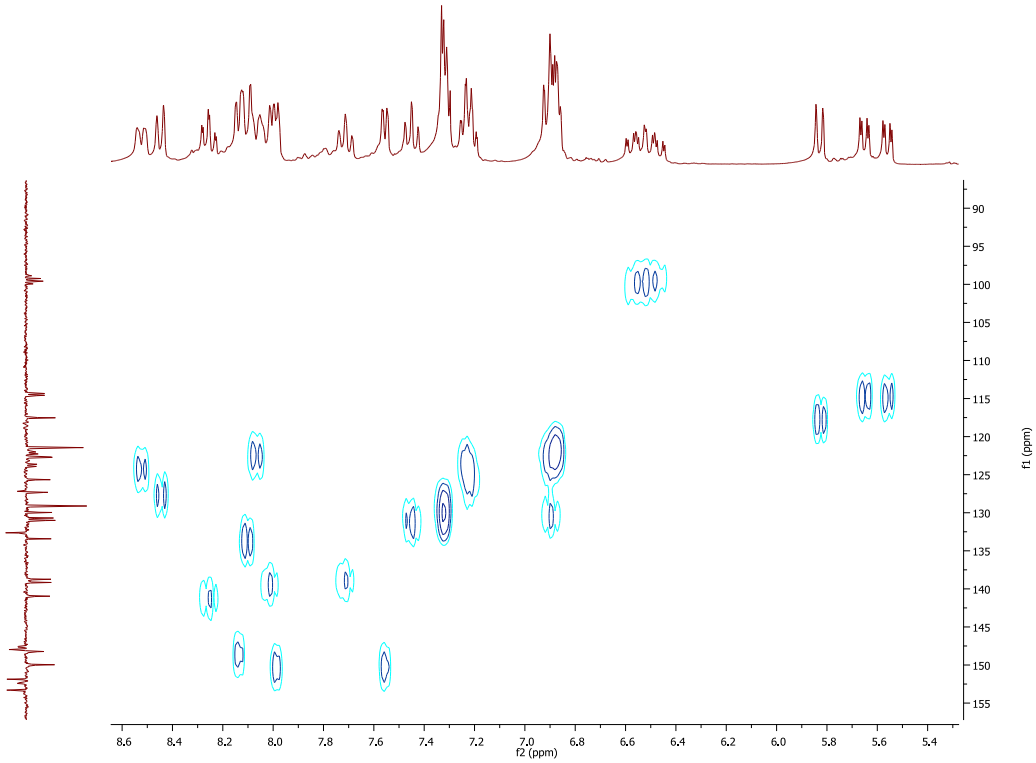
^{1}H NMR (300 MHz, $CDCl_3$) 0.1M:



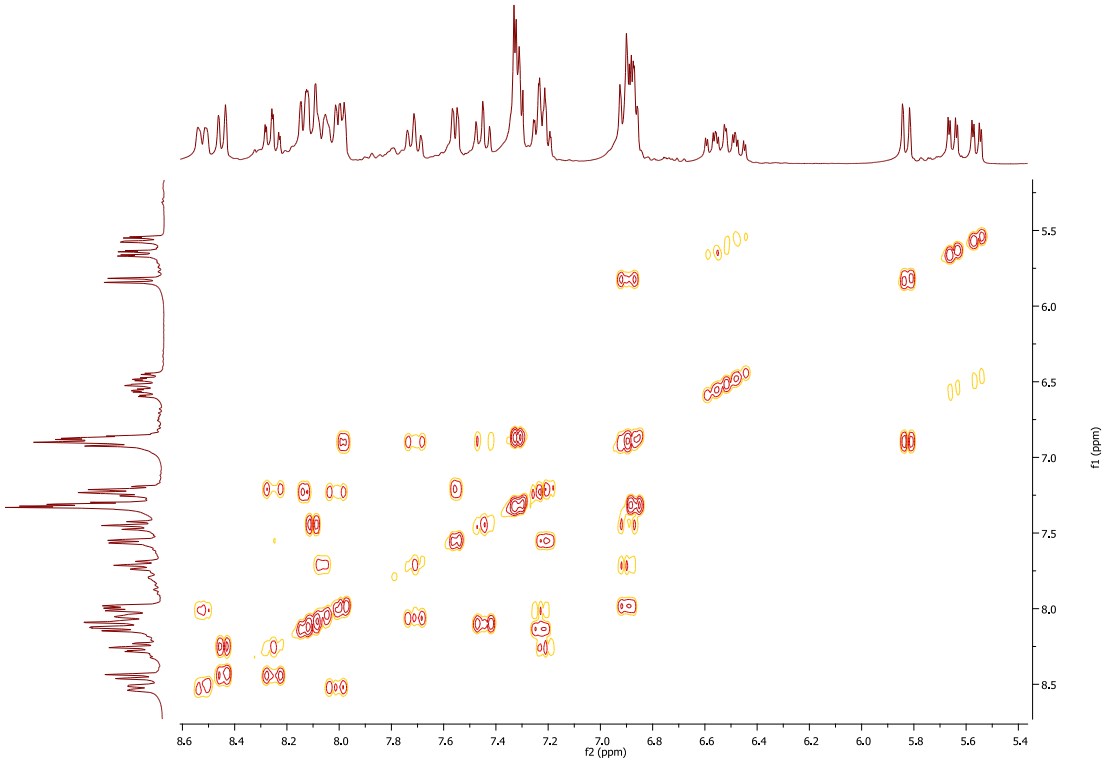
^{13}C APT NMR (75 MHz, $CDCl_3$) 0.1M:



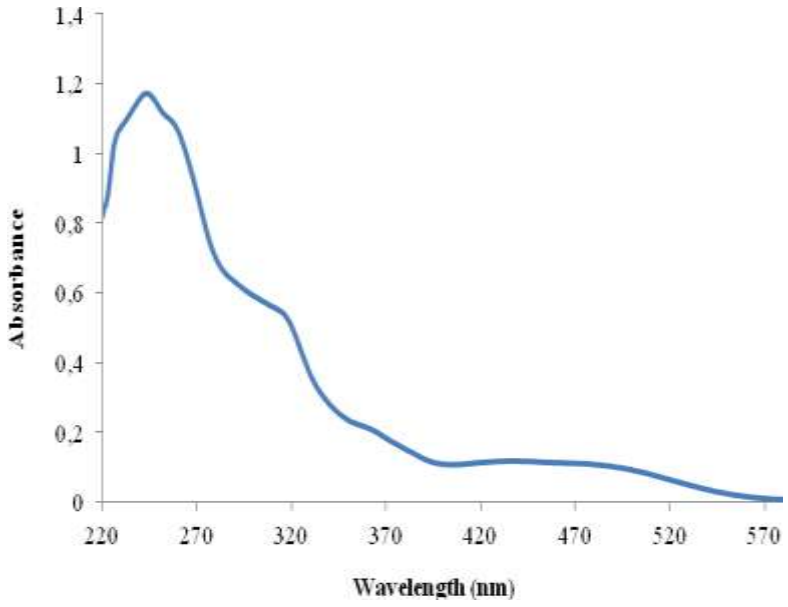
HSQC-NMR, 0.1 M:



COSY.NMR, 0.1M:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
230 ($4.2 \cdot 10^4$), 244 ($4.6 \cdot 10^4$), 255 ($4.3 \cdot 10^4$), 310 ($2.5 \cdot 10^4$), 361 ($7.7 \cdot 10^3$), 440 ($4.7 \cdot 10^3$), 477 ($4.5 \cdot 10^3$)

[Ir(Fppy)$_2$**2**], **B2**

SYNTHESIS:

$[Ir(Fppy)_2Cl]_2$ (0.150 g, 0.123 mmol) and silver triflate (0.95 g, 0.37 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **2** (0.128 g, 0.492 mmol) and triethylamine (0.130 mL, 0.932 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as light-orange solid (0.031 g, 15%).

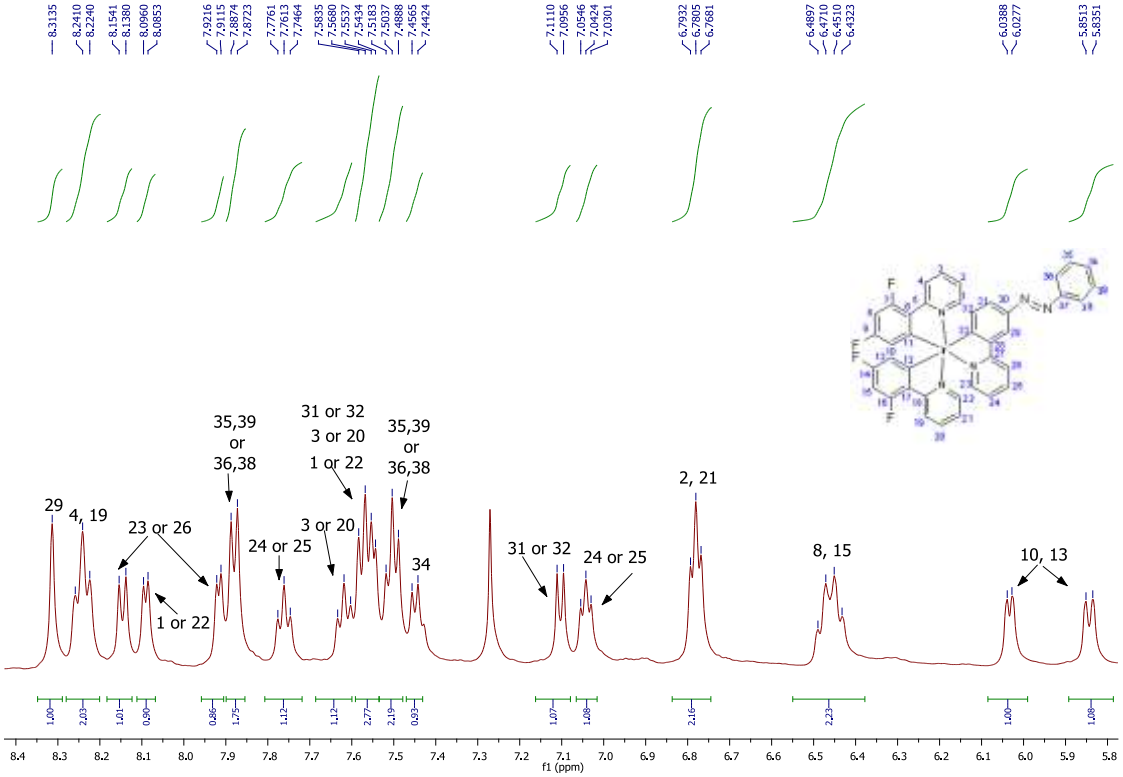
Elemental Analysis: calculated for $C_{39}H_{24}F_4IrN_5 \cdot C_3H_6O$: C, 56.75; H, 3.40; N, 7.88. Found: C, 56.46; H, 3.43; N, 7.43.

Exact mass (EI) - m/z: 830.1677 for $[M+H]^+$ with (^{193}Ir).

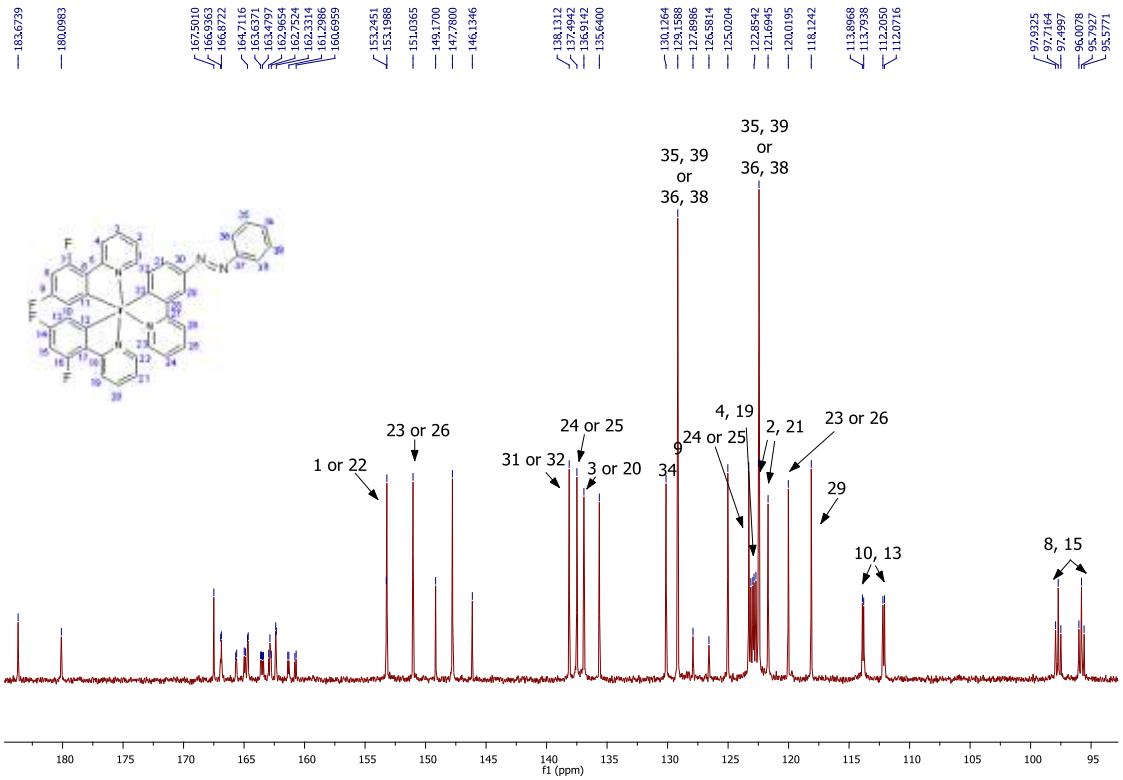
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (s, 1H, C_6H_3), 8.24 (t, J = 8.6, 2H, C_5H_4N ($C_{11}H_6NF_2$)), 8.15 (d, J = 8.0, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 8.09 (d, J = 5.3, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 7.92 (d, J = 5.0, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 7.88 (d, J = 7.5, 2H, C_6H_5), 7.76 (t, J = 7.4, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 7.62 (t, J = 7.7, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 7.58–7.54 (m, 3H), 7.52–7.49 (m, 2H, C_6H_5), 7.45 (d, J = 7.1, 1H, C_6H_5), 7.10 (d, J = 7.7, 1H, C_6H_3), 7.04 (t, J =6.1, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 6.78 (t, J = 6.3, 2H, C_5H_4N ($C_{11}H_6NF_2$)), 6.47 (t, J =9.4, 1H, $C_6H_2F_2$), 6.45 (t, J =9.4, 1H, $C_6H_2F_2$), 6.03 (d, J = 5.6, 1H, $C_6H_2F_2$), 5.84 (d, J = 8.1, 1H, $C_6H_2F_2$).

^{13}C NMR (126 MHz, $CDCl_3$): δ 183.67 (1C, $C_{quat.\ C16H12N3}$), 180.10 (1C, $C_{quat.\ C11H6NF2}$), 167.50 (1C, $C_{quat.\ C16H12N3}$), 166.90 (d, J =8.1, 1C, $C_{quat.\ C11H6NF2}$), 164.68 (d, J =6.9, 1C, $C_{quat.\ C11H6NF2}$), 164.62 (dd, J =10.1, J =259, 1C, $C_{quat.C-F}$), 163.93 (dd, J =12.5, J = 254, 1C, $C_{quat.C-F}$), 162.38 (dd, J =10.9, J =263, 1C, $C_{quat.C-F}$), 162.36 (d, J = 6.4, 1C, $C_{quat.\ C11H6NF2}$), 161.78 (dd, J =13.4, J =259, 1C, $C_{quat.C-F}$), 153.25 (1C, $C_{quat.\ C16H12N3}$), 153.20 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 151.04 (1C, CH, C_5H_4N ($C_{16}H_{12}N_3$)), 149.17 (1C, $C_{quat.\ C16H12N3}$), 147.78 (1C, CH), 146.13 (1C, $C_{quat.\ C16H12N3}$), 138.13 (1C, CH, C_6H_3), 137.49, (1C, CH, C_5H_4N ($C_{16}H_{12}N_3$)) 136.91 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 135.64 (1C, CH), 130.13 (1C, CH, C_6H_5), 129.16 (2C, CH, C_6H_5), 127.90 (1C, $C_{quat.\ C11H6NF2}$), 126.58 (1C, $C_{quat.\ C11H6NF2}$), 125.02 (1C, CH), 123.29 (1C, CH, C_5H_4N ($C_{16}H_{12}N_3$)), 123.04 (d, J =20.8, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.78 (d, J =19.7, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.49 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.44 (2C, CH, C_6H_5), 121.69 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 120.02 (1C, CH, C_5H_4N ($C_{16}H_{12}N_3$)), 118.12 (1C, CH, C_6H_3), 113.85 (d, J =13.0, 1C, CH, $C_6H_2F_2$), 112.14 (d, J =16.8, 1C, CH, $C_6H_2F_2$), 97.72 (pst, J =27.2, 1C, CH, $C_6H_2F_2$), 95.79 (pst, J =27.2, 1C, CH, $C_6H_2F_2$).

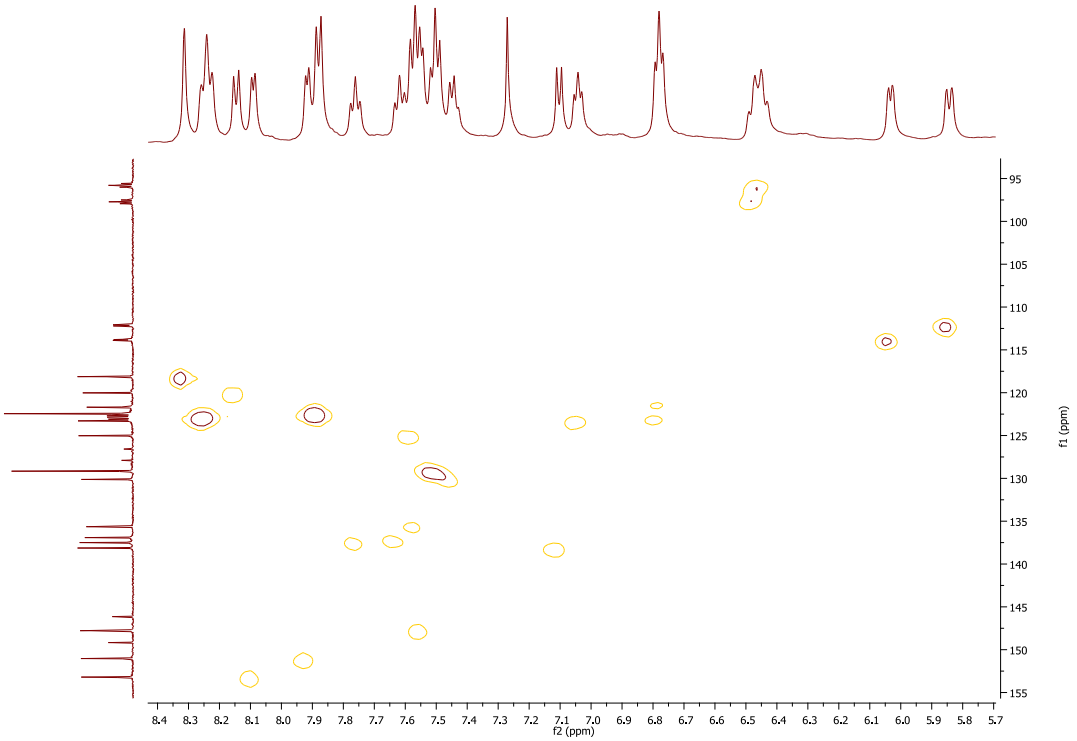
^{1}H NMR (500 MHz, $CDCl_3$):



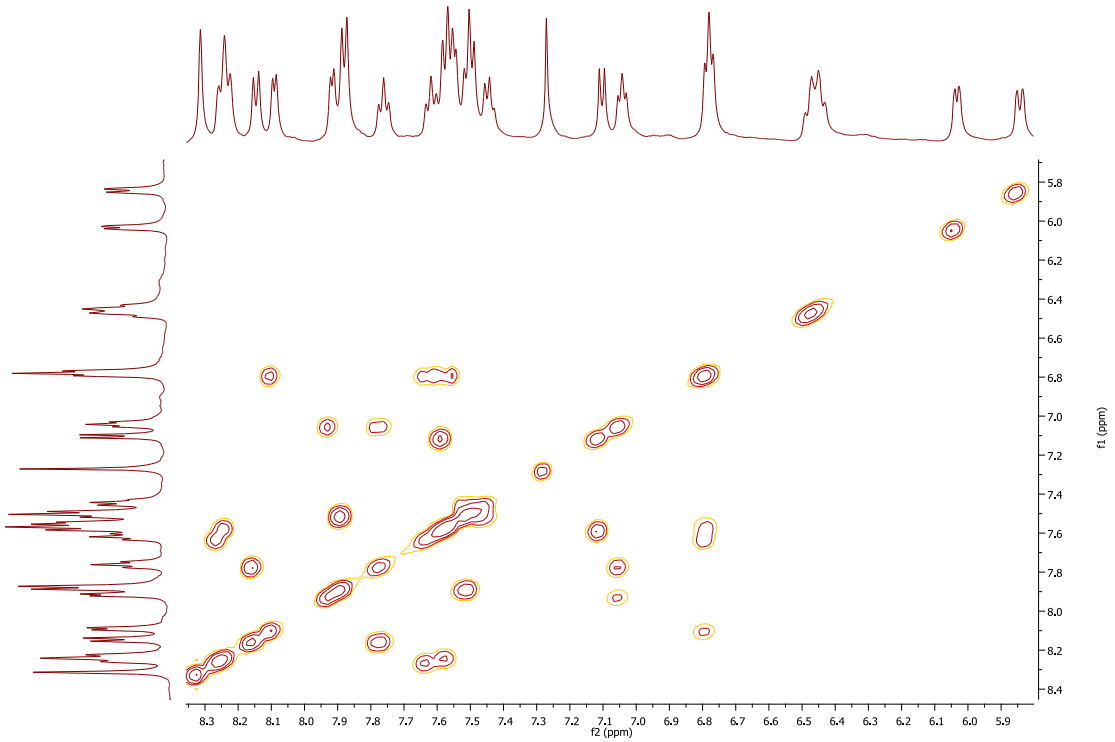
^{13}C NMR (126 MHz, $CDCl_3$):



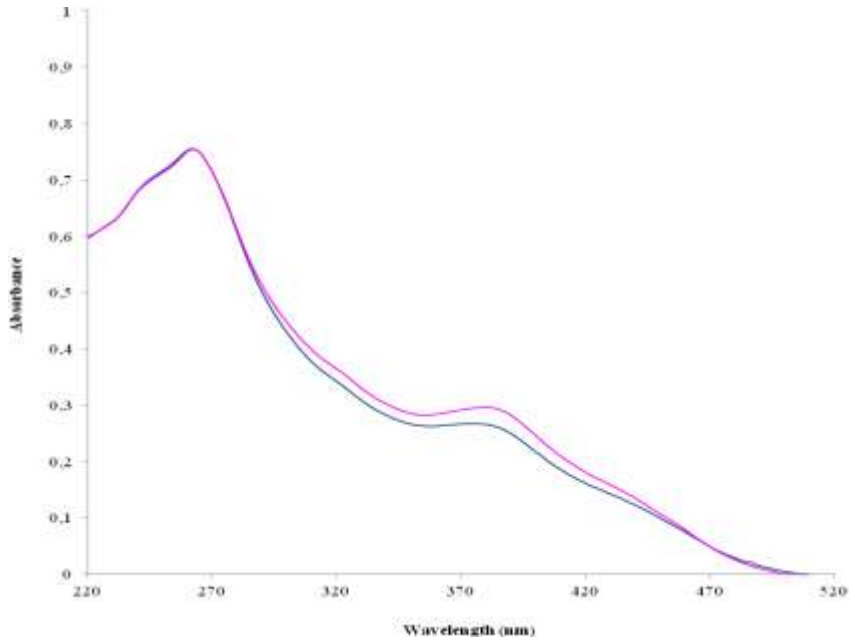
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 389 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
387 ($1.8 \cdot 10^4$), 436 ($9.0 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 389 nm. ($2.5 \cdot 10^{-5}$M).

Due to its low photoisomerization, it has been impossible to calculate k value.

[Ir(Fppy)$_2$**3**], **B3**

SYNTHESIS:

$[Ir(Fppy)_2Cl]_2$ (0.150 g, 0.123 mmol) and silver triflate (0.095 g, 0.370 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of **3** (0.128 g, 0.492 mmol) and triethylamine (0.130 mL, 0.932 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as dark-orange solid (0.143 g, 70%).

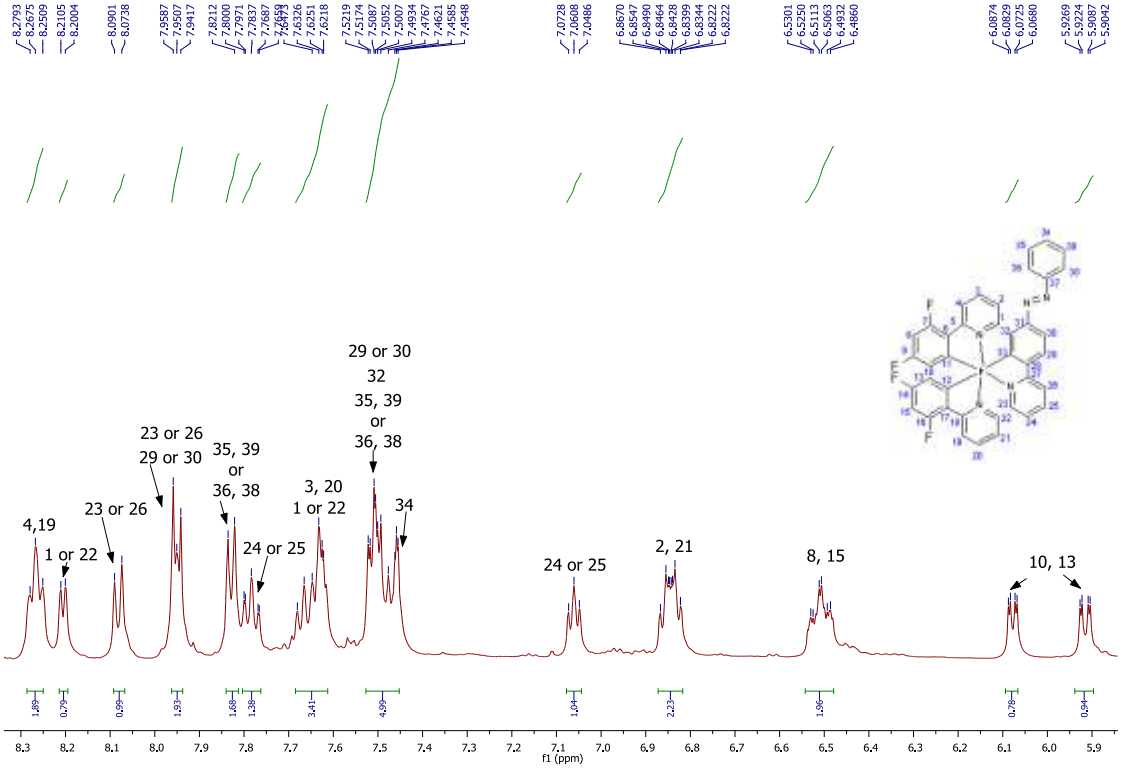
Elemental Analysis: calculated for $C_{39}H_{24}F_4IrN_5$: C, 56.38; H, 2.91; N, 8.43. Found: C, 56.84; H, 2.64; N, 8.25.

Exact mass (EI) - m/z: 832.1656 for $[M+H]^+$ with (^{193}Ir).

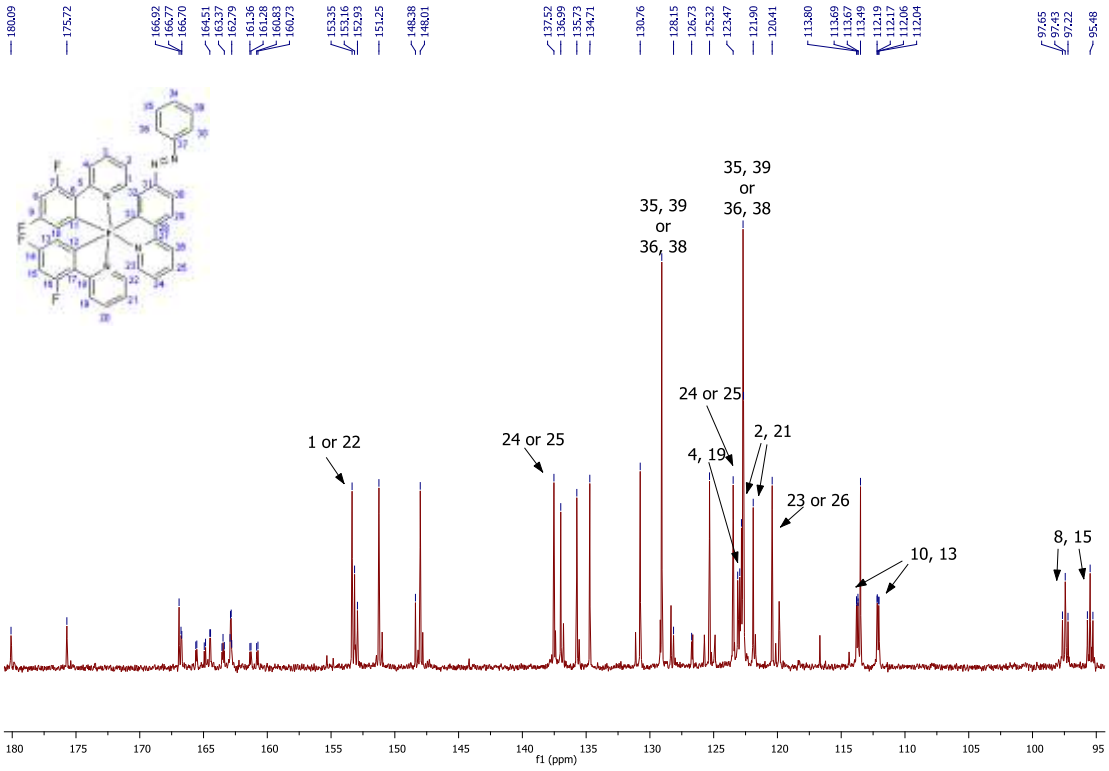
^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.27 (t, J = 7.1, 2H, C_5H_4N ($C_{11}H_6NF_2$)), 8.21 (d, J = 5.0, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 8.08 (d, J = 8.2, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 7.96–7.94 (m, 2H, $C_{16}H_{12}N_3$), 7.83 (d, J = 7.3, 2H, C_6H_5), 7.78 (td, J = 8.1, J =1.4, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 7.68–7.61 (m, 3H, C_5H_4N ($C_{11}H_6NF_2$)), 7.53–7.45 (m, 5H, $C_{16}H_{12}N_3$), 7.06 (t, J = 6.0, 1H, C_5H_4N ($C_{16}H_{12}N_3$)), 6.86 (ddd, J = 7.4, 6.0, 1.4, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 6.83 (ddd, J = 7.3, 6.0, 1.3, 1H, C_5H_4N ($C_{11}H_6NF_2$)), 6.53–6.49 (m, 2H, $C_6H_2F_2$), 6.08 (dd, J = 7.4, 2.3, 1H, $C_6H_2F_2$), 5.92 (dd, J = 9.1, 2.2, 1H, $C_6H_2F_2$).

^{13}C NMR (126 MHz, CD_2Cl_2): δ 180.09 (1C, $C_{quat.\ C11H6NF2}$), 175.72 (1C, $C_{quat.\ C16H12N3}$), 166.92 (1C, $C_{quat.\ C16H12N3}$), 166.74 (d, J =7.9, 1C, $C_{quat.\ C11H6NF2}$), 164.54 (dd, J =10.0, J =260, 1C, $C_{quat.C-F}$), 164.48 (d, J =7.2, 1C, $C_{quat.\ C11H6NF2}$), 163.90 (dd, J =12.7, J = 254, 1C, $C_{quat.C-F}$), 162.86 (d, J = 7.6, 1C, $C_{quat.\ C11H6NF2}$), 162.39 (dd, J =10.9, J =263, 1C, $C_{quat.C-F}$), 161.80 (dd, J =12.9, J =260, 1C, $C_{quat.C-F}$), 153.35 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 153.16 (1C, $C_{quat.\ C16H12N3}$), 152.93 (1C, $C_{quat.\ C16H12N3}$), 151.25 (1C, CH), 148.38 (1C, $C_{quat.\ C16H12N3}$), 148.01 (1C, CH), 137.52 (1C, CH, C_5H_4N ($C_{16}H_{12}N_3$)), 136.99, (1C, CH) 135.73 (1C, CH), 134.71 (1C, CH), 130.76 (1C, CH), 129.07 (2C, CH, C_6H_5), 128.15 (1C, $C_{quat.\ C11H6NF2}$), 126.73 (1C, $C_{quat.\ C11H6NF2}$), 125.32 (1C, CH), 123.47 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 123.04 (d, J =21.4, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.74 (d, J =20.2, 1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.70 (2C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 122.66 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)) 121.90 (1C, CH, C_5H_4N ($C_{11}H_6NF_2$)), 120.41 (1C, C_5H_4N ($C_{16}H_{12}N_3$)), 113.74 (dd, J =13.8, 2.0 1C, CH, $C_6H_2F_2$), 113.49 (1C, CH), 112.11 (dd, J =16.2, 2.0, 1C, CH, $C_6H_2F_2$), 97.43 (pst, J =27.2, 1C, CH, $C_6H_2F_2$), 95.48 (pst, J =27.2, 1C, CH, $C_6H_2F_2$).

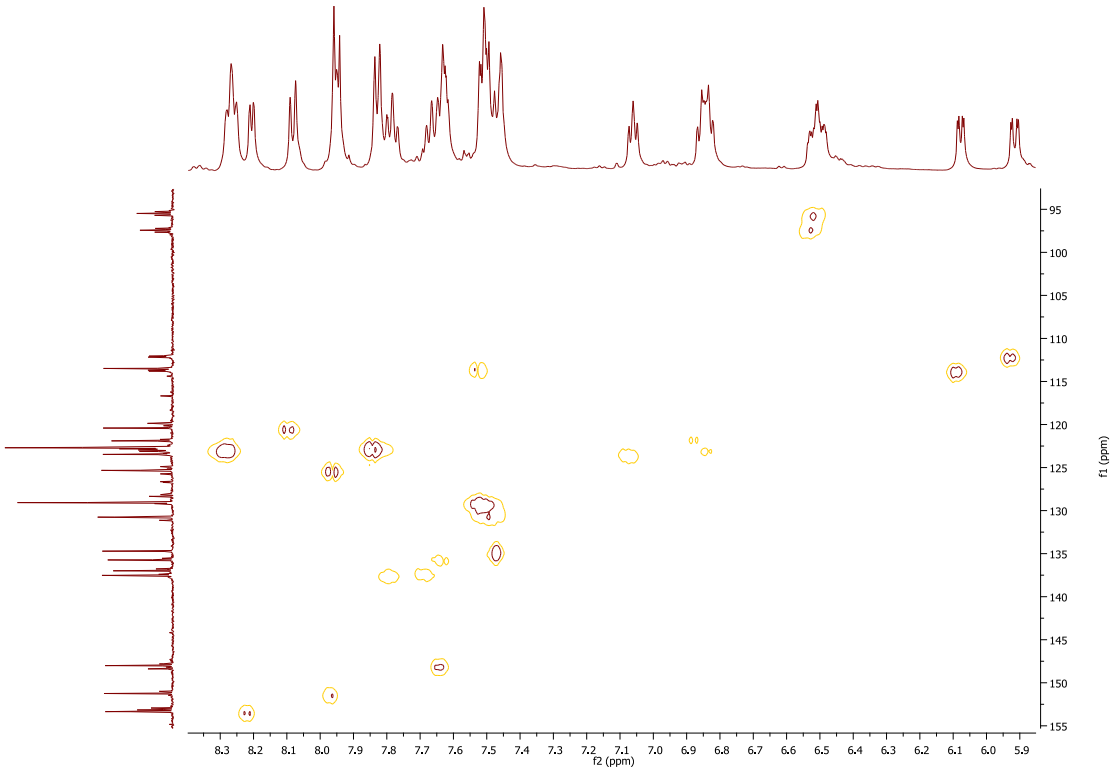
^{1}H NMR (500 MHz, CD_2Cl_2):



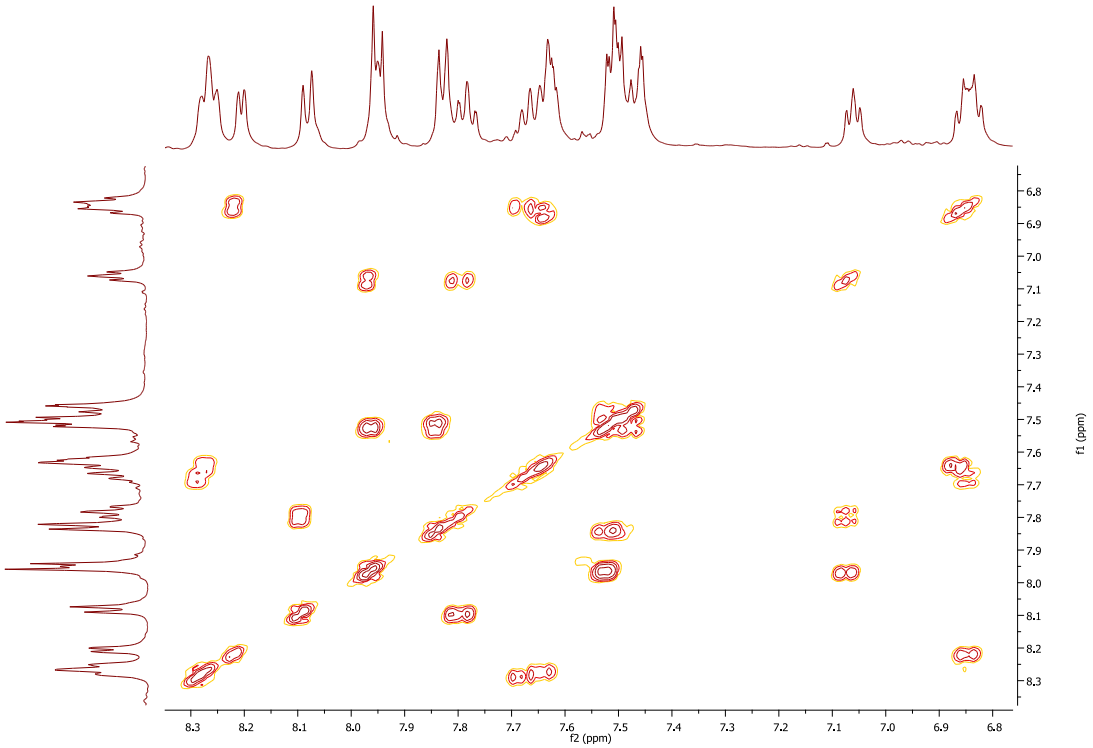
^{13}C NMR (126 MHz, CD_2Cl_2):



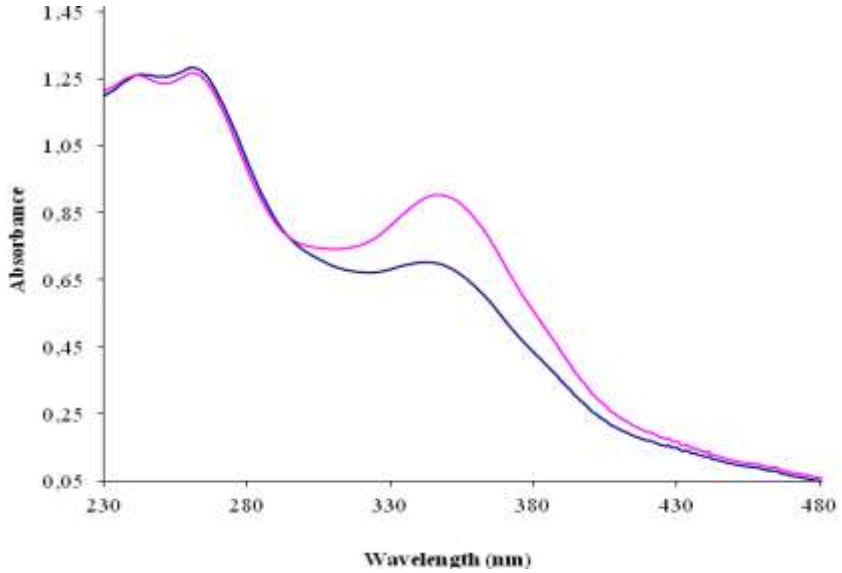
HSQC-NMR:



COSY.NMR:

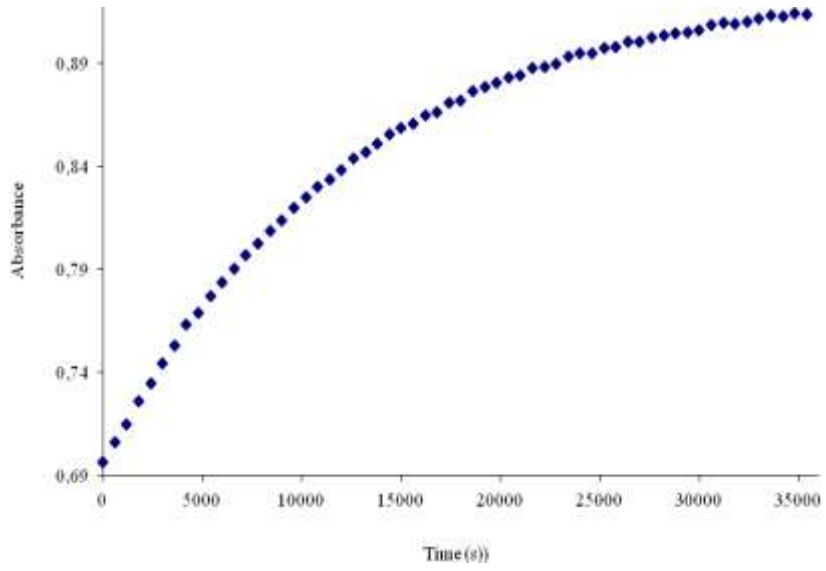


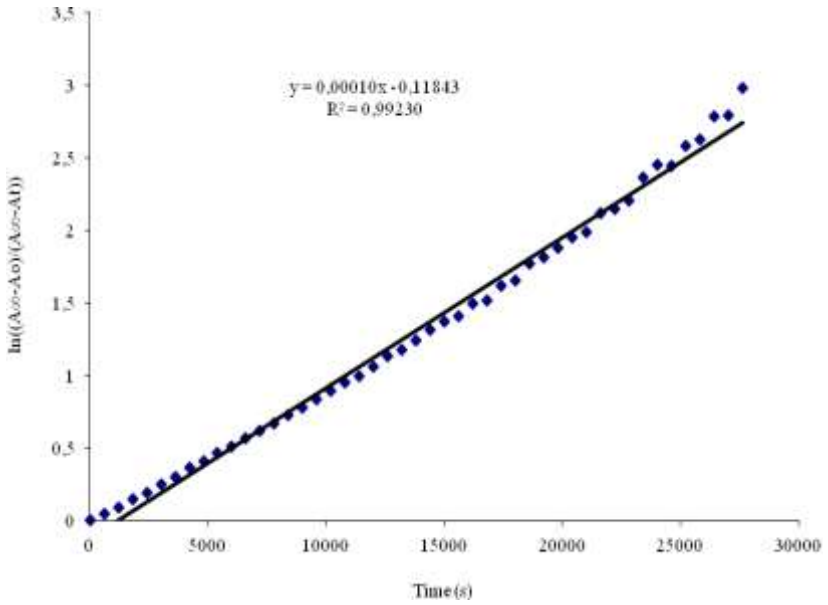
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 355 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
348 ($2.8 \cdot 10^4$), 433 ($5.5 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 355 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$1.0 \cdot 10^{-4}$**
Half-life (s)	**6700**

[Ir(Fppy)$_2$((5-bromo-2-pyridyl)phenyl)], **D**

SYNTHESIS:

$[Ir(Fppy)_2Cl]_2$ (0.150 g, 0.123 mmol) and silver triflate (0.095 g, 0.37 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of 2-(4-bromophenyl)pyridine) (0.115 g, 0.492 mmol) and triethylamine (0.130 mL, 0.932 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as yellow powder (0.060 g, 30%).

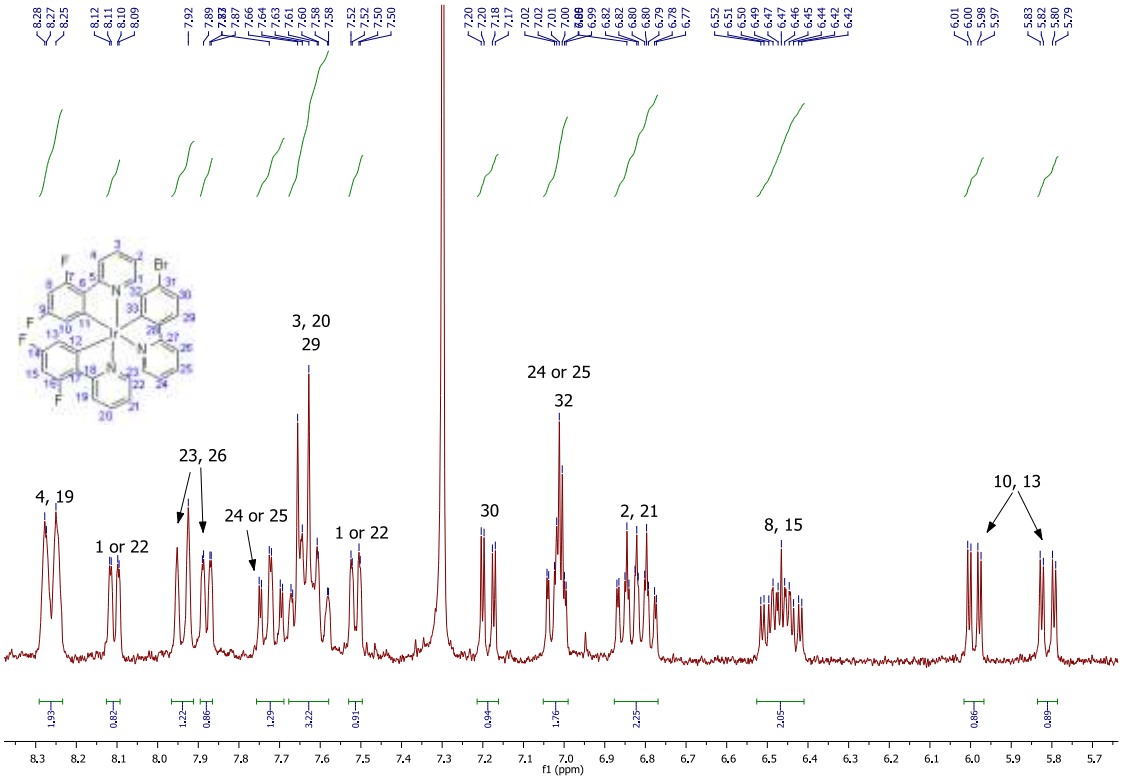
Elemental Analysis: calculated for $C_{33}H_{19}BrF_4IrN_3 \cdot 3C_3H_6O$: C, 51.48; H, 3.81; N, 4.29. Found: C, 51.57; H, 3.55; N, 4.52.

Exact mass (EI) - m/z: 806.0396 for $[M+H]^+$ with (^{193}Ir)(^{79}Br).

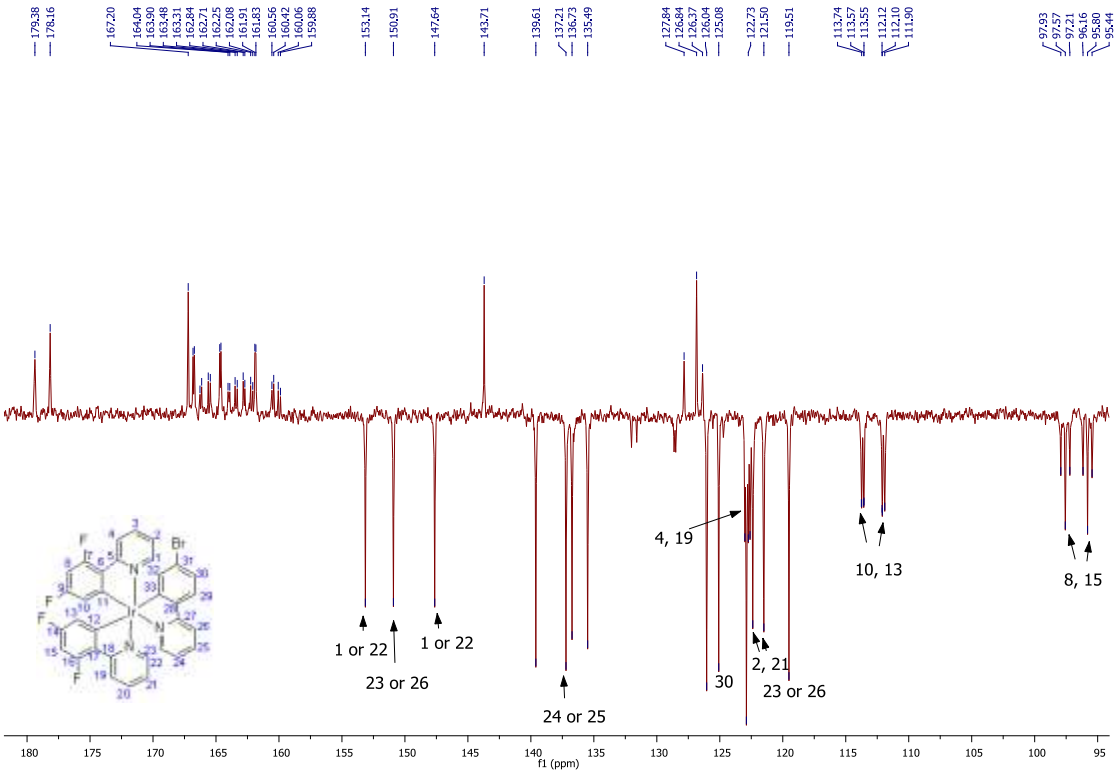
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.29–8.23 (d, J =8.3, 2H, $C_5H_5N(C_{11}H_6NF_2)$), 8.11 (dd, J = 5.9, 1.1, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 7.92 (d, J =8.22, 1H, $C_5H_5N(C_{11}H_7NBr)$), 7.88 (dd, J = 5.6, 0.9, 1H $C_5H_5N(C_{11}H_7NBr)$), 7.72 (t, J =7.4, 1.7, 1H $C_5H_5N(C_{11}H_7NBr)$), 7.66–7.58 (m, 3H), 7.51 (dd, J = 5.9, 0.9, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 7.19 (dd, J = 8.3, 2.1, 1H, C_6H_3Br), 7.02 (ddd, J =7.2, 5.6, 1.3, 1H), 7.01 (d, J = 2.19, 1H), 6.84 (ddd, J = 7.3, 5.9, 1.4, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 6.82 (ddd, J = 7.3, 5.9, 1.4, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 6.53–6.41 (m, 2H, $C_6H_2F_2$), 5.99 (dd, J = 7.5, 2.4, 1H, $C_6H_2F_2$), 5.81 (dd, J = 9.1, 2.4, 1H, $C_6H_2F_2$).

^{13}C NMR (75 MHz, $CDCl_3$): δ 179.38 (1C, $C_{quat.}$ $C_{11}H_6NF_2$), 178.16 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 167.20 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 166.77 (d, J =7.9, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 164.65 (d, J =7.1, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 164.49 (dd, J =10.0, J =257, 1C, $C_{quat.C\text{-}F}$), 163.85 (dd, J =12.5, J = 252, 1C, $C_{quat.C\text{-}F}$), 162.23 (dd, J =10.8, J =261, 1C, $C_{quat.C\text{-}F}$), 161.87 (d, J = 6.4, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 161.69 (dd, J =13.1, J =257, 1C, $C_{quat.C\text{-}F}$), 153.14 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 150.91 (1C, CH, $C_5H_5N(C_{11}H_7NBr)$), 147.64 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 143.71 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 139.61 (1C, CH), 137.21 (1C, CH, C_5H_5N ($C_{11}H_7NBr$)), 136.73, (1C, CH) 135.49 (1C, CH), 127.84 (1C, $C_{quat.}$ $C_{11}H_6NF_2$), 126.84 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 126.37 (1C, $C_{quat.}$ $C_{11}H_6NF_2$), 126.04 (1C, CH), 125.08 (1C, CH, C_6H_3Br), 122.89 (1C, CH), 122.87 (d, J =20.3, 1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 122.8 (d, J =21, 1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 122.38 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 121.50 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 119.51 (1C, CH, $C_5H_5N(C_{11}H_7NBr)$), 113.65 (d, J =14.1, 1.9, 1C, CH, $C_6H_2F_2$), 111.99 (d, J =16.5, 2.1, 1C, CH, $C_6H_2F_2$), 97.56 (pst, J =27.2, 1C, CH, $C_6H_2F_2$), 95.80 (pst, J =27.1, 1C, CH, $C_6H_2F_2$).

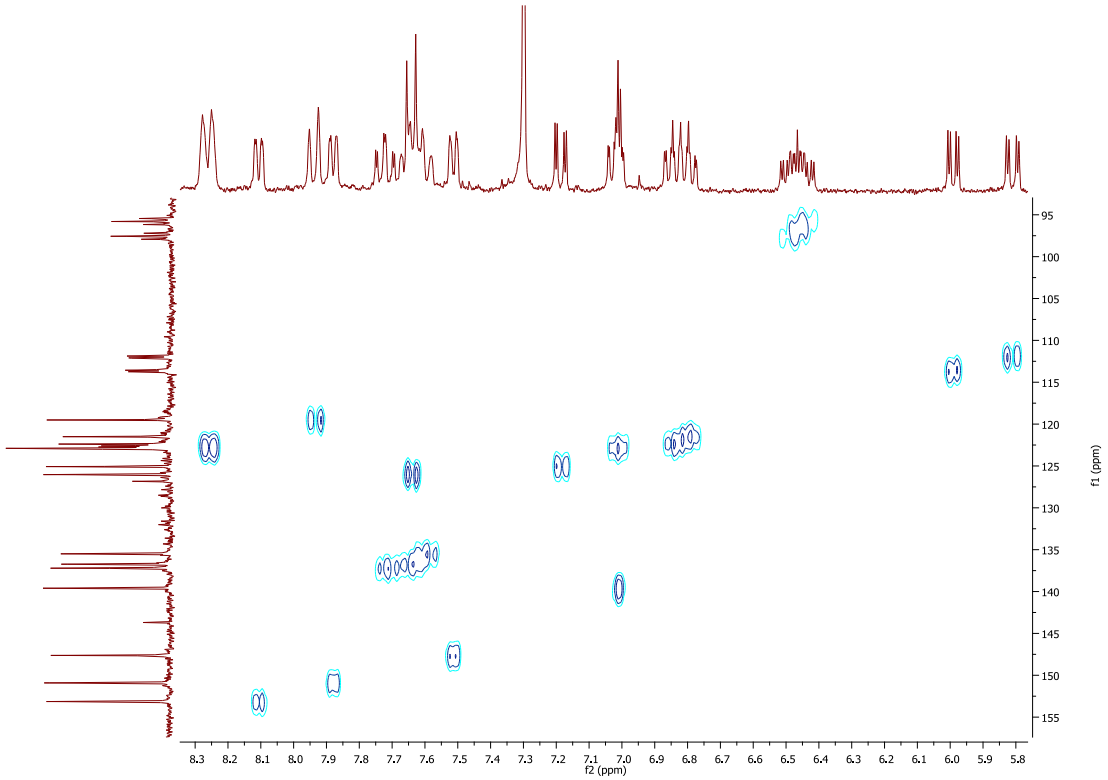
^{1}H NMR (300 MHz, $CDCl_3$):



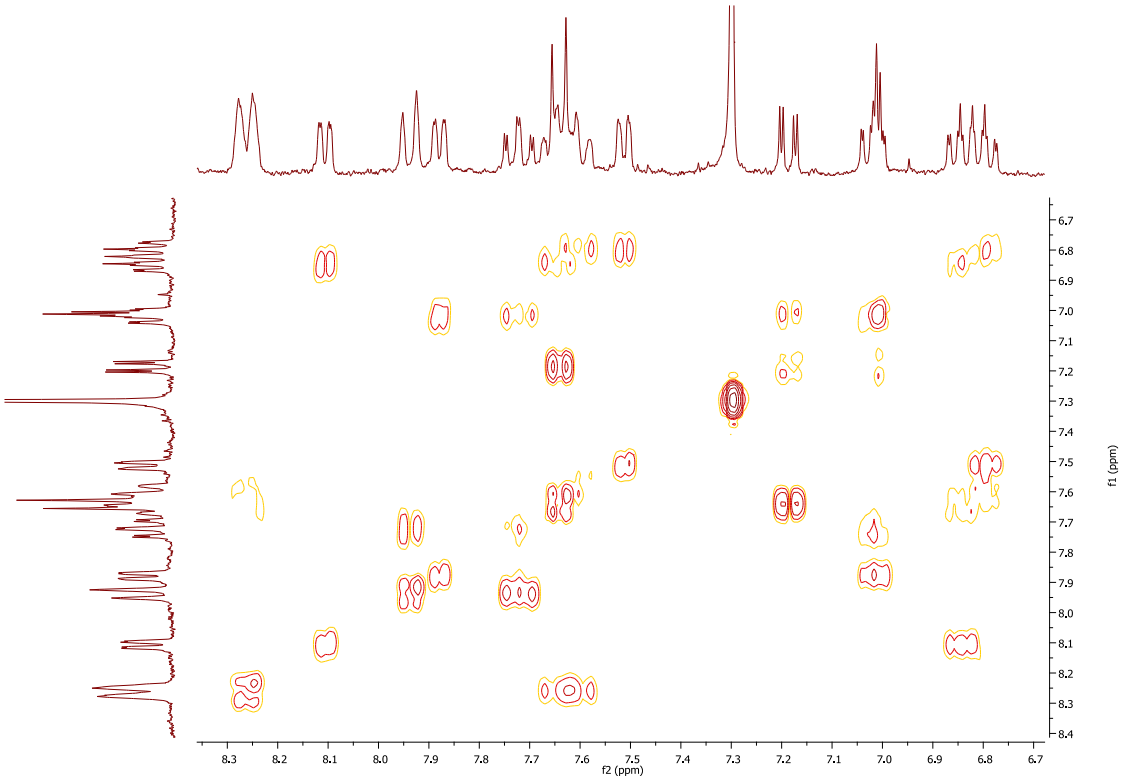
^{13}C APT NMR (75 MHz, $CDCl_3$):



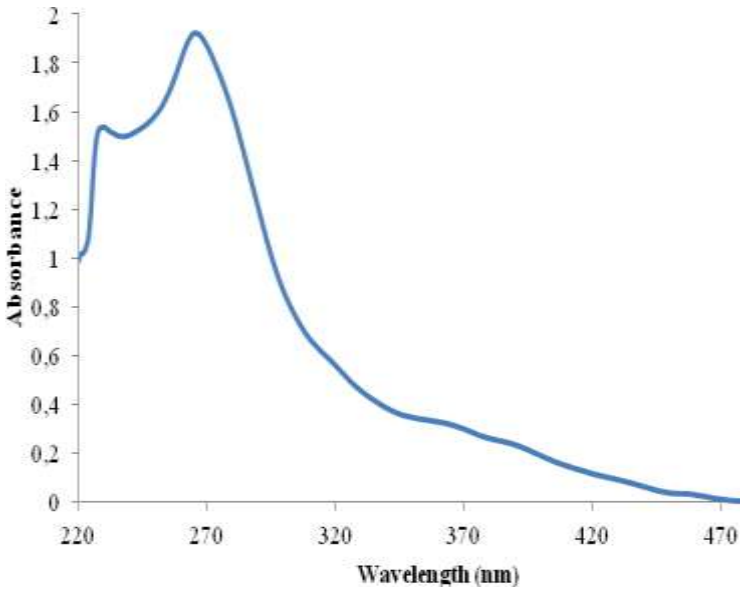
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
226 ($3.9 \cdot 10^4$), 263 ($4.7 \cdot 10^4$), 312 ($1.4 \cdot 10^4$), 356 ($7.5 \cdot 10^3$), 388 ($5.2 \cdot 10^3$), 431 ($1.5 \cdot 10^3$), 458 ($0.3 \cdot 10^3$)

[Ir((5-bromo-2-pyridyl)phenyl))$_2$(ppy)], **F-ppy**

SYNTHESIS:

[Ir((5-bromo-2-pyridyl)phenyl)$_2$Cl]$_2$ (0.150 g, 0.108 mmol) and silver triflate (0.084 g, 0.324 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of 2-phenylpyridine (0.067 g, 0.060 mL, 0.432 mmol) and triethylamine (0.113 mL, 0.810 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane:hexane (5:1). The product was obtained as yellow powder (0.105 g, 60%).

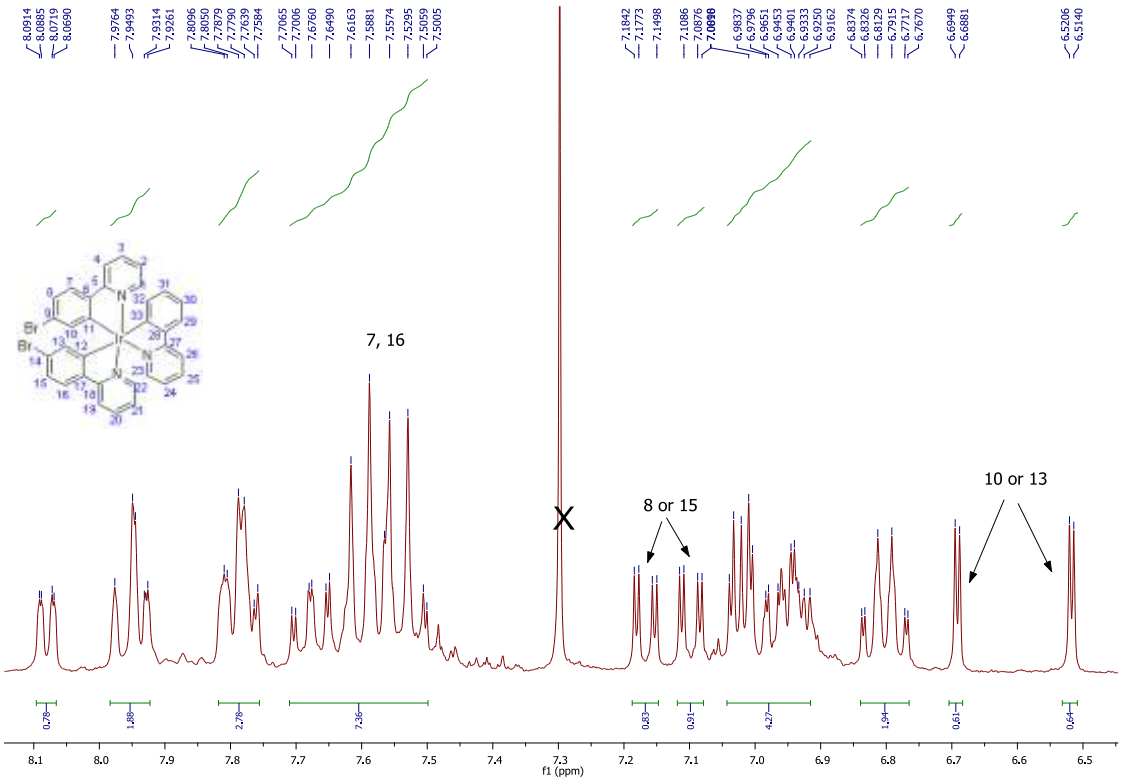
Elemental Analysis: calculated for $C_{33}H_{22}Br_2IrN_3 \cdot C_6H_{14}$: C, 57.19; H, 6.02; N, 3.92. Found: C, 57.20; H, 6.11; N, 3.77.

Exact mass (MALDI) - m/z: 810.9785 for $[M]^+$ with (^{193}Ir)(^{79}Br).

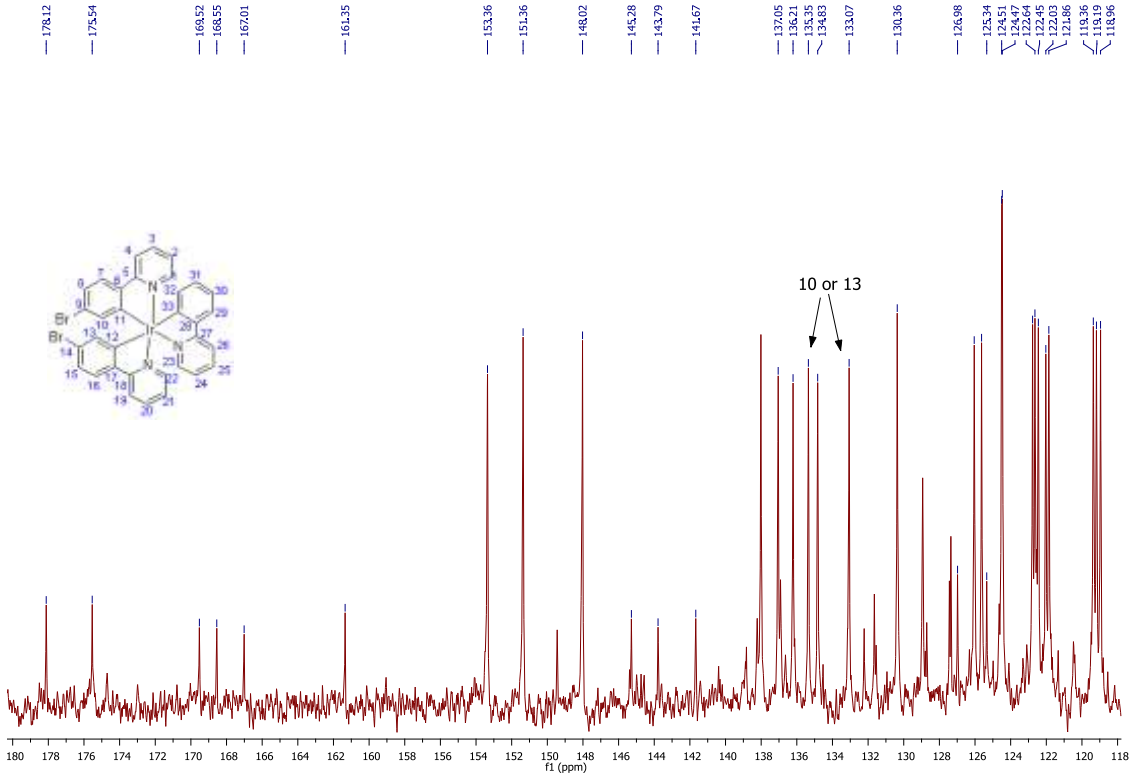
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.08 (dd, J = 5.8, 0.9, 1H), 7.98–7.92 (m, 2H), 7.78 (m, 3H), 7.71–7.50 (m, 6H), 7.17 (dd, J = 8.3, 2.1, 1H, C_5H_3Br), 7.10 (dd, J = 8.3, 2.0, 1H, C_5H_3Br), 7.04–6.92 (m, 4H), 6.81 (ddd, J = 7.4, 1.4, 2H), 6.79 (ddd, J = 7.4, 1.4, 2H), 6.69 (d, J = 2.0, 1H, C_5H_3Br), 6.52 (d, J = 2.0, 1H, C_5H_3Br).

^{13}C NMR (75 MHz, $CDCl_3$): δ 178.34 (1C, $C_{quat.}$), 175.75 (1C, $C_{quat.}$), 169.74 (1C, $C_{quat.}$), 168.76 (1C, $C_{quat.}$), 167.23 (1C, $C_{quat.}$), 161.56 (1C, $C_{quat.}$), 153.57 (1C, CH, C_5H_4N), 151.58 (1C, CH), 148.24 (1C, CH), 145.50 (1C, $C_{quat.}$), 144.00 (1C, $C_{quat.}$), 141.89 (1C, $C_{quat.}$), 138.23 (1C, CH), 137.26 (1C, CH), 136.43 (1C, CH), 135.57 (1C, CH C_5H_3Br), 135.05 (1C, CH), 133.28 (1C, CH, C_5H_3Br), 130.58 (1C, CH), 127.20 (1C, $C_{quat.}$), 126.26 (1C, CH), 125.56 (1C, $C_{quat.}$), 125.85 (1C, CH), 124.72 (1C, CH), 124.69 (1C, CH), 122.99 (1C, CH), 122.86 (1C, CH), 122.66 (1C, CH), 122.24 (1C, CH), 122.07 (1C, CH), 119.58 (1C, CH), 119.40 (1C, CH), 119.17 (1C, CH).

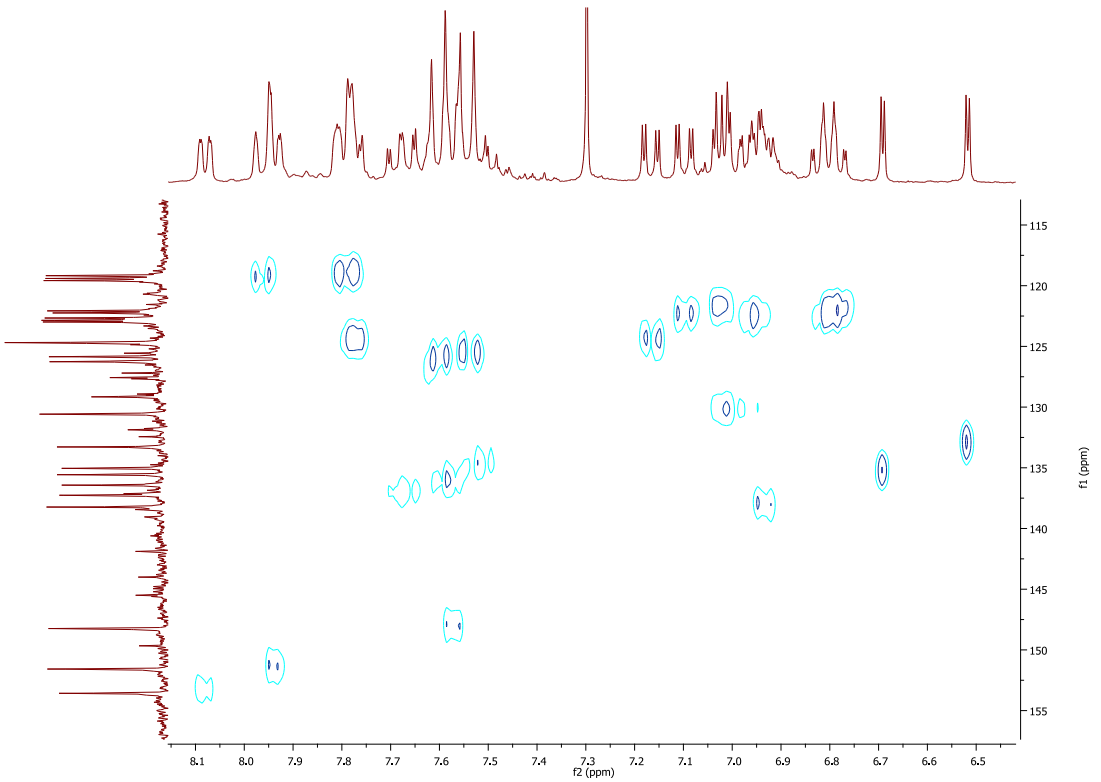
^{1}H NMR (300 MHz, $CDCl_3$):



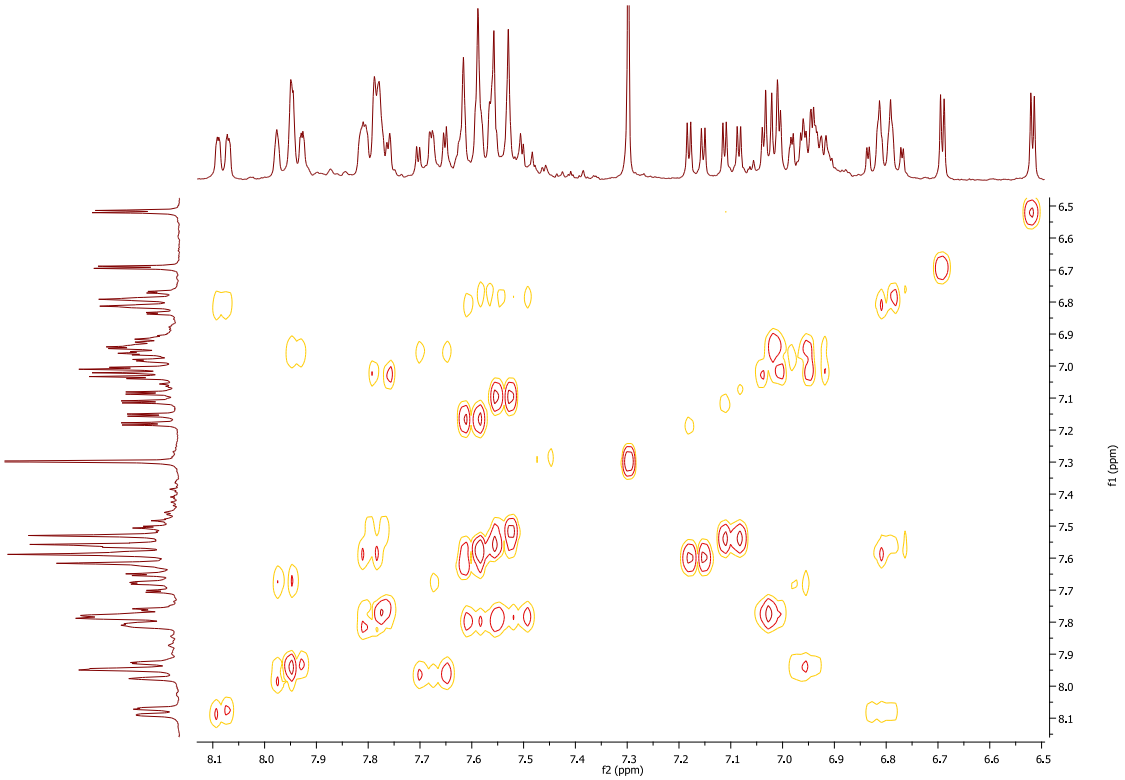
^{13}C NMR (75 MHz, $CDCl_3$):



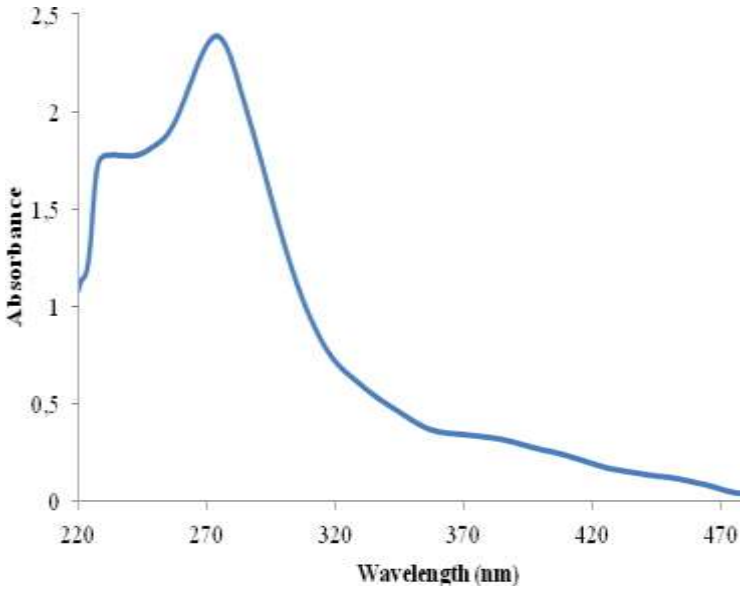
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
228 (36900), 267 (47300), 366 (5500), 399 (3900), 446 (1400), 476 (200)

[Ir((5-bromo-2-pyridyl)phenyl))$_2$(Fppy)] **F-Fppy**

SYNTHESIS:

[Ir((5-bromo-2-pyridyl)phenyl)$_2$Cl]$_2$ (0.150 g, 0.108 mmol) and silver triflate (0.084 g, 0.324 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of Fppy (0.083 g, 0.066 mL, 0.432 mmol) and triethylamine (0.113 mL, 0.810 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as yellow powder (0.110 g, 60%).

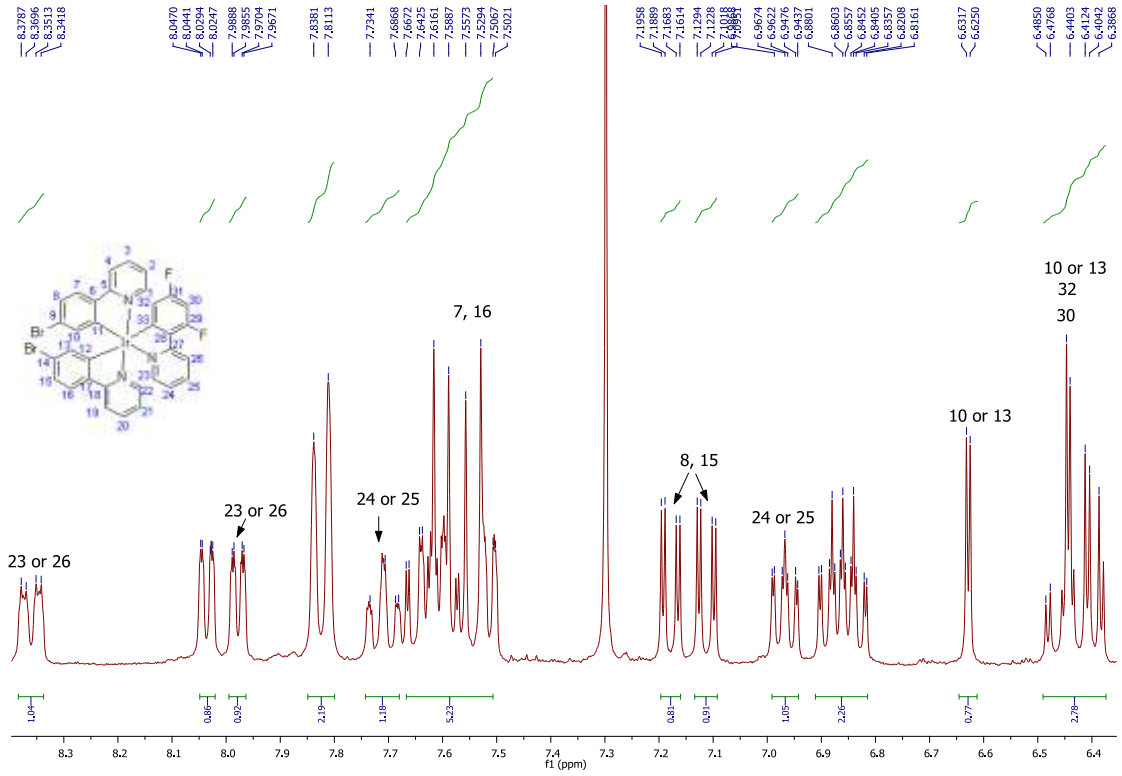
Elemental Analysis: calculated for $C_{33}H_{20}Br_2F_2IrN_3 \cdot CH_2Cl_2$: C, 43.75; H, 2.38; N, 4.50. Found: C, 43.92; H, 1.98; N, 4.28.

Exact mass (MALDI) - m/z: 846.9603 for $[M]^+$ with (^{193}Ir)(^{79}Br).

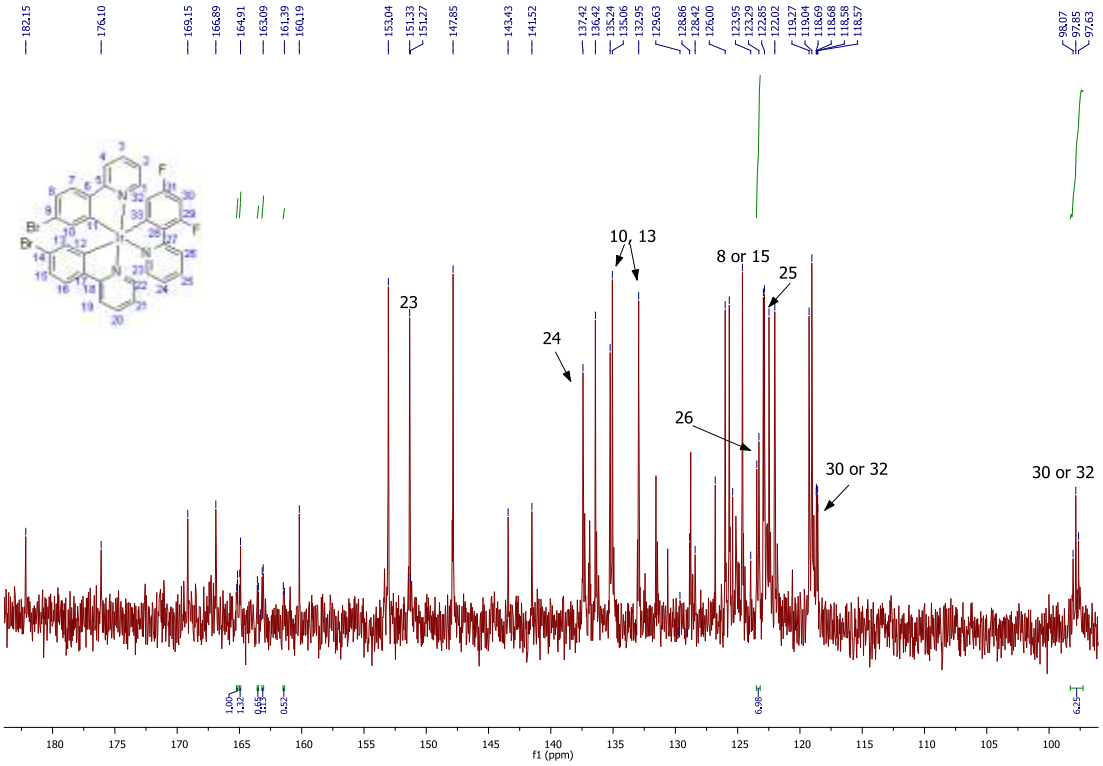
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.36 (ddd, $^5J_{F-H}$ = 1.7, J = 8.3, 1.0, 1H, $C_5H_4N(C_{11}H_6NF_2)$), 8.04 (brdd, J = 5.8, 1.4, 1H, $C_5H_4N(C_{11}H_7NBr)$), 7.98 (brdd, J = 5.5, 1.6, 1H, $C_5H_4N(C_{11}H_6NF_2)$), 7.82 (d, J = 8.1, 2H, $C_5H_4N(C_{11}H_7NBr)$), 7.70 (brddd, J = 8.3, 7.3, 1.6, 1H, $C_5H_4N(C_{11}H_6NF_2)$), 7.67–7.51 (m, 5H, $C_{11}H_7NBr$), 7.18 (dd, J = 8.3, 2.1, 1H, C_6H_4Br), 7.11 (dd, J = 8.3, 2.0, 1H, C_6H_4Br), 6.97 (ddd, J = 7.1, 5.6, 1.2, 1H, $C_5H_4N(C_{11}H_6NF_2)$), 6.88 (ddd, J = 7.3, 5.9, 1.4, 1H, $C_5H_4N(C_{11}H_7NBr)$), 6.84 (ddd, J = 7.3, 5.9, 1.4, 1H, $C_5H_4N(C_{11}H_7NBr)$), 6.63 (d, J = 2.0, 1H, C_6H_4Br), 6.49–6.37 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 182.15 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 176.10 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 169.15 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 166.89 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 164.94 (d, J =7.6, 1C, $C_{quat.}$ $C_{11}H_7NBr$), 164.16 (dd, J =9.1, J = 258, 1C, $C_{quat.C-F}$), 162.48 (dd, J =10.6, J = 262, 1C, $C_{quat.C-F}$), 160.19 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 153.04 (1C, CH C_6H_3Br), 151.33 (1C, CH, $C_5H_4N(C_{11}H_6NF_2)$), 147.85 (1C, CH), 143.43 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 141.52 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 137.42 (1C, CH, $C_5H_4N(C_{11}H_6NF_2)$), 136.42 (1C, CH), 135.24 (1C, CH), 135.06 (1C, CH, C_6H_4Br), 132.95 (1C, CH, C_6H_4Br), 128.42 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 126.80 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 126.00 (1C, CH), 125.67 (1C, CH), 125.40 (1C, $C_{quat.}$ $C_{11}H_7NBr$), 124.62 (1C, CH, C_6H_4Br), 123.38 (d, J =21.7, 1C, CH, $C_5H_4N(C_{11}H_6NF_2)$), 122.93 (1C, CH), 122.85 (1C, CH), 122.48 (1C, CH, $C_5H_4N(C_{11}H_6NF_2)$), 122.02 (1C, CH), 119.27 (1C, CH, $C_5H_4N(C_{11}H_7NBr)$), 119.04 (1C, CH, $C_5H_4N(C_{11}H_7NBr)$), 118.63 (d, J =13.7, 2.0, 1C, CH, $C_6H_2F_2$), 97.85 (pst, J =27.5, 1C, CH, $C_6H_2F_2$)

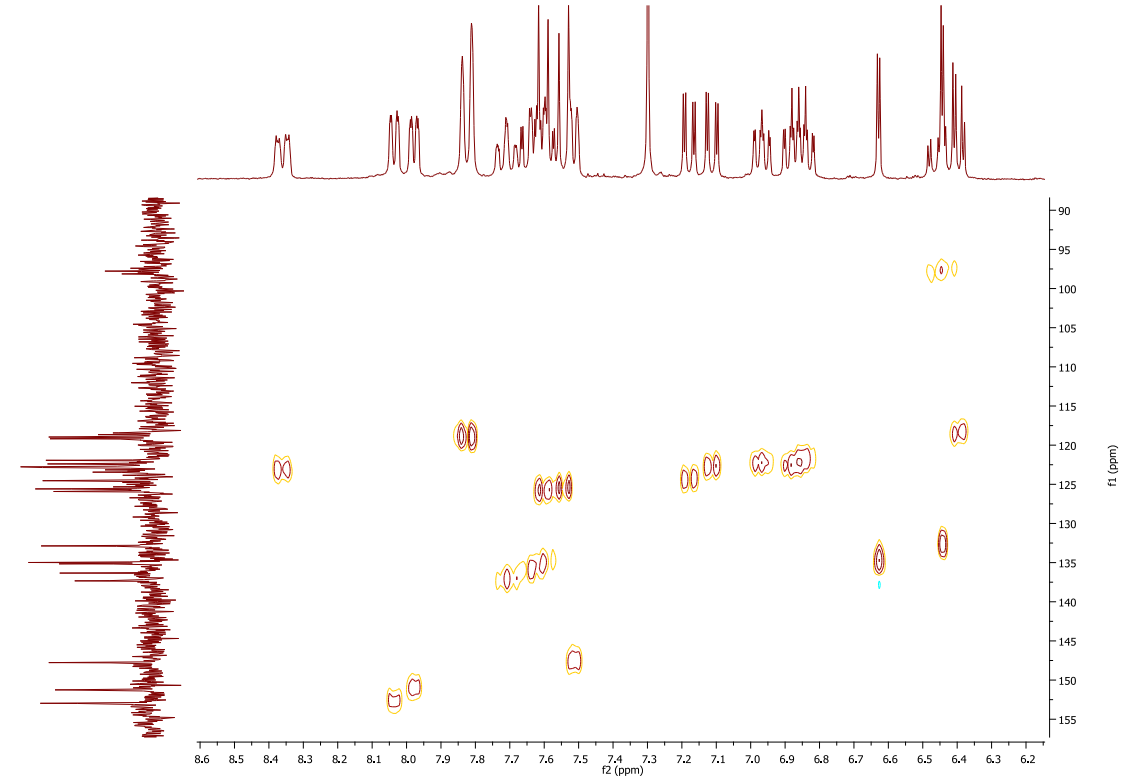
^{1}H NMR (300 MHz, $CDCl_3$):



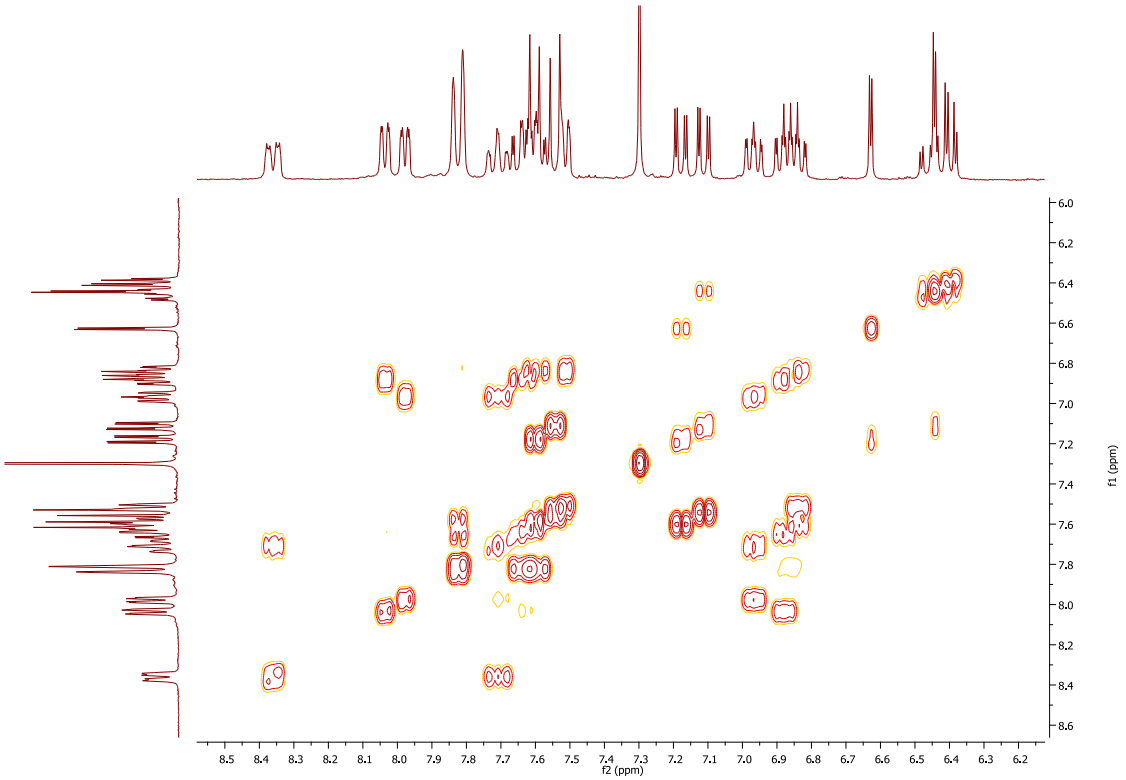
^{13}C NMR (126 MHz, $CDCl_3$):



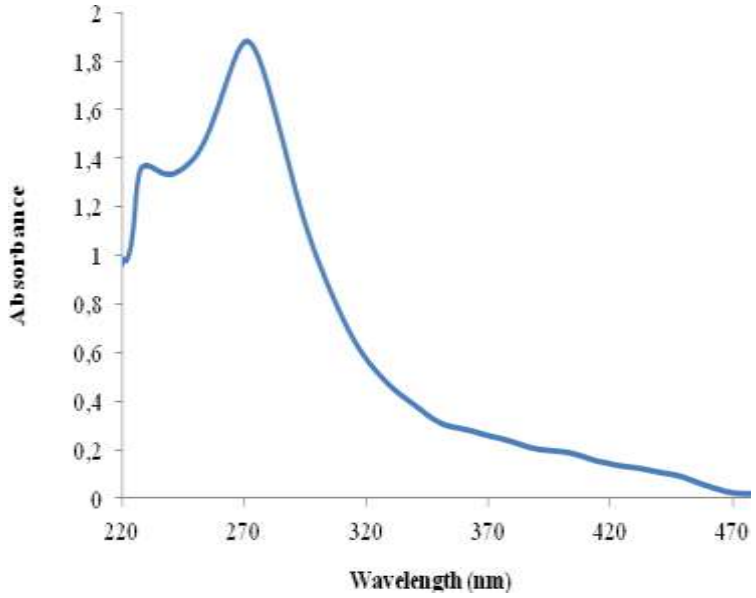
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
228 ($3.7 \cdot 10^4$), 267 ($4.7 \cdot 10^4$), 366 ($5.5 \cdot 10^3$), 399 ($3.9 \cdot 10^3$), 446 ($1.4 \cdot 10^3$), 476 ($0.2 \cdot 10^3$)

[Ir(ppy)$_2$**4**], **A4**

SYNTHESIS:

C (0.100 g, 0.136 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.046 g, 0.150 mmol), $Pd(PPh_3)_4$ (2 mol %, 3.143 mg, 0.003 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as orange powder (0.097 g, 85%).

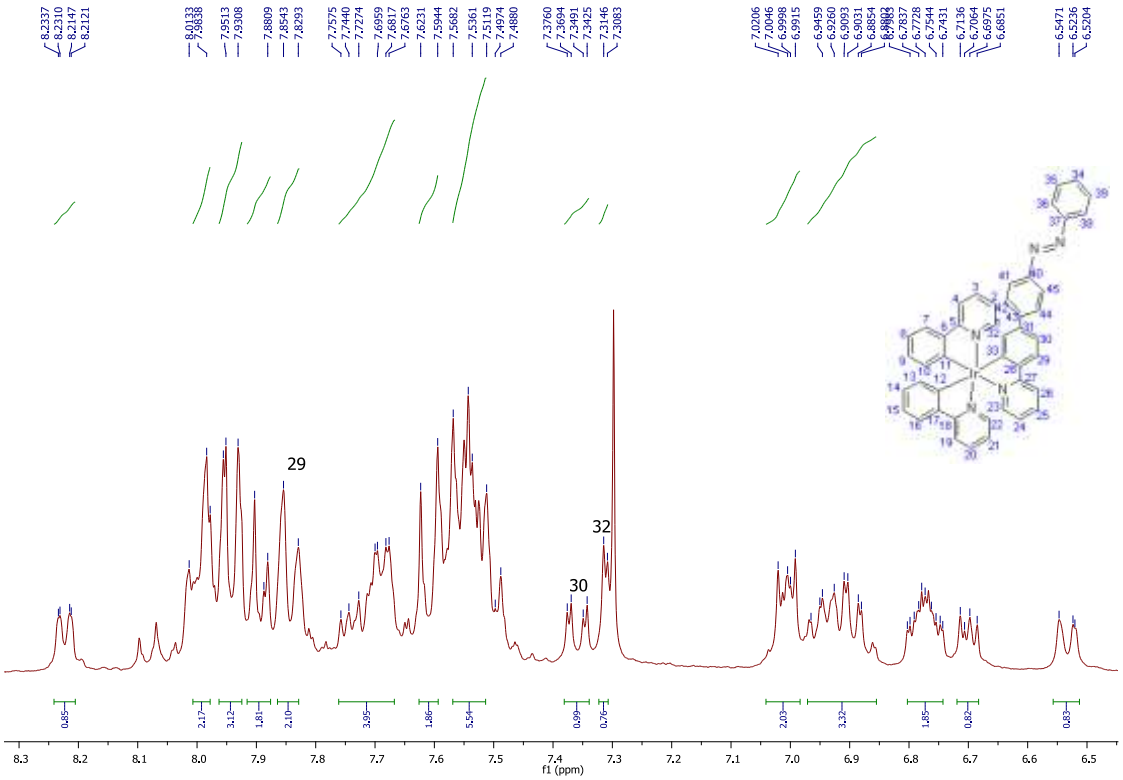
Elemental Analysis: calculated for $C_{45}H_{32}IrN_5 \cdot 1.5C_3H_6O$: C, 64.48; H, 4.48; N, 7.59. Found: C, 63.97; H, 4.08; N, 7.72.

Exact mass (MALDI) - m/z: 835.2299 for $[M]^+$ with (^{193}Ir).

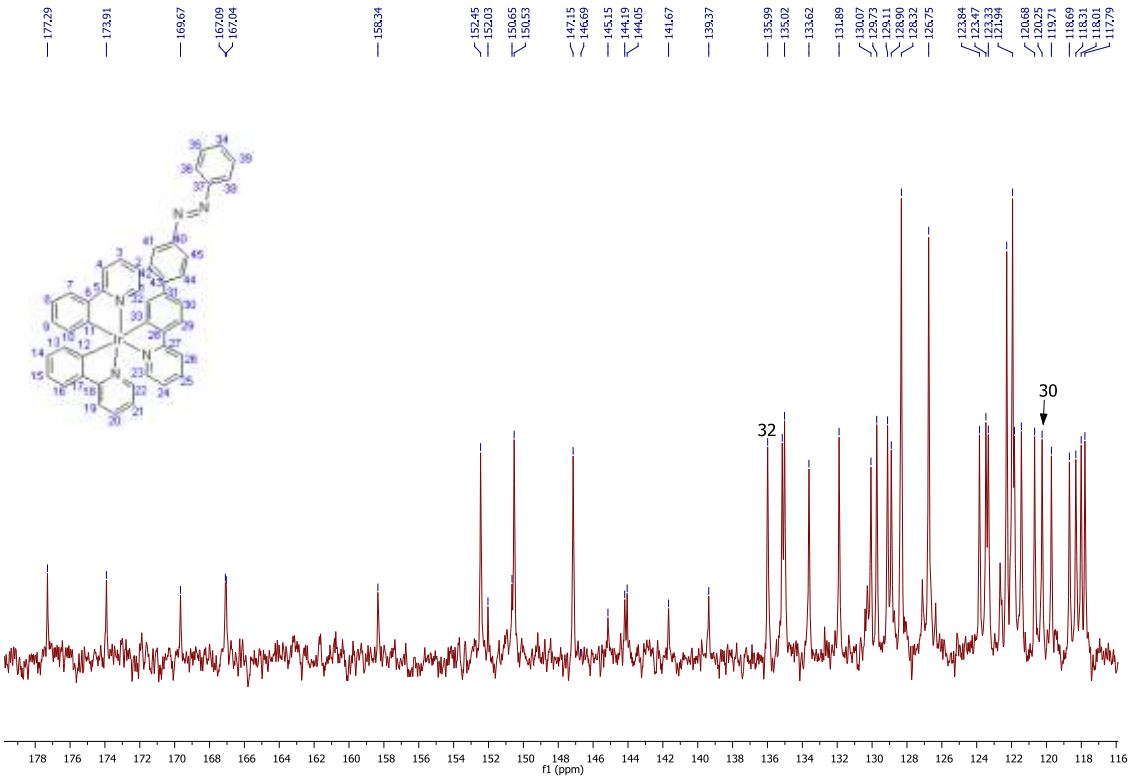
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22 (dd, J = 5.7, 0.8, 1H), 8.01–7.83 (m, 9H), 7.76–7.67 (m, 4H), 7.62–7.49 (m, 7H), 7.36 (dd, J = 8.1, 2.0, 1H, C_6H_3), 7.31 (d, J = 1.9, 1H, C_6H_3), 7.00–6.99 (m, 2H), 6.97–6.86 (m, 3H), 6.80–6.74 (m, 2H), 6.71–6.69 (m, 1H), 6.53 (dd, J = 7.1, 1.4 1H).

^{13}C NMR (75 MHz, CD_2Cl_2): δ 177.29 (1C, $C_{quat.}$), 173.91 (1C, $C_{quat.}$), 169.67 (1C, $C_{quat.}$), 167.09 (1C, $C_{quat.}$), 167.04 (1C, $C_{quat.}$), 158.34 (1C, $C_{quat.}$), 152.45 (1C, CH), 152.03 (1C, $C_{quat.}$), 150.65 (1C, $C_{quat.}$), 150.53 (1C, CH), 147.15 (1C, CH), 145.15 (1C, $C_{quat.}$), 144.19 (1C, $C_{quat.}$), 144.05 (1C, $C_{quat.}$), 141.67 (1C, $C_{quat.}$), 139.37 (1C, $C_{quat.}$), 135.99 (1C, CH, C_6H_3), 135.15 (1C, CH) 135.02 (1C, CH), 133.62 (1C, CH), 131.89 (1C, CH), 130.07 (1C, CH), 129.73 (1C, CH), 129.11 (1C, CH), 128.90 (1C, CH), 128.32 (2C, CH, $C_{12}H_9N_2$), 126.75 (2C, CH, $C_{12}H_9N_2$), 123.84 (1C, CH), 123.47 (1C, CH), 123.33 (1C, CH), 122.28 (2C, CH, $C_{12}H_9N_2$), 121.94 (2C, CH, $C_{12}H_9N_2$), 121.83 (1C, CH), 121.44 (1C, CH), 120.68 (1C, CH), 120.25 (1C, CH, C_6H_3), 119.71 (1C, CH), 118.69 (1C, CH), 118.31 (1C, CH), 118.01 (1C, CH), 117.79 (1C, CH).

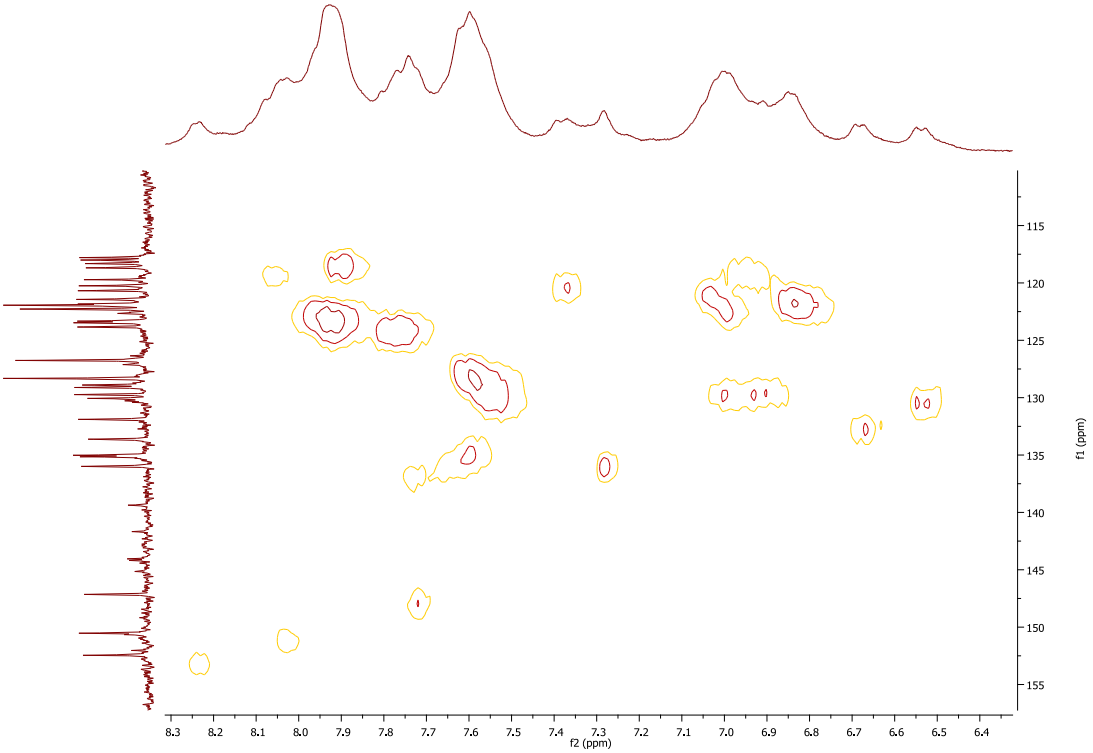
^{1}H NMR (300 MHz, $CDCl_3$):



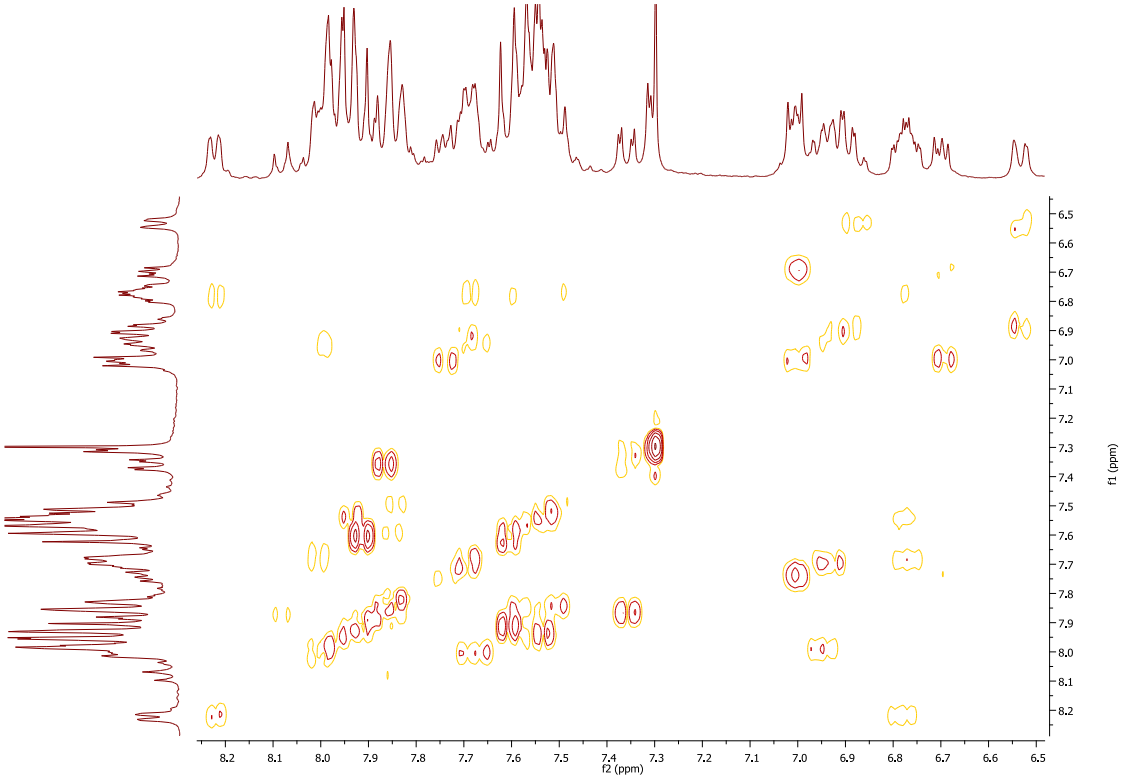
^{13}C NMR (75 MHz, CD_2Cl_2):



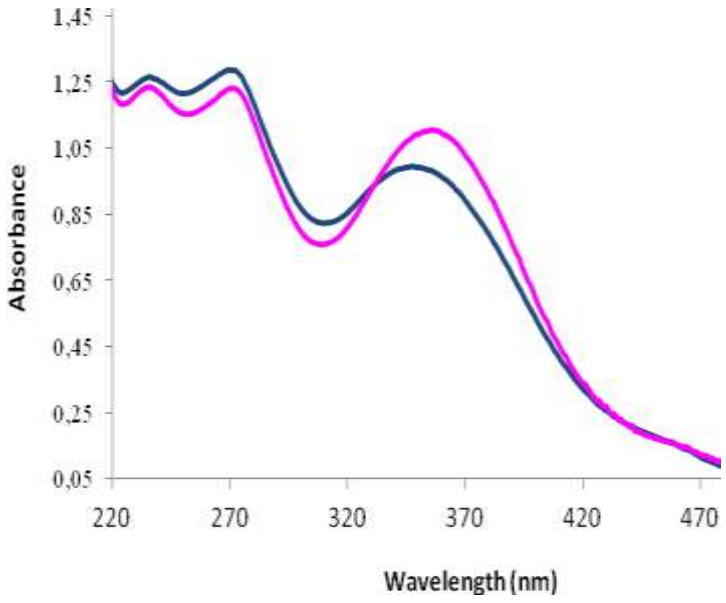
HSQC-NMR:



COSY.NMR:

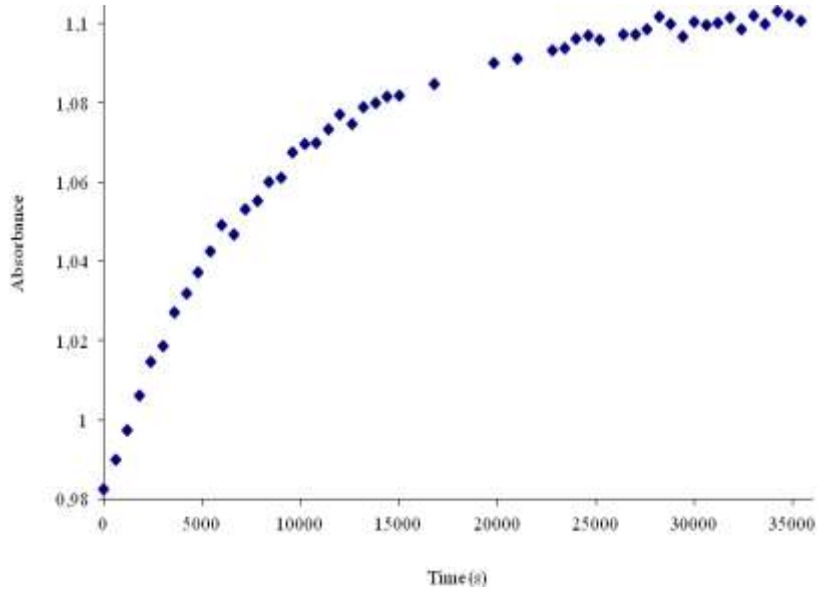


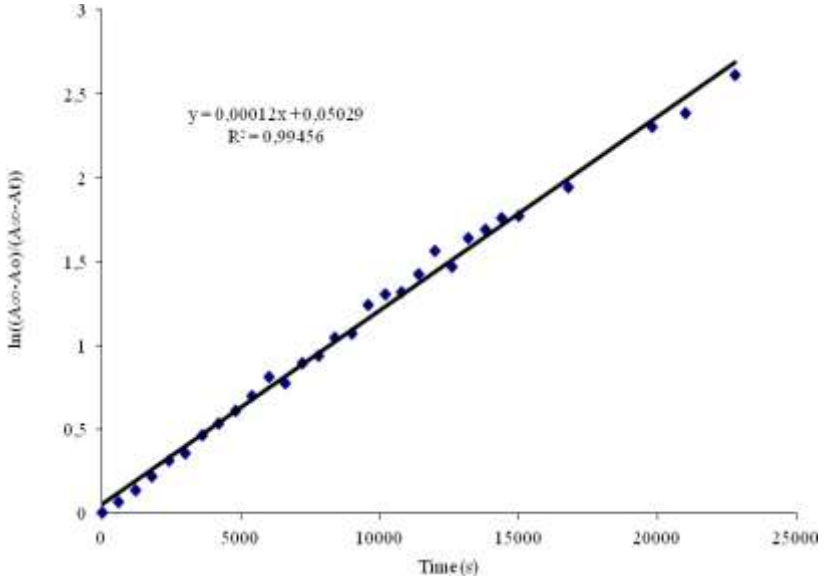
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 367 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
356 ($3.7 \cdot 10^4$), 464 ($5.4 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 367 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$1.2 \cdot 10^{-4}$**
Half-life (s)	**6000**

[Ir(Fppy)$_2$**4**], **B4**

SYNTHESIS:

D (0.100 g, 0.124 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.042 g, 0.137 mmol), $Pd(PPh_3)_4$ (2 mol %, 2.867 mg, 0.002 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as orange powder (0.099 g, 88%).

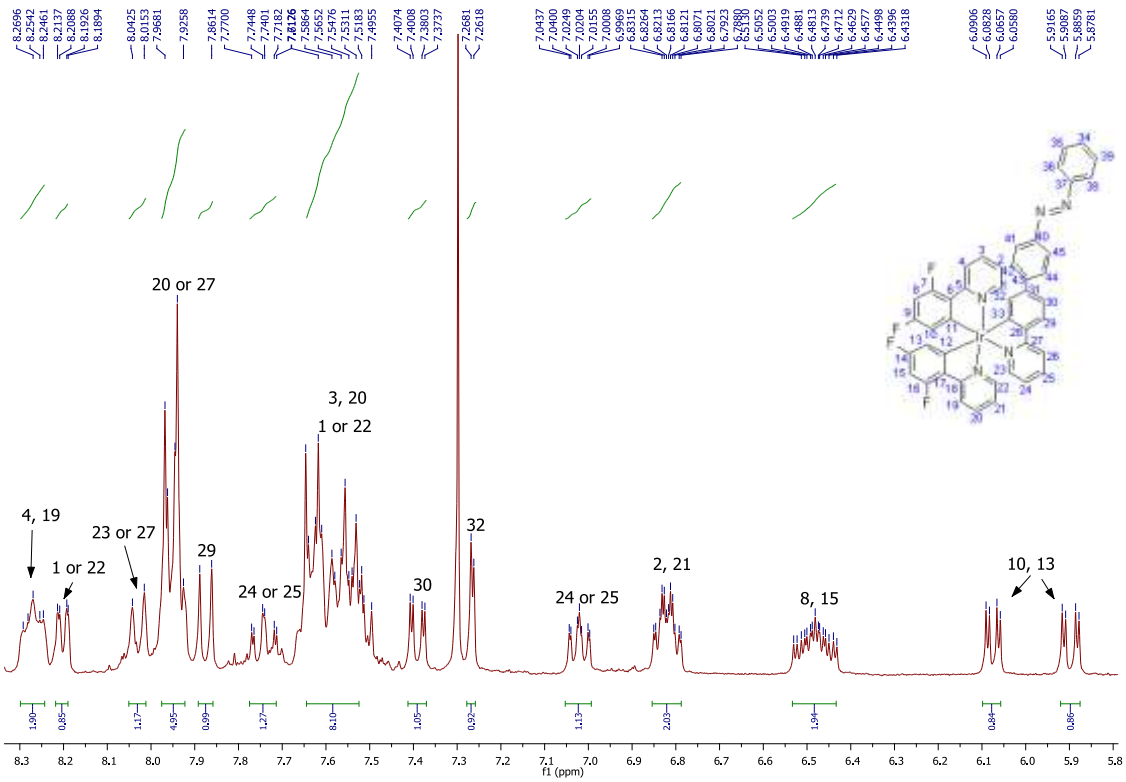
Elemental Analysis: calculated for $C_{45}H_{28}F_4IrN_5 \cdot {}_2CH_2Cl_2$: C, 52.42; H, 3.00; N, 6.50. Found: C, 52.18; H, 2.49; N, 6.43.

Exact mass (MALDI) - m/z: 907.1906 for $[M]^+$ with (^{193}Ir).

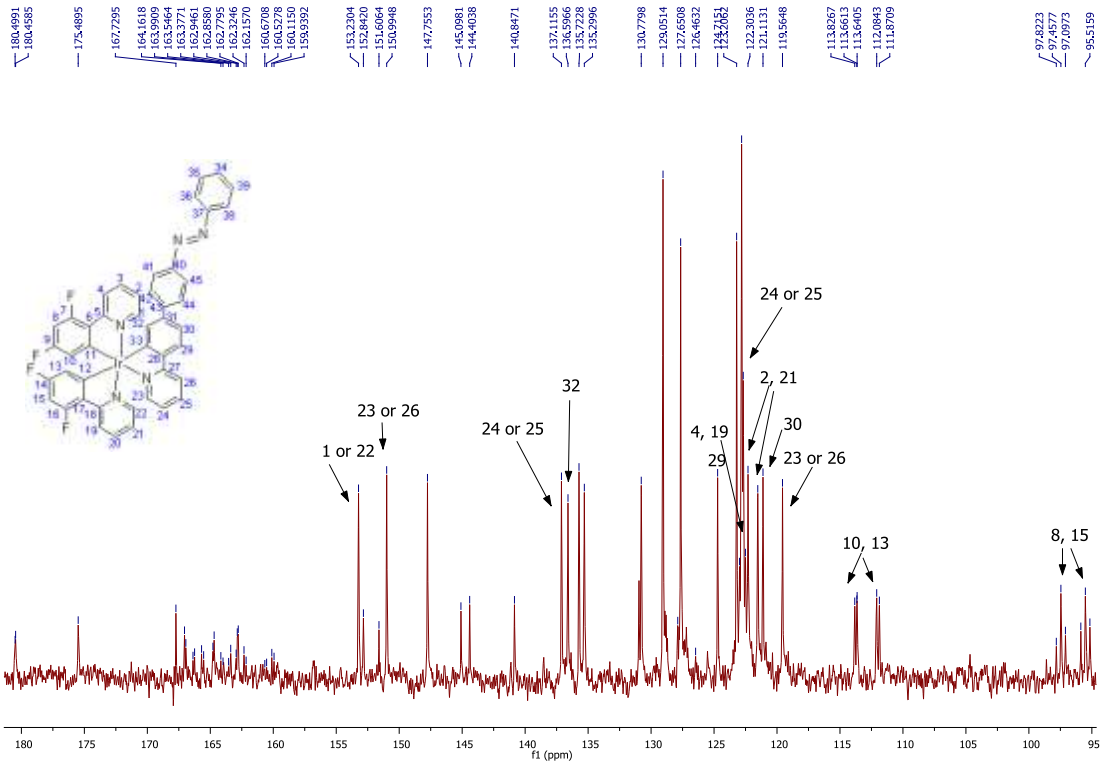
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.30–8.24 (m, 2H, $C_5H_5N(C_{11}H_6NF_2)$), 8.21 (dd, J =5.8, 1.1, 1H $C_5H_5N(C_{11}H_6NF_2)$), 8.03 (d, J = 8.1, 1H, $C_5H_5N(C_{23}H_{16}N_3)$), 7.98–7.92 (m, 5H), 7.87 (d, J = 8.2, 1H C_6H_3), 7.74 (td, J =7.6, 1.7, 1H, $C_5H_5N(C_{23}H_{16}N_3)$), 7.65–7.52 (m, 8H), 7.39 (dd, J =8.1, 2.0, 1H, C_6H_3), 7.26 (d, J = 1.9, 1H, C_6H_3), 7.02 (ddd, J = 7.1, 5.6, 1.1, 1H, $C_5H_5N(C_{23}H_{16}N_3)$), 6.83 (ddd, J = 7.2, 5.7, 1.4, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 6.81 (ddd, J = 7.2, 5.7, 1.4, 1H, $C_5H_5N(C_{11}H_6NF_2)$), 6.53–6.43 (m, 2H, $C_6H_2F_2$), 6.07 (dd, J = 7.5, 2.3, 1H, $C_6H_2F_2$), 5.90 (dd, J = 9.2, 2.3, 1H, $C_6H_2F_2$).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.48 (1C, J =3.1, $C_{quat.}$ $C_{11}H_6NF_2$), 175.49 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 167.73 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 166.99 (d, J =8.0, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 164.74 (d, J =7.2, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 164.57 (dd, J =9.6, J =257, 1C, $C_{quat.C\text{-}F}$), 163.93 (dd, J =12.6, J = 253, 1C, $C_{quat.C\text{-}F}$), 162.82 (d, J = 5.9, 1C, $C_{quat.}$ $C_{11}H_6NF_2$), 162.67 (dd, J =10.8, J =262, 1C, $C_{quat.C\text{-}F}$), 161.75 (dd, J =13.1, J =257, 1C, $C_{quat.C\text{-}F}$), 153.23 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 152.84 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 151.61 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 150.99 (1C, CH, $C_5H_5N(C_{23}H_{16}N_3)$), 147.76 (1C, CH), 145.10 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 144.40 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 140.85 (1C, $C_{quat.}$ $C_{23}H_{16}N_3$), 137.12 (1C, CH, $C_5H_5N(C_{23}H_{16}N_3)$), 136.60 (1C, CH, C_6H_3) 135.72 (1C, CH), 135.30 (1C, CH), 130.78 (1C, CH), 129.05 (2C, CH, $C_{12}H_9N_2$), 127.93 (1C, $C_{quat.}$ $C_{11}H_6NF_2$), 127.65 (2C, CH, $C_{12}H_9N_2$), 126.46 (1C, $C_{quat.}$ $C_{11}H_6NF_2$), 124.72 (1C, CH, C_6H_3), 123.21 (2C, CH, $C_{12}H_9N_2$), 122.84 (d, J =20.3, 1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 122.81 (2C, CH, $C_{12}H_9N_2$), 122.68 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 122.65 (d, J =21, 1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 122.30 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 121.53 (1C, CH, $C_5H_5N(C_{11}H_6NF_2)$), 121.11 (1C, CH, C_6H_3), 119.56 (1C, CH, $C_5H_5N(C_{23}H_{16}N_3)$), 113.74 (d, J =14.0, 1.6, 1C, CH, $C_6H_2F_2$), 111.98 (d, J =16.0, 1.7, 1C, CH, $C_6H_2F_2$), 97.46 (pst, J =27.4, 1C, CH, $C_6H_2F_2$), 95.52 (pst, J =27.2, 1C, CH, $C_6H_2F_2$).

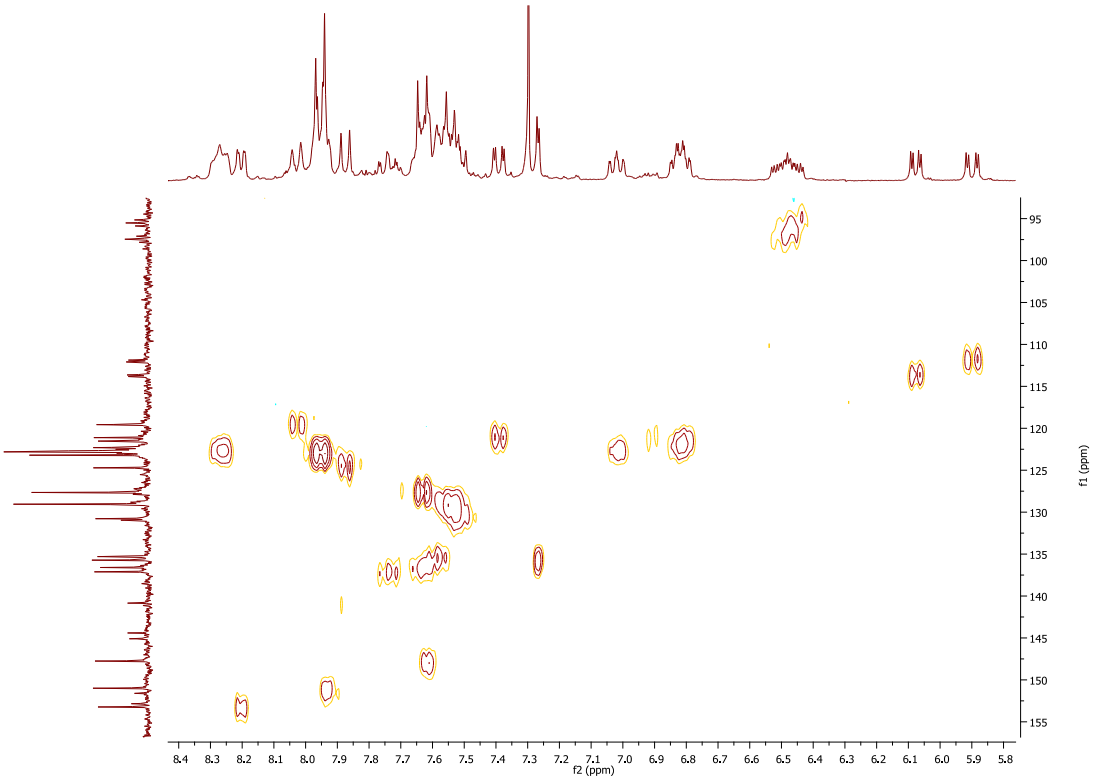
^{1}H NMR (300 MHz, $CDCl_3$):



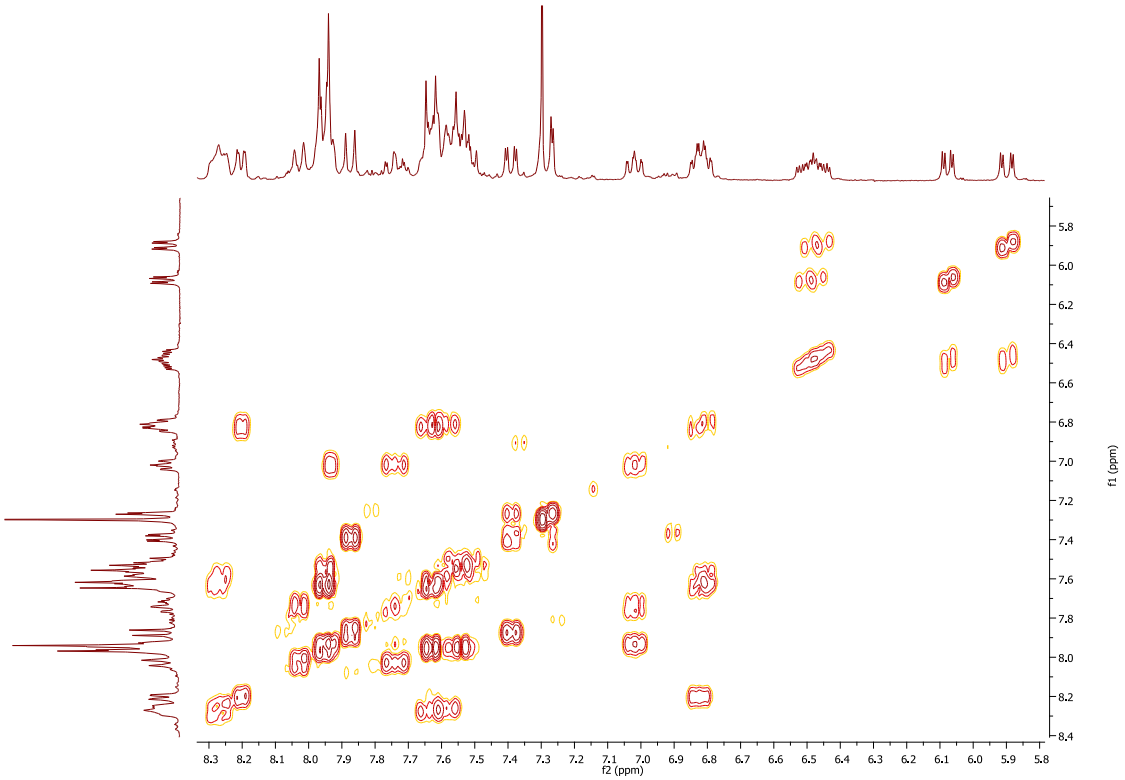
^{13}C NMR (75 MHz, $CDCl_3$):



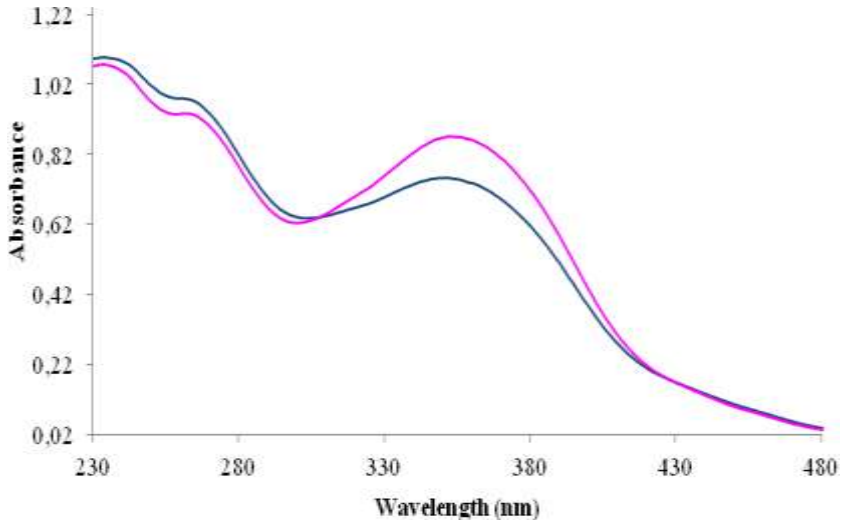
HSQC-NMR:



COSY.NMR:

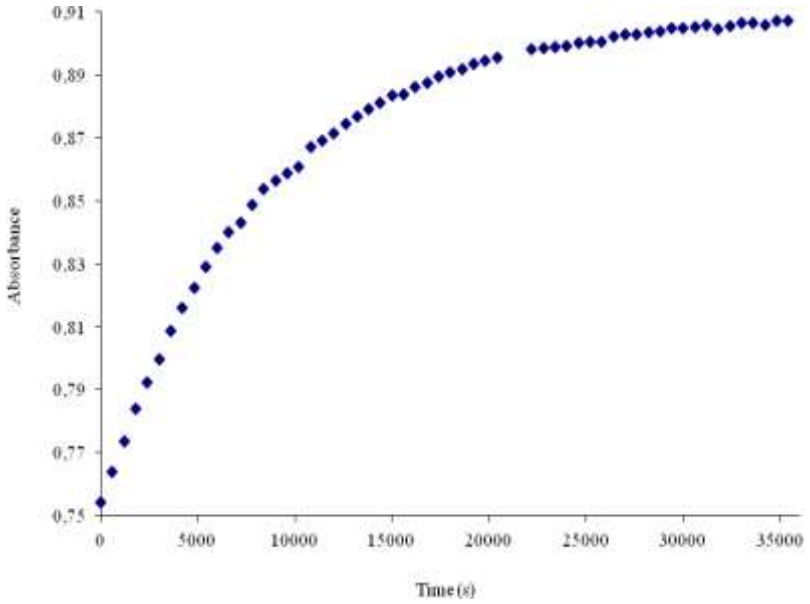


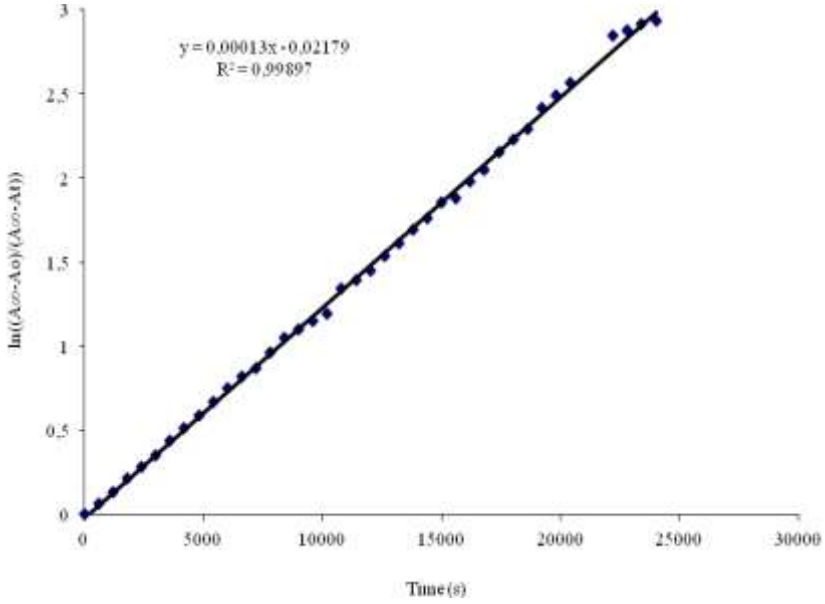
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 359 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
352 ($3.8 \cdot 10^4$), 449 ($5.6 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 359 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$1.3 \cdot 10^{-4}$**
Half-life (s)	**5500**

[Ir(**4**)$_2$(ppy)], **G-ppy**

SYNTHESIS:

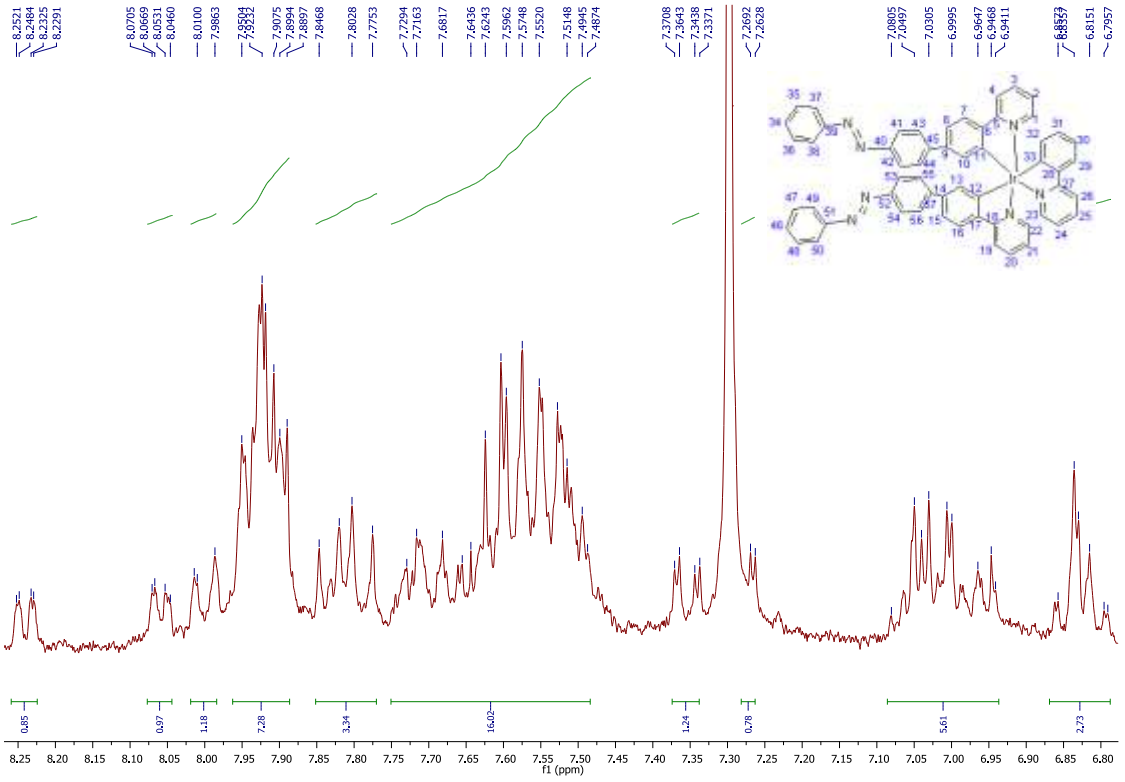
F-ppy (0.100 g, 0.123 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.080 g, 0.258 mmol), $Pd(PPh_3)_4$ (2 mol %, 2.843 mg, 0.002 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The product was obtained as insoluble dark-orange powder (0.110 g, 88%), less than 3 mg in 10 mL of Chloroform (0.0003M). A little part of the product was purified on an alumina column, eluting with dichloromethane.

Elemental Analysis: calculated for $C_{57}H_{40}IrN_7 \cdot 2C_3H_6O$: C, 66.88; H, 4.63; N, 8.67. Found: C, 66.20; H, 4.06; N, 8.28.

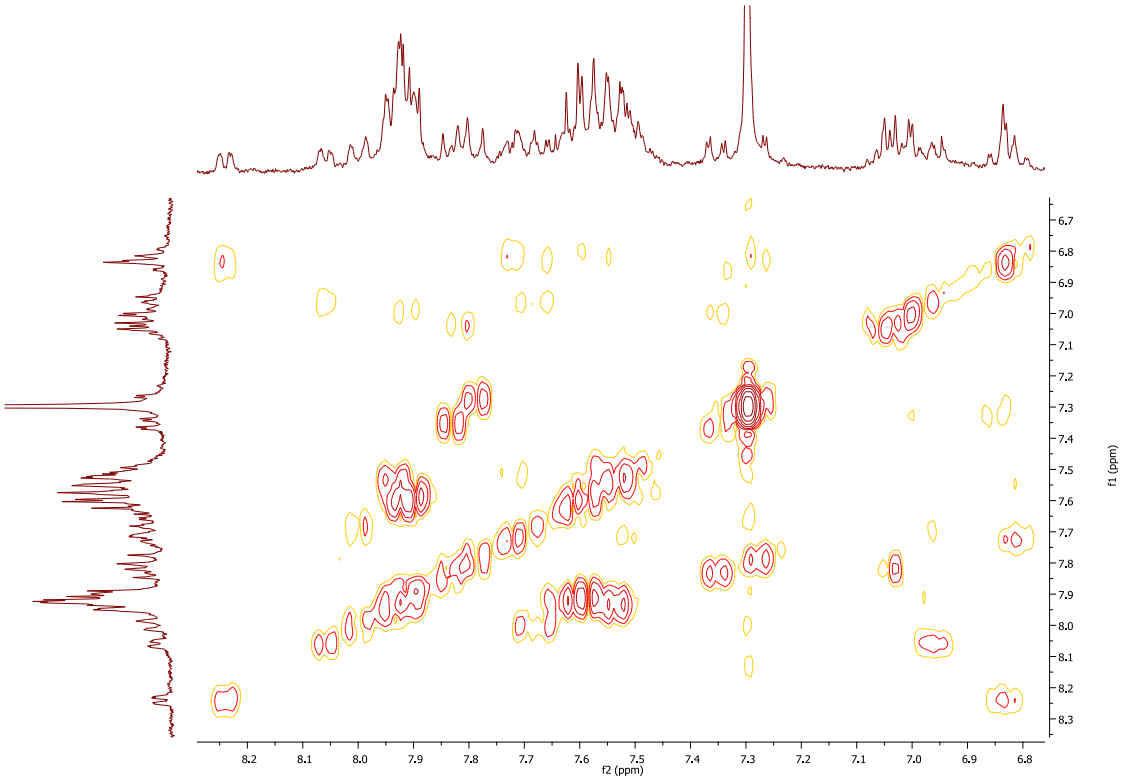
Exact mass (MALDI) - m/z: 1015.2990 for $[M]^+$ with (^{193}Ir).

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.24 (dd, J = 5.8, 1.1, 1H), 8.06 (dd, J = 5.7, 1.1, 1H), 8.00 (dd, J = 8.3, 1.2, 1H), 7.96–7.89 (m, 7H), 7.85–7.78 (m, 3H), 7.75–7.48 (m, 16H), 7.36 (dd, J =8.1, 2.0, 1H), 7.27 (dd, J =8.1, 1.9, 1H), 7.09–6.94 (m, 6H), 6.86–6.79 (m, 3H).

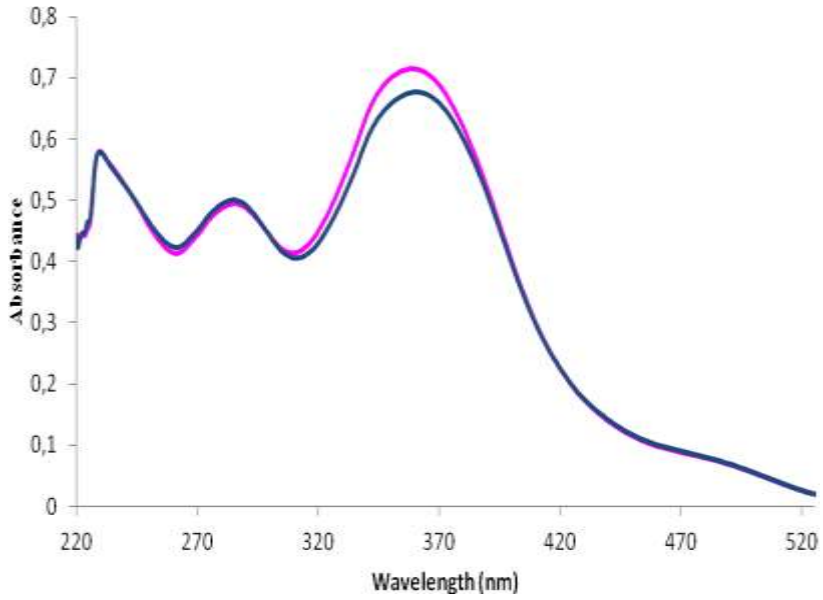
^{1}H NMR (300 MHz, $CDCl_3$)



COSY.NMR:



UV-vis spectra (CH_2Cl_2), before (pink line) and after (blue line) irradiation at 363 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
354 ($6.5 \cdot 10^4$), 481 ($7.1 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 339 K in CH_3CN after irradiation at 363 nm.

Due to low solubility of the complex, we couldn't calculate k value because the solubitity of the complex increase with heat, and the kinetics measures were made at 339 K.

[Ir(**4**)$_2$(Fppy)], **G-Fppy**

SYNTHESIS:

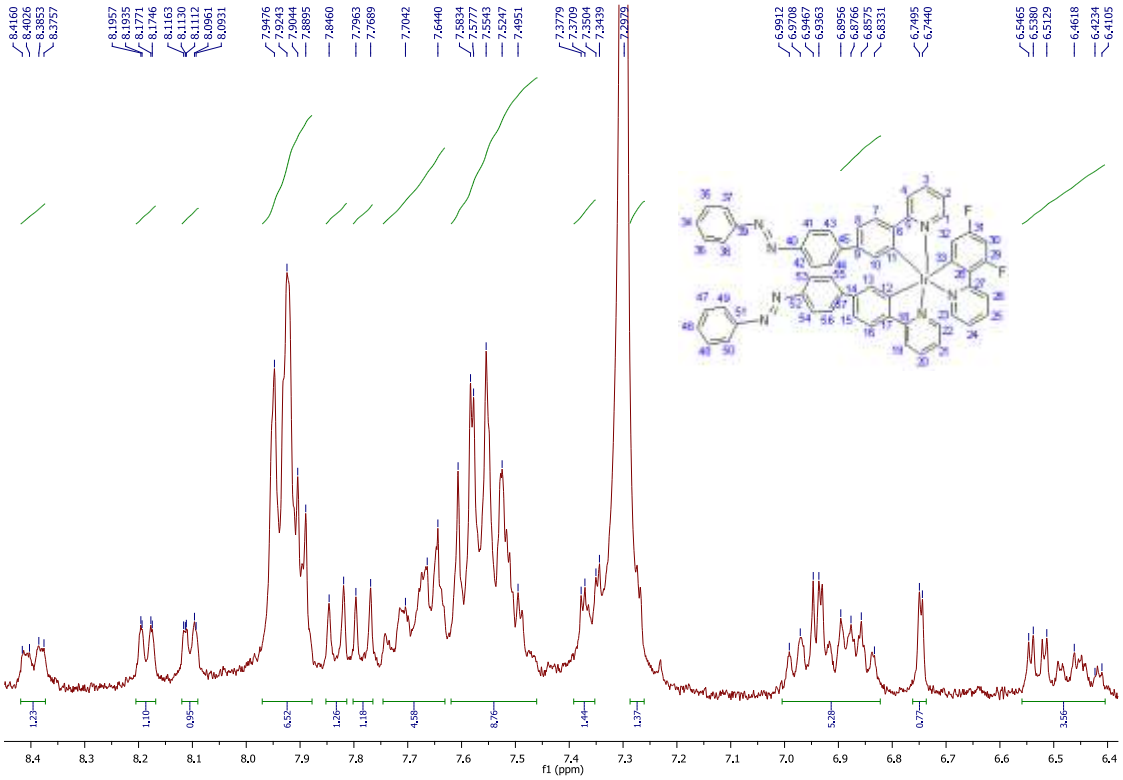
F-Fppy (0.100 g, 0.118 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.076 g, 0.247 mmol), $Pd(PPh_3)_4$ (2 mol %, 2.727 mg, 0.002 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The product was obtained as insoluble orange powder (0.111 g, 90%), less than 1.5 mg in 10 mL of Chloroform (0.0002M). A little part of the product was purified on an alumina column, eluting with dichloromethane.

Elemental Analysis: calculated for $C_{57}H_{38}F_2IrN7$: C, 65.13; H, 3.64; N, 9.33. Found: C, 64.75; H, 3.456; N, 8.816.

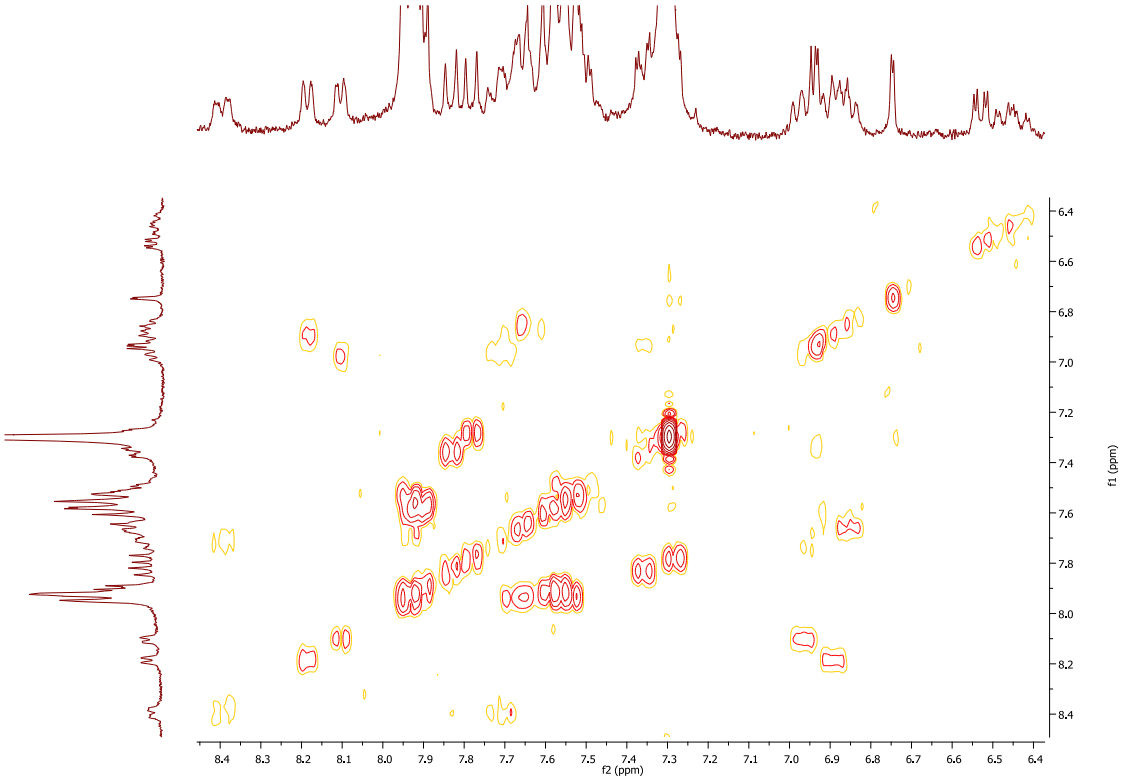
Exact mass (MALDI) - m/z: 1051.2782 for $[M]^+$ with (^{193}Ir).

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.42–8.38 (m, 1H), 8.19 (dd, J = 5.6, 0.7, 1H), 8.12–8.09 (m, 1H), 7.95–7.89 (m, 7H), 7.83 (d, J = 8.1, 1H), 7.78 (d, J = 8.8, 1H), 7.74–7.46 (m, 14H), 7.36 (dd, J =8.2, 2.0, 1H), 7.27 (dd, J =8.1, 1.9, 1H, 1H), 6.99 –6.83 (m, 5H), 6.75 (d, J = 1.7, 1H), 6.55–6.41 (m, 4H).

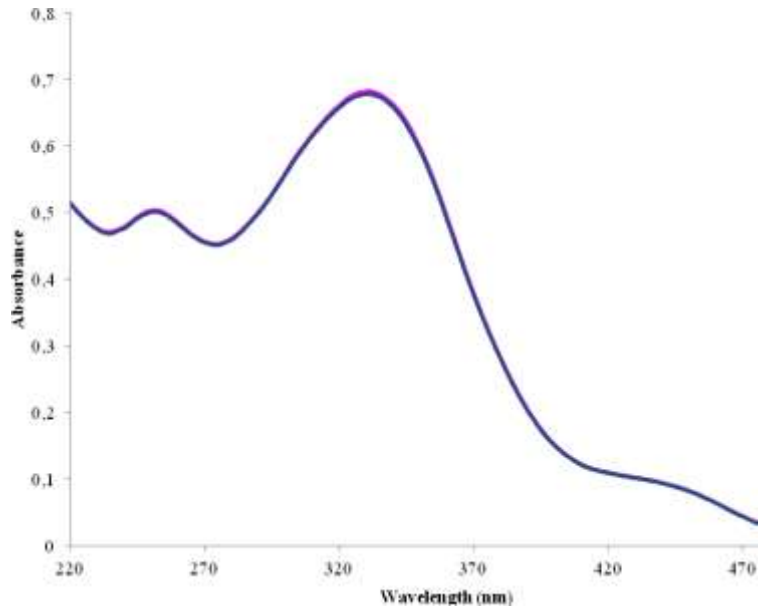
^{1}H NMR (300 MHz, $CDCl_3$):



COSY.NMR:



UV-vis spectra (CH_2Cl_2), before (pink line) and after (blue line) irradiation at 339 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
350 ($6.4 \cdot 10^4$), 469 ($8.7 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 339 K in CH_3CN after irradiation at 339 nm.

Due to low solubility of the complex, we couldn't calculate k value because the solubitity of the complex increase with heat, and the kinetics measures were made at 339 K.

[Ir(**4**)$_2$(acac)], **G-acac**

SYNTHESIS:

F-acac (0.100 g, 0.132 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.085 g, 0.277 mmol), $Pd(PPh_3)_4$ (2 mol %, 3.051 mg, 0.003 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The resulting solid was purified on an alumina column, eluting with dichloromethane. The product was obtained as orange powder (0.101 g, 80%).

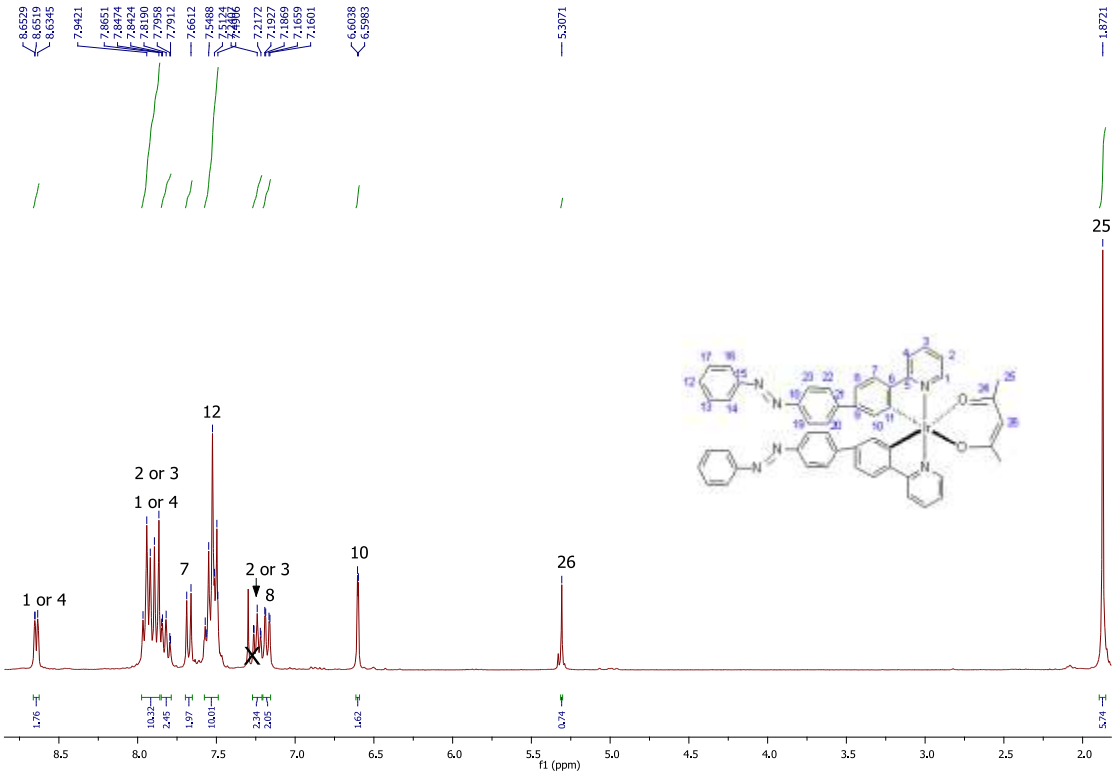
Elemental Analysis: calculated for $C_{51}H_{39}IrN_6O_2$: C, 63.80; H, 4.09; N, 8.75. Found: C, 63.67; H, 4.11; N, 8.23.

Exact mass (EI) - m/z: 960.2753 $(M)^+$ with (^{193}Ir).

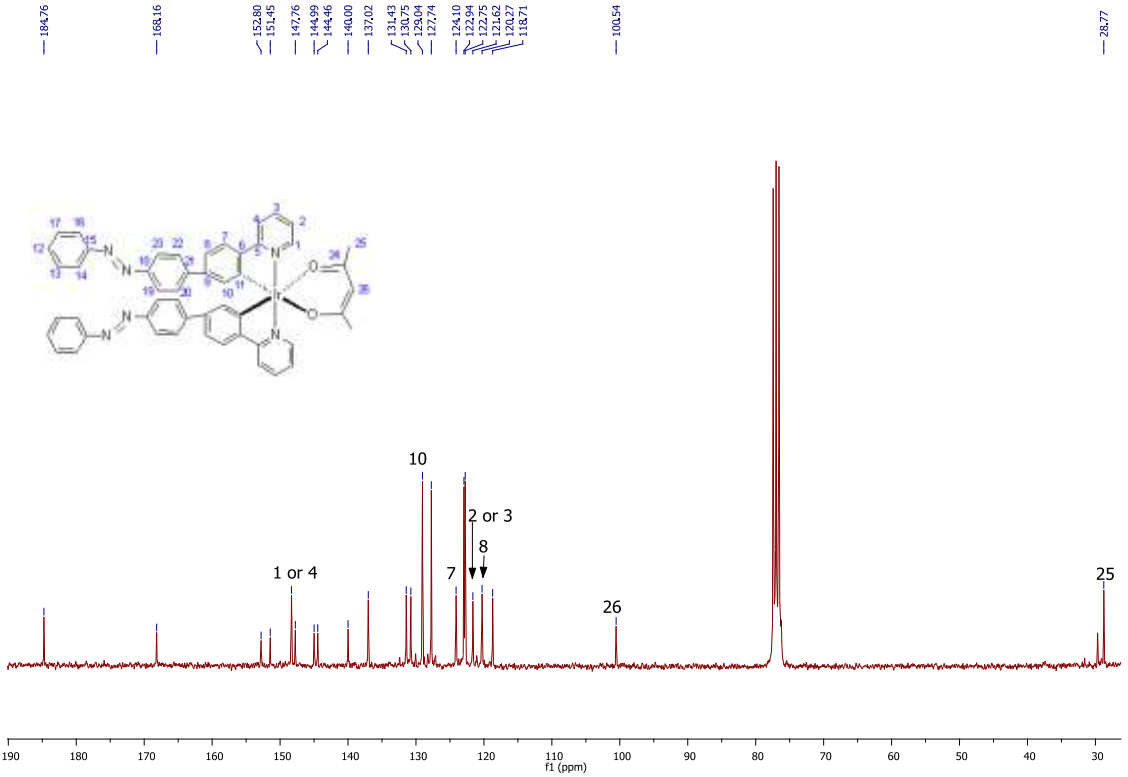
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.64 (dd, J = 5.7, 0.8, 2H, C_5H_4N), 7.97–7.79 (m, 12H), 7.67 (d, J = 8.1, 2H, C_6H_3), 7.58–7.49 (m, 10H), 7.24 (ddd, J = 7.2, 5.8, 1.4, 2H, C_5H_4N), 7.18 (dd, J = 8.1, 1.7, 2H, C_6H_3), 6.60 (d, J = 1.7, 2H, C_6H_3), 5.31 (s, 1H, HAcac), 1.87 (s, 6H, Hacac).

^{13}C NMR (75 MHz, $CDCl_3$): δ 184.76 (2C, $C_{quat.}$), 168.16 (2C, $C_{quat.}$), 152.80 (2C, $C_{quat.}$), 151.45 (2C, $C_{quat.}$), 148.32 (2C, CH), 147.76 (2C, $C_{quat.}$), 144.99 (2C, $C_{quat.}$), 144.46 (2C, $C_{quat.}$), 140.00 (2C, $C_{quat.}$), 137.02 (2C, CH, C_5H_4N), 131.43 (2C, CH), 130.75 (2C, CH, C_6H_3), 129.04 (4C, CH, $C_{12}H_9N_2$), 127.74 (4C, CH, $C_{12}H_9N_2$), 124.10 (2C, CH, C_6H_3), 122.94 (4C, CH, $C_{12}H_9N_2$), 122.75 (4C, CH, $C_{12}H_9N_2$), 121.62 (2C, CH, C_5H_4N), 120.27 (2C, CH, C_6H_3), 118.71 (2C, CH), 100.54 (1C, CH, Hacac), 28.77 (2C, CH_3, Hacac).

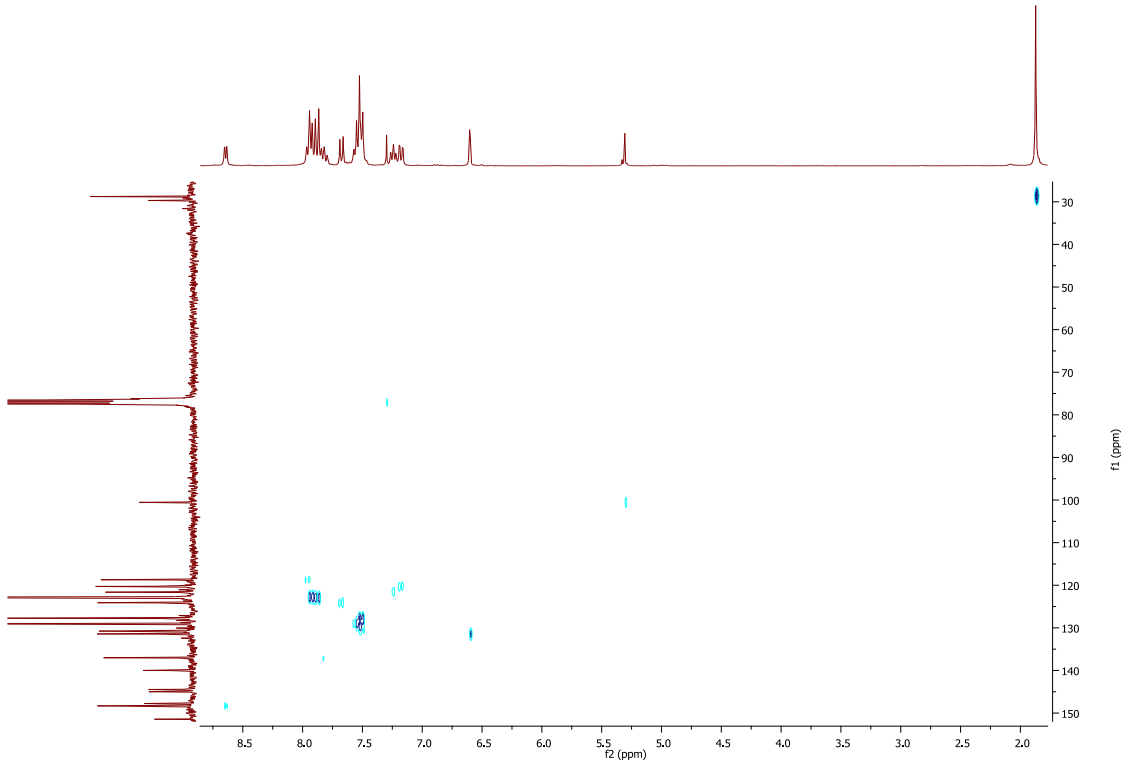
^{1}H NMR (300 MHz, $CDCl_3$):



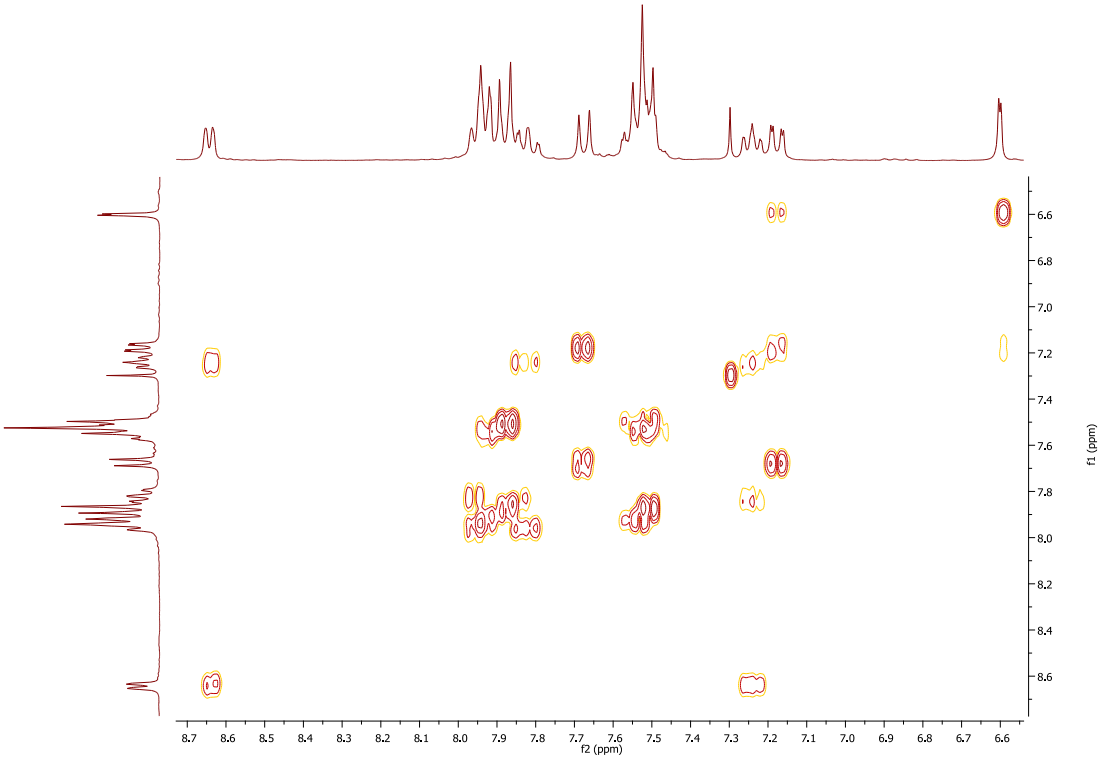
^{13}C NMR (75 MHz, $CDCl_3$):



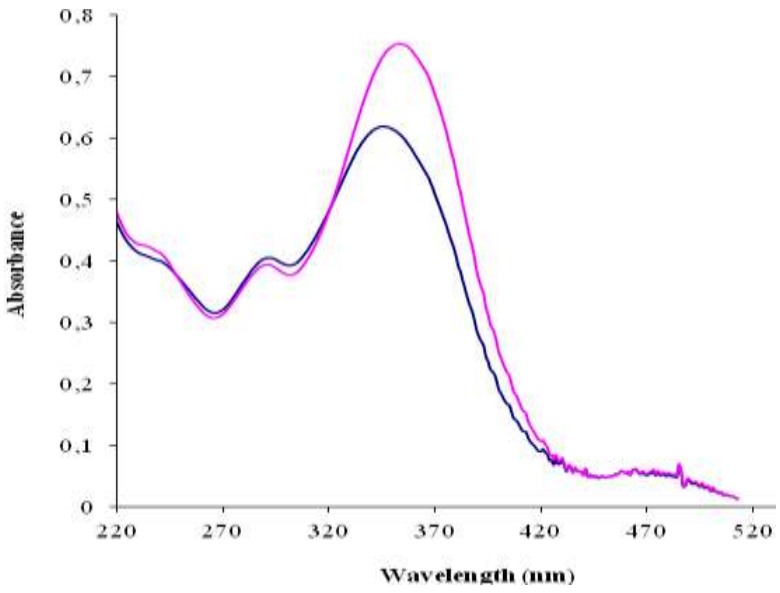
HSQC-NMR:



COSY.NMR:

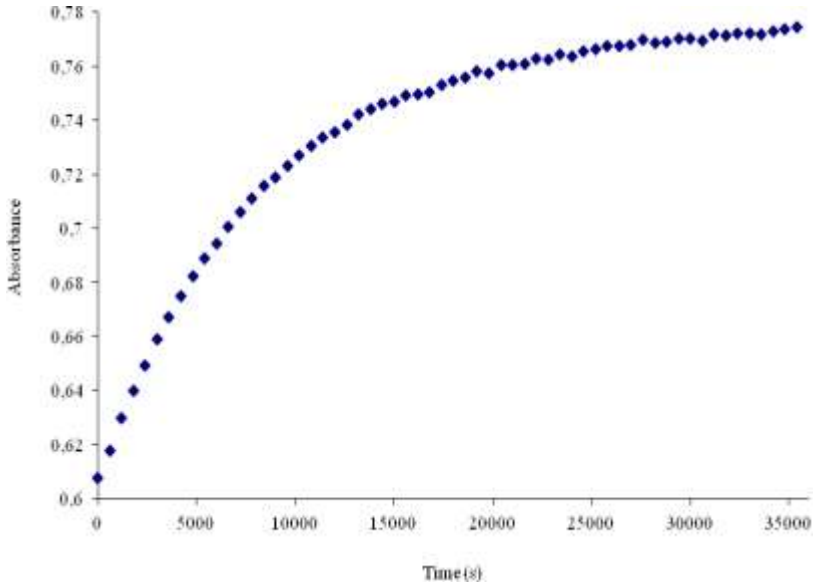


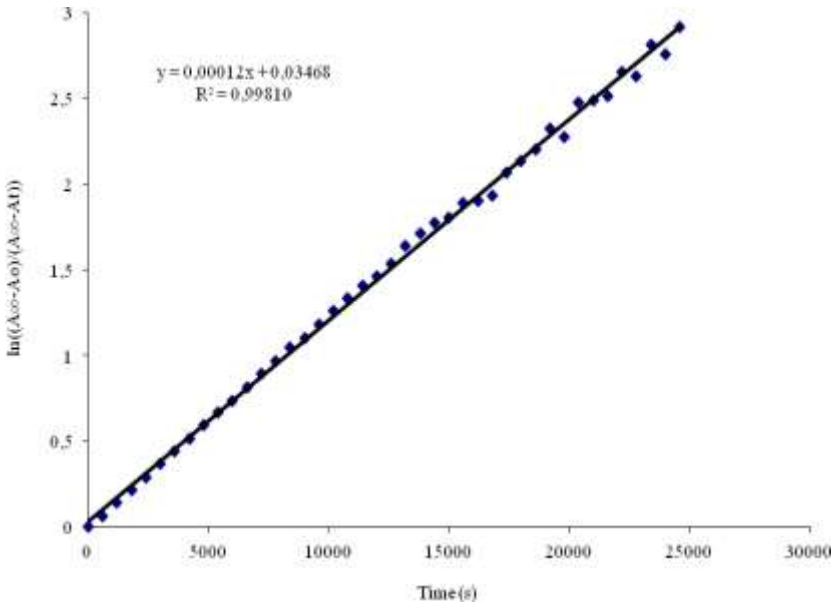
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 366 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
353 ($6.8 \cdot 10^4$), 470 ($8.4 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 366 nm. ($1.0 \cdot 10^{-5}$M).





K (s^{-1})	**$1.2 \cdot 10^{-4}$**
Half-life (s)	**5900**

[Ir((5-bromo-2-pyridyl)phenyl)$_3$], **H**

SYNTHESIS:

[Ir((5-bromo-2-pyridyl)phenyl)$_2$Cl]$_2$ (0.150 g, 0.108 mmol) and silver triflate (0.084 g, 0.324 mmol) were dissolved in degassed acetone (8 mL) and refluxed under nitrogen for 2 h. The solution was cooled to room temperature and gravity-filtered to remove AgCl. The filtrate was refluxed under nitrogen for 1 h and added to a 1 h refluxed solution of 2-(4-bromophenyl)pyridine (0.101 g, 0.432 mmol) and triethylamine (0.113 mL, 0.810 mmol) dissolved in degassed acetone (4 mL). The solution was then stirred and refluxed overnight under nitrogen. After concentrating in *vacuo*, the resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as yellow powder (0.116 g, 60%).

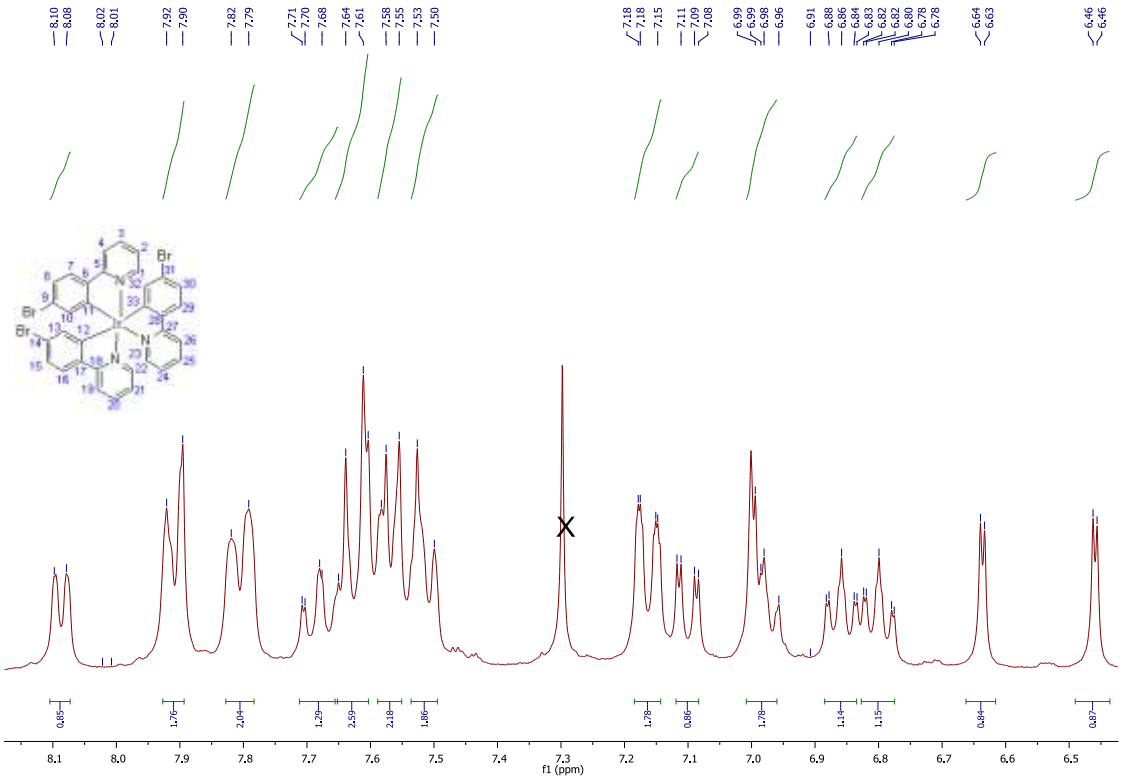
Elemental Analysis: calculated for $C_{33}H_{21}Br_3IrN_3 \cdot 3C_3H_6O$: C, 47.33; H, 3.69; N, 3.94. Found: C, 47.26; H, 3.36; N, 4.04.

Exact mass (EI) - m/z: 889.8982 for $[M+H]^+$ with (^{193}Ir)(^{79}Br).

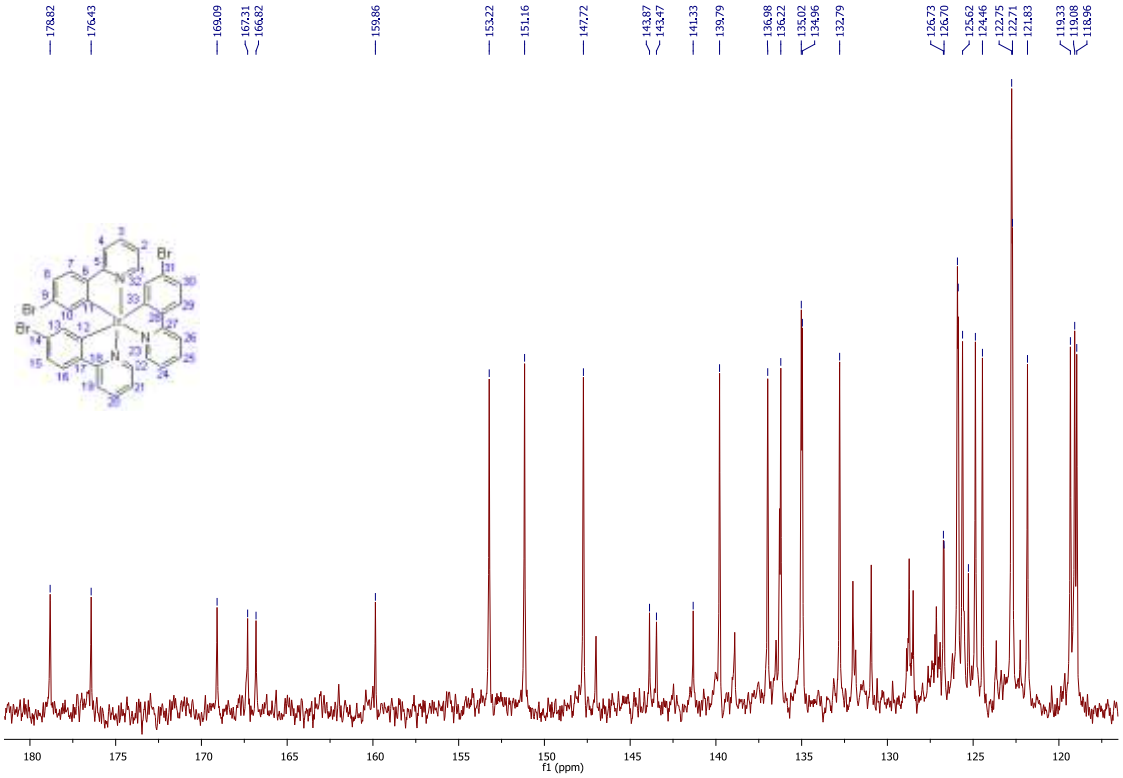
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.09 (dd, J =5.8, 0.9, 1H, C_5H_4N), 7.91 (m, 2H, C_5H_4N), 7.81 (m, 2H, C_5H_4N), 7.71–7.50 (m, 7H), 7.16 (dd, J = 8.3, 2.0, 2H, C_5H_3Br), 7.10 (dd, J = 8.3, 1.9, 1H, C_5H_3Br), 7.00 (d, J = 2.0, 1H, C_5H_3Br), 6.98 (ddd, J =7.1, J = 5.4, J =1.4, 1H, C_5H_4N), 6.86 (ddd, J = 7.3, 5.9, 1.4, 1H, C_5H_4N), 6.80 (ddd, J = 7.3, 5.9, 1.4, 1H, C_5H_4N), 6.64 (d, J = 2.0, 1H, C_5H_3Br), 6.46 (d, J = 1.9, 1H, C_5H_3Br).

^{13}C NMR (75 MHz, $CDCl_3$): δ 178.82 (1C, $C_{cuat.}$), 176.43 (1C, $C_{cuat.}$), 169.09 (1C, $C_{cuat.}$), 167.31 (1C, $C_{cuat.}$), 166.82 (1C, $C_{cuat.}$), 159.86 (1C, $C_{cuat.}$), 153.22 (1C, CH, C_5H_4N), 151.16 (1C, CH, C_5H_4N), 147.72 (1C, CH), 143.87 (1C, $C_{cuat.}$), 143.47 (1C, $C_{cuat.}$), 141.33 (1C, $C_{cuat.}$), 139.79 (1C, CH, C_5H_3Br), 136.98 (1C, CH,), 136.22 (1C, CH), 135.02 (1C, CH), 134.96 (1C, CH), 132.79 (1C, CH, C_5H_3Br), 126.73 (1C, $C_{cuat.}$), 126.69 (1C, $C_{cuat.}$), 125.27 (1C, $C_{cuat.}$), 125.92 (1C, CH), 125.87 (1C, CH), 125.62 (1C, CH), 125.28 (1C, 1$C_{cuat.}$), 124.87 (1C, CH, C_5H_3Br), 124.46 (1C, CH, C_5H_3Br), 122.75 (2C, CH), 122.71 (1C, CH), 121.83 (1C, CH, C_5H_4N), 119.33 (1C, CH, C_5H_4N), 119.08 (1C, CH, C_5H_4N), 118.96 (1C, CH, C_5H_4N).

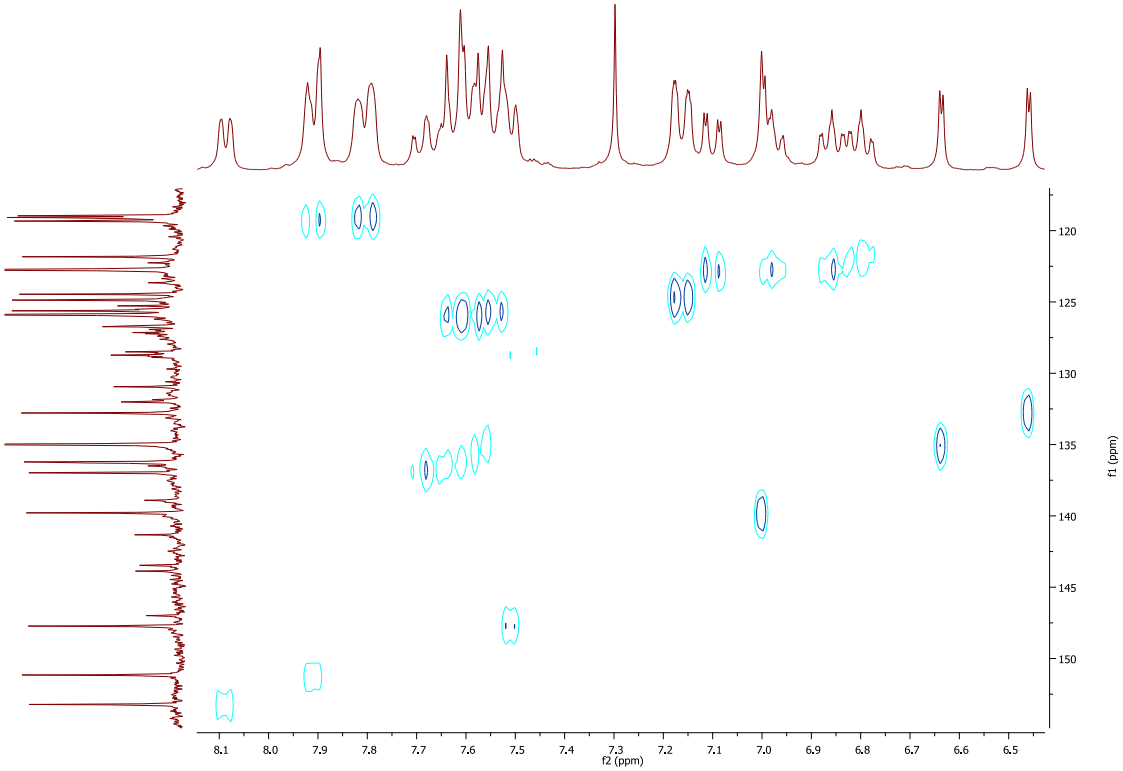
^{1}H NMR (300 MHz, $CDCl_3$):



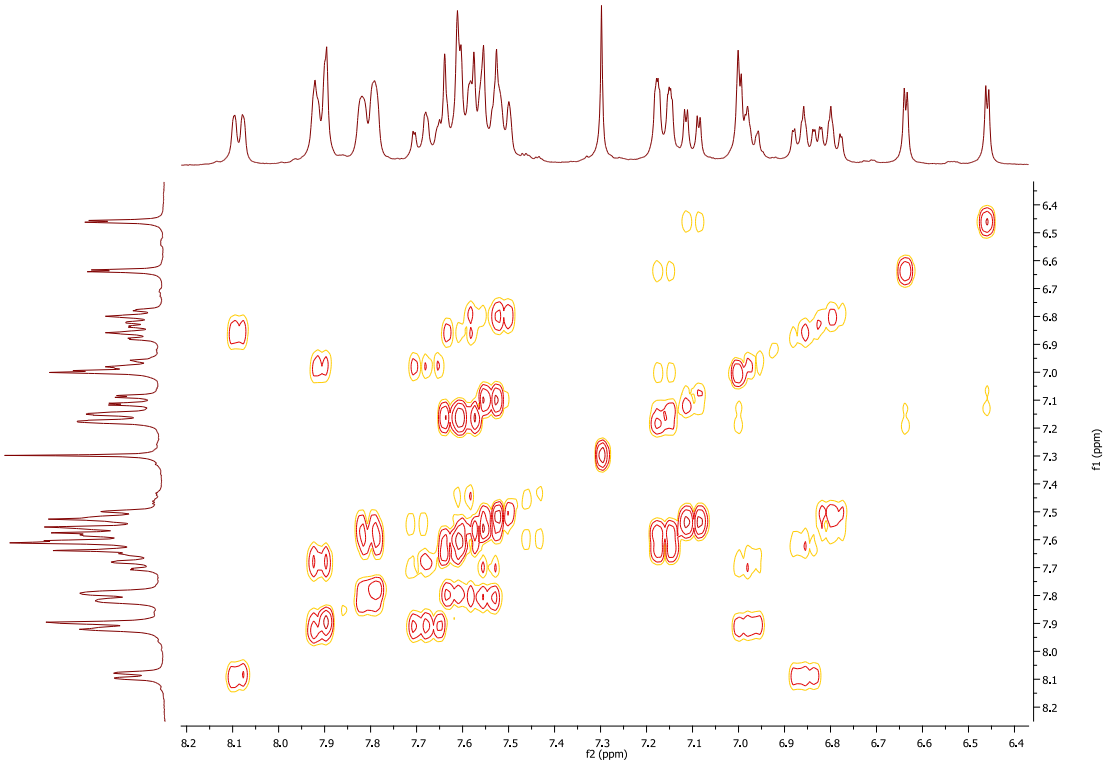
^{13}C NMR (75 MHz, $CDCl_3$):



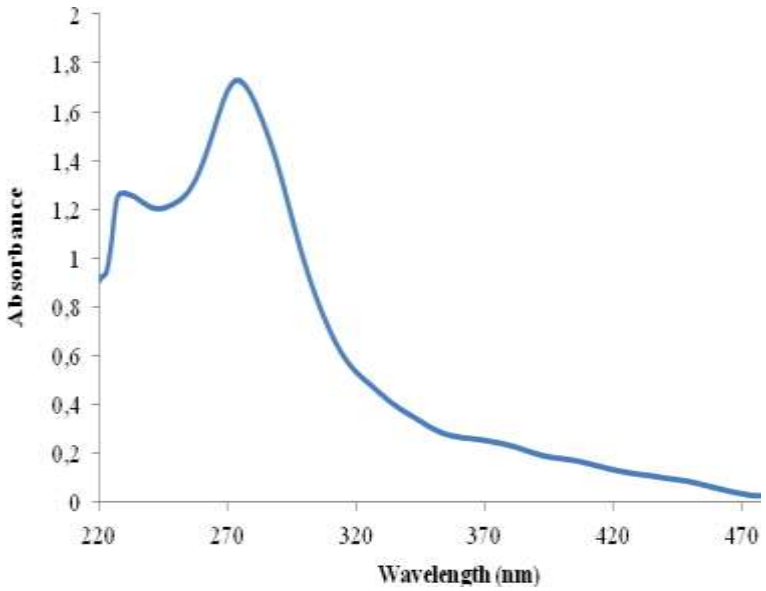
HSQC-NMR:



COSY.NMR:



UV-vis spectra (CH_3CN):



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
230 ($3.9 \cdot 10^4$), 271 ($5.1 \cdot 10^4$), 368 ($6.0 \cdot 10^3$), 404 ($4.0 \cdot 10^3$), 443 ($1.7 \cdot 10^3$), 482 ($0.3 \cdot 10^3$)

[Ir(**4**)$_3$], **I**

SYNTHESIS:

H (0.100 g, 0.112 mmol) was dissolved in 4 mL of degassed THF. To this mixture, 1-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-diazene (0.110 g, 0.359 mmol), $Pd(PPh_3)_4$ (2 mol %, 2.588 mg, 0.002 mmol), Na_2CO_3 (1M aq., 2 mL) were added successively under nitrogen, and heated overnight at 80ºC with continuous stirring. The reaction mixture was heated overnight at 80ºC with continuous stirring. The reaction was cooled to room temperature and 50 mL of water were added to precipitate the formed compound. The solution was gravity filtered and the solid was washed with hexane (20 mL). The resulting solid was purified on a silica gel column, eluting with dichloromethane. The product was obtained as orange powder (0.123 g, 92%).

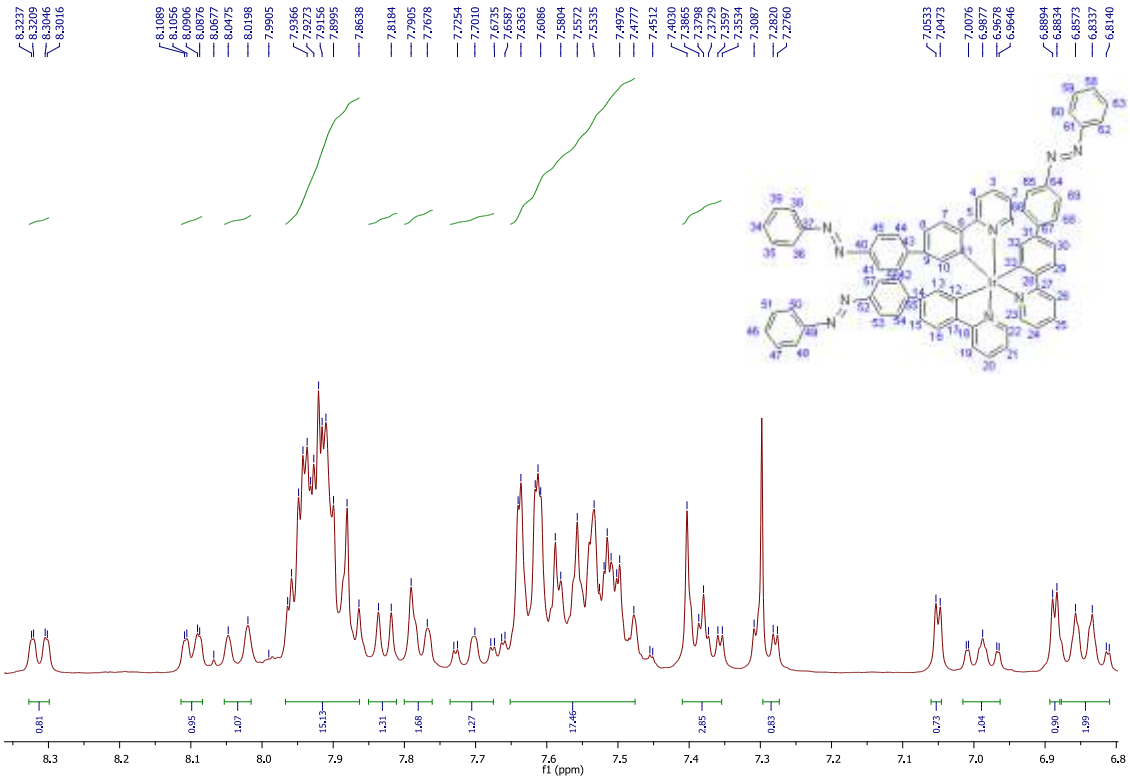
Elemental Analysis: calculated for $C_{69}H_{48}IrN_9 \cdot 2C_3H_6O$: C, 68.68; H, 4.61; N, 9.61. Found: C, 68.88; H, 4.16; N, 9.68.

Exact mass (MALDI) - m/z: 1195.3662 for $[M]^+$ with (^{193}Ir).

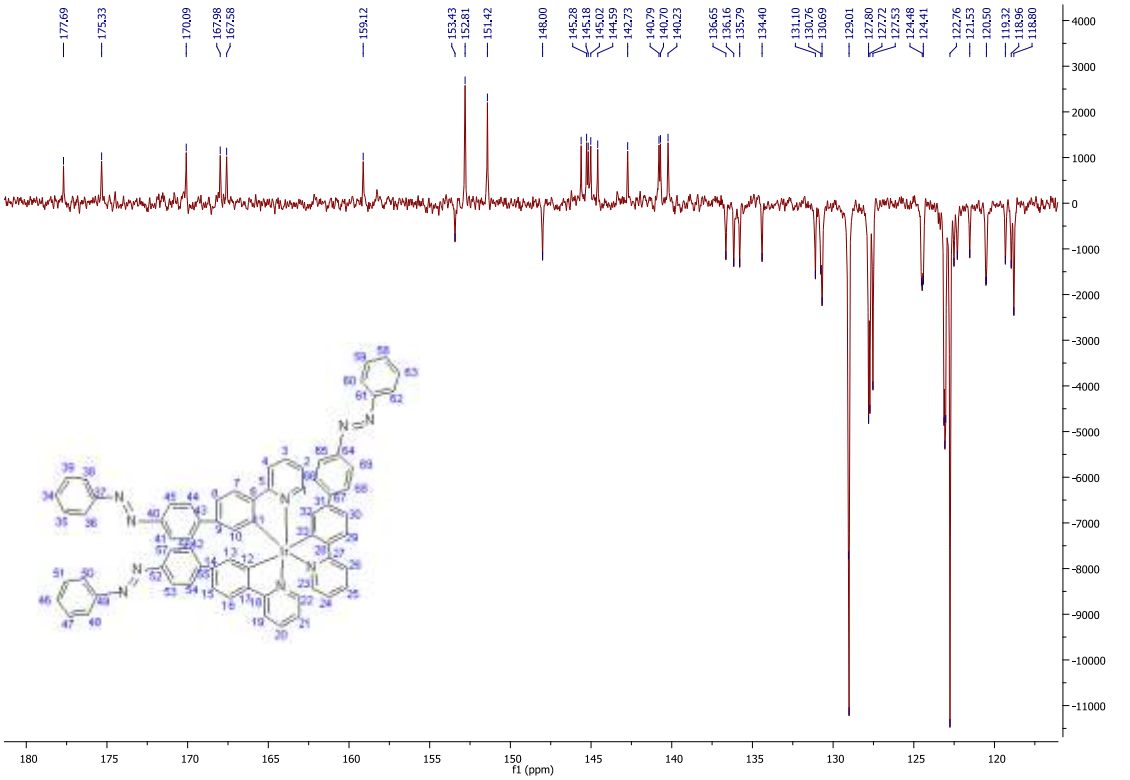
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.31 (dd, *J* = 5.8, 0.9, 1H, C_5H_5N), 8.10 (dd, *J* = 5.4, 0.9, 1H, C_5H_5N), 8.03 (d, *J* = 8.3, 1H, C_5H_5N), 7.97–7.86 (m, 15H), 7.83 (d, *J* = 5.4, 1H), 7.79–7.77 (m, 2H), 7.70 (td, J = 7.32, 1.56, 1H, C_5H_5N), 7.65–7.49 (m, 17H), 7.41–7.35 (m, 3H), 7.30 (dd, J =8.0, 1.8 ,1H, C_6H_3), 7.05 (d, *J* = 1.8, 1H, C_6H_3), 6.99 (ddd, J = 6.9, 5.6, 0.9, 1H, C_5H_5N), 6.89 (d, *J* = 1.8, 1H, C_6H_3), 6.88–6.81 (m, 2H, C_5H_5N).

^{13}C NMR (75 MHz, $CDCl_3$): δ 177.69 (1C, $C_{quat.}$), 175.33 (1C, $C_{quat.}$), 170.09 (1C, $C_{quat.}$), 167.98 (1C, $C_{quat.}$), 167.58 (1C, $C_{quat.}$), 159.12 (1C, $C_{quat.}$), 153.43 (1C, CH), 152.81 (3C, $C_{quat.}$), 151.42 (3C, $C_{quat.}$), 151.42 (1C, CH), 148.00 (1C, CH), 145.62 (1C, $C_{quat.}$), 145.28 (1C, $C_{quat.}$), 145.18 (1C, $C_{quat.}$), 145.02 (1C, $C_{quat.}$), 144.59 (1C, $C_{quat.}$), 142.73 (1C, $C_{quat.}$), 140.79 (1C, $C_{quat.}$), 140.70 (1C, $C_{quat.}$), 140.23 (1C, $C_{quat.}$), 136.65 (1C, CH), 136.16 (1C, CH), 135.79 (1C, CH), 134.40 (1C, CH), 131.10 (1C, CH), 130.76 (1C, CH), 130.69 (2C, CH), 129.05 (1C, CH), 129.01 (6C, CH), 127.80 (2C, CH), 127.72 (2C, CH), 127.53 (2C, CH), 124.53 (1C, CH), 124.48 (1C, CH), 124.41 (1C, CH), 123.13 (2C, CH), 123.07 (2C, CH), 123.02 (2C, CH), 122.76 (6C, CH), 122.51 (1C, CH), 122.30 (1C, CH), 121.53 (1C, CH), 120.53 (1C, CH), 120.50 (1C, CH), 119.32 (1C, CH), 118.96 (1C, CH), 118.80 (2C, CH).

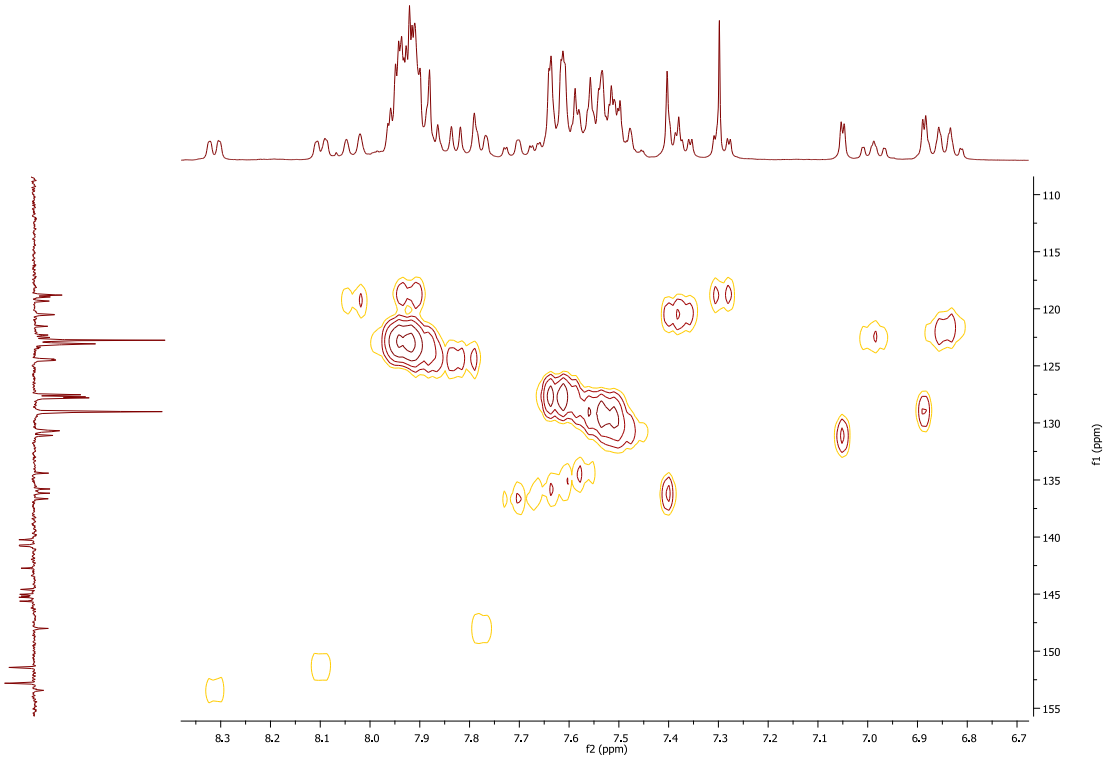
^{1}H NMR (300 MHz, $CDCl_3$):



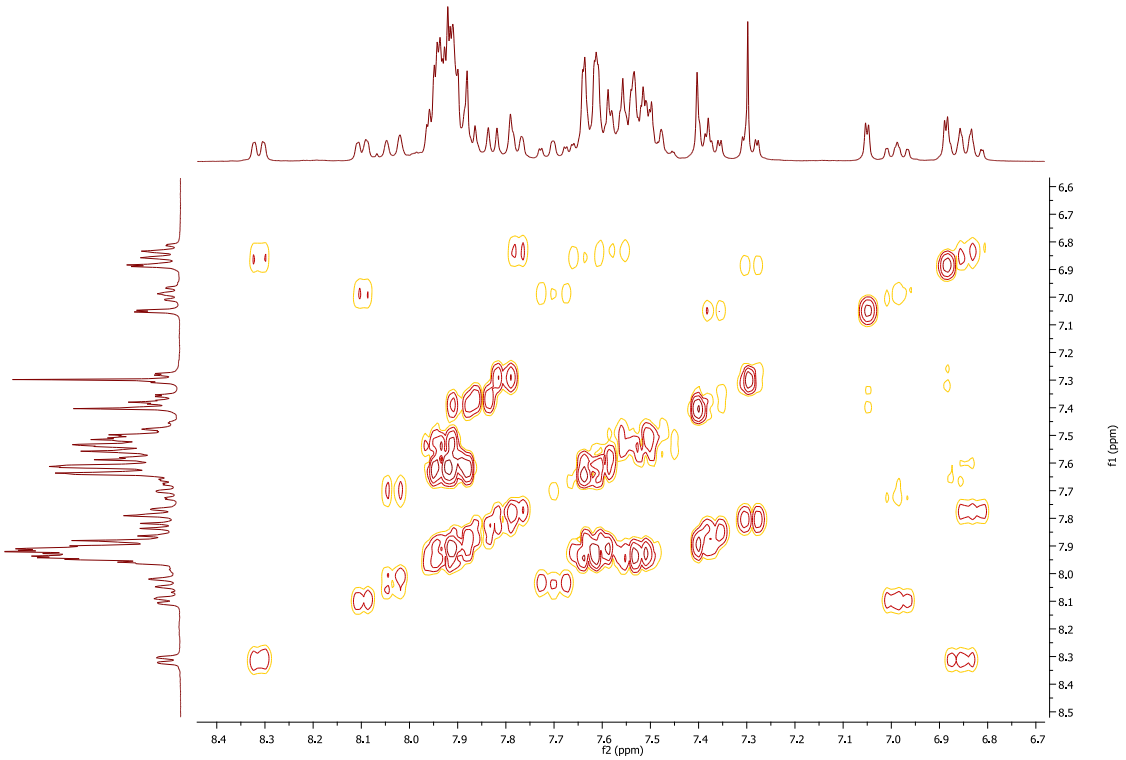
^{13}C APT NMR (75 MHz, $CDCl_3$):



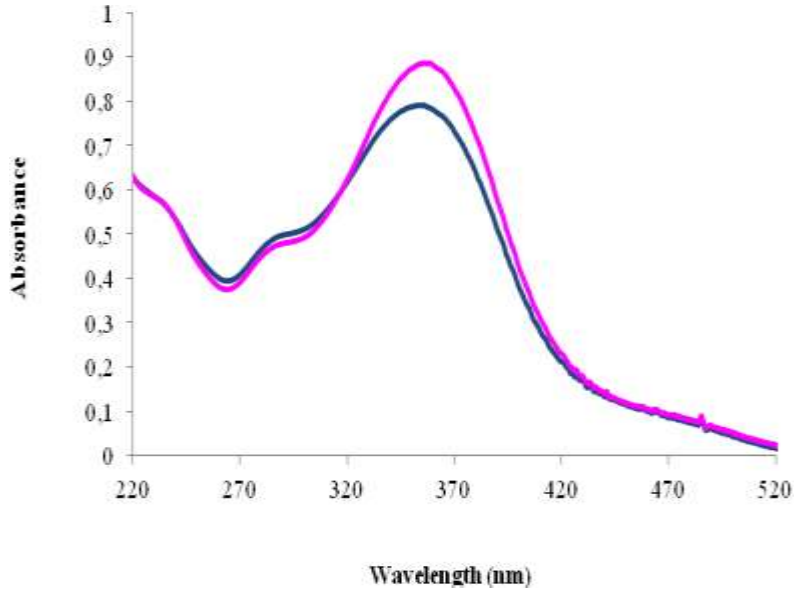
HSQC-NMR:



COSY.NMR:

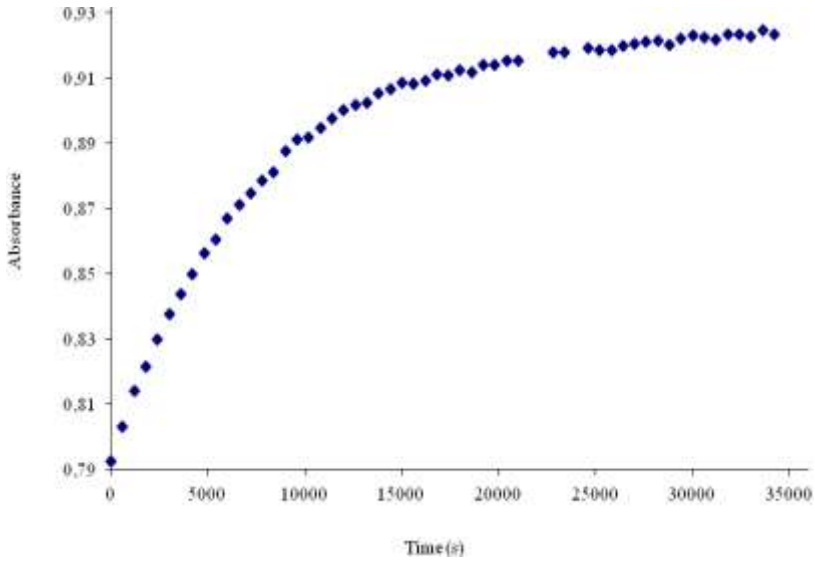


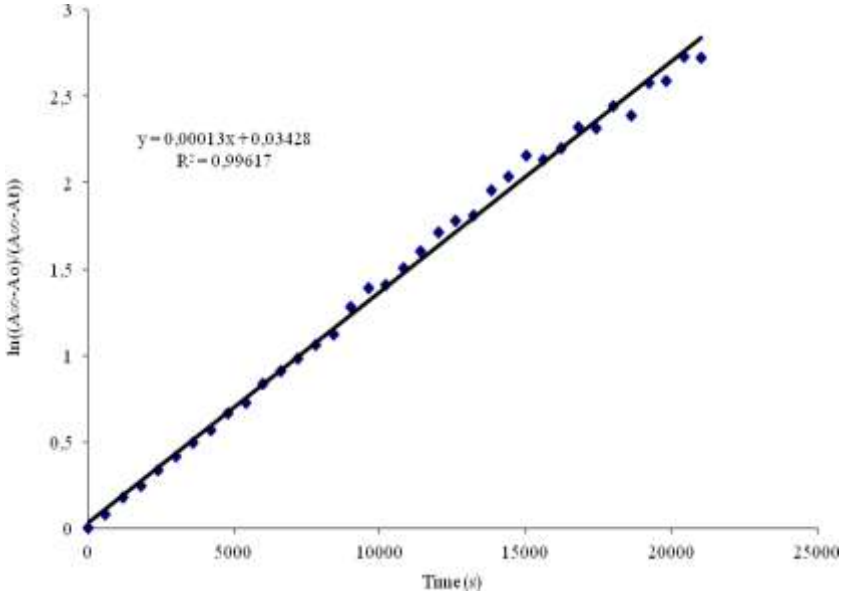
UV-vis spectra (CH_3CN), before (pink line) and after (blue line) irradiation at 358 nm:



λ_{abs} (nm), (ε (L mol^{-1} cm^{-1}))
355 ($8.9 \cdot 10^4$), 476 ($9.2 \cdot 10^3$)

Cis to trans thermal isomerization kinetics. All k values were calculated from the first-order plots of absorption change at 328 K in CH_3CN after irradiation at 358 nm. ($2.5 \cdot 10^{-5}$M).





K (s^{-1})	**$1.3 \cdot 10^{-4}$**
Half-life (s)	**5200**

Cyclic Voltammetry

The measurements of 10^{-3}M solution of A-I were carried out in anhydrous DMF solution containing 0.1 M [*TBA*][PF_6] supporting electrolyte and ferrocene as an internal standard.($1 \cdot 10^{-3}$M) at 100 mV/s. The potentials were controlled using a Metrohm Ag/AgCl reference electrode.

Series A:

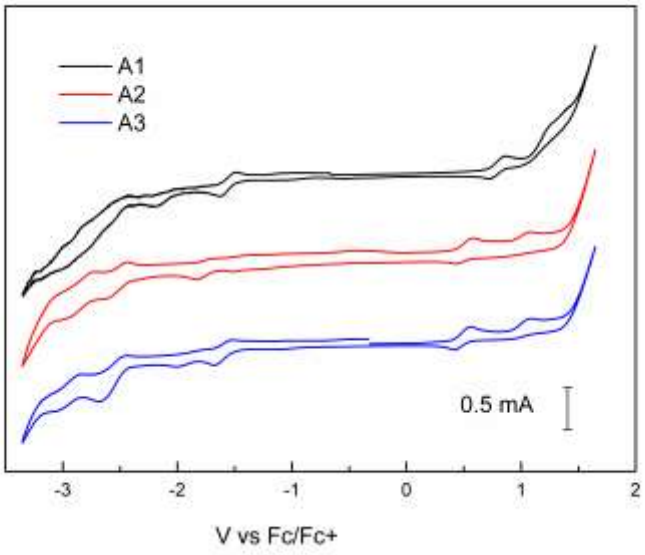


Figura S1. Cyclic voltammograms of compounds A1', A2 and A3.

Series B:

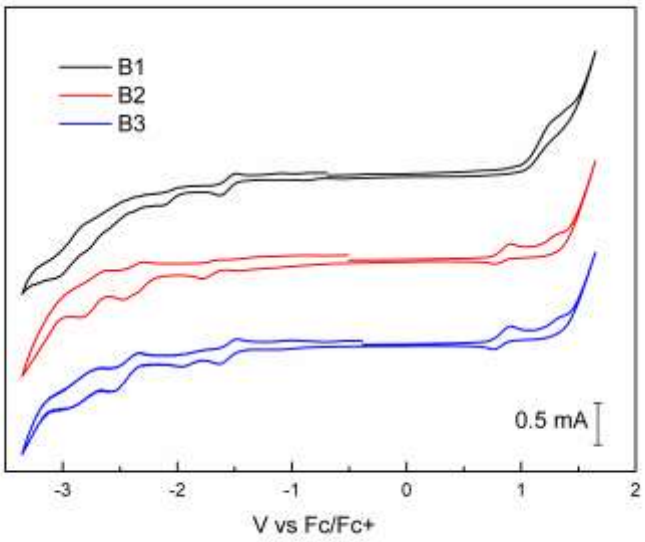


Figura S2. Cyclic voltammograms of compounds B1', B2 and B3.

Series CDA4 B4:

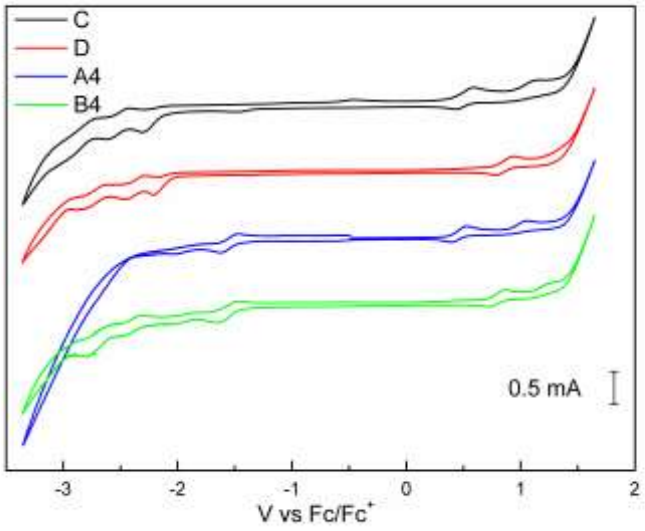


Figura S3. Cyclic voltammograms of compounds C, D, A4 and B4.

Series F:

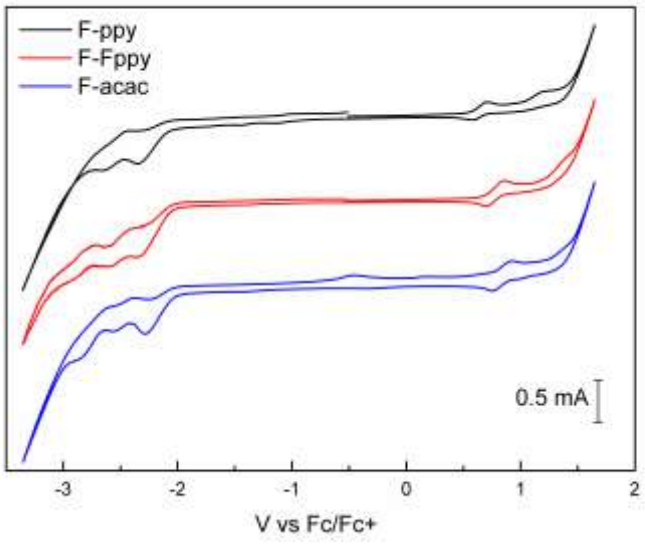


Figura S4. Cyclic voltammograms of compounds F-ppy, F-Fppy and F-acac.

Series G:

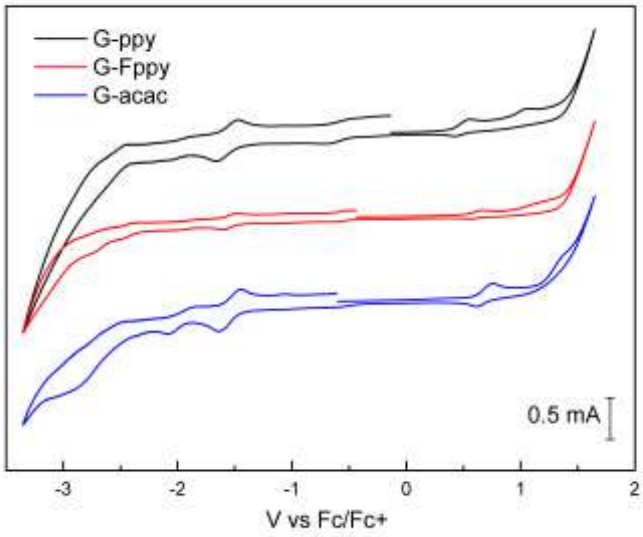


Figura S5. Cyclic voltammograms of compounds G-ppy, G-Fppy and G-acac.

Series HI:

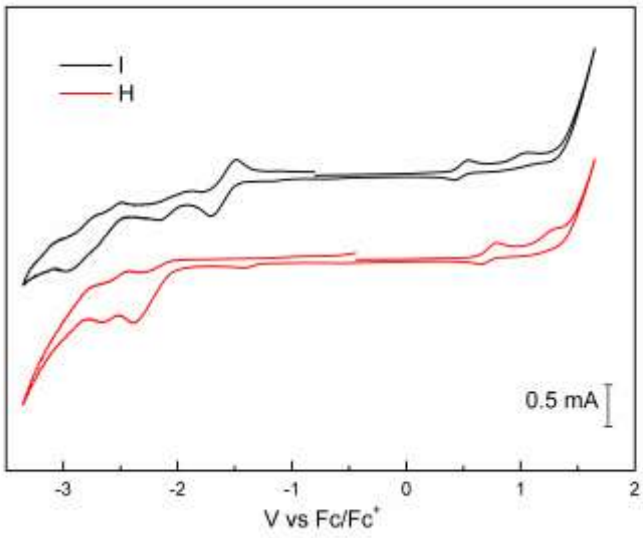


Figura S6. Cyclic voltammograms of compounds H and I.

Computational details

All the calculations were obtained with the Gaussian09 suite of programs.[1] In optimizations, electron correlation was partially taken into account by using the hybrid functional B3LYP[2] and the standard 6-31G* basis set[3] for hydrogen, carbon, nitrogen and fluorine, and the Hay-Wadt small core effective potential (ECP) including double-□ valence basis set[4] for iridium atoms (LANL2DZ). All stationary points were characterized by harmonic analysis in order to verify that each configuration is a minimum on the potential energy surface. All the optimized compounds have positive definite Hessian matrices. Zero-point vibrational energy corrections were computed at the B3LYP/6-31G*&LANL2DZ level and were not scaled. Solvent effects were considered by means of polarized continuum method (PCM) developed by Tomasi and co.[5] Time dependent calculations of the optimized geometries were performed using CAM-B3LYP functional[6] with the same basis set used in geometry optimizations. This functional was shown to give reliable results on the study of iridium complexes.[7]

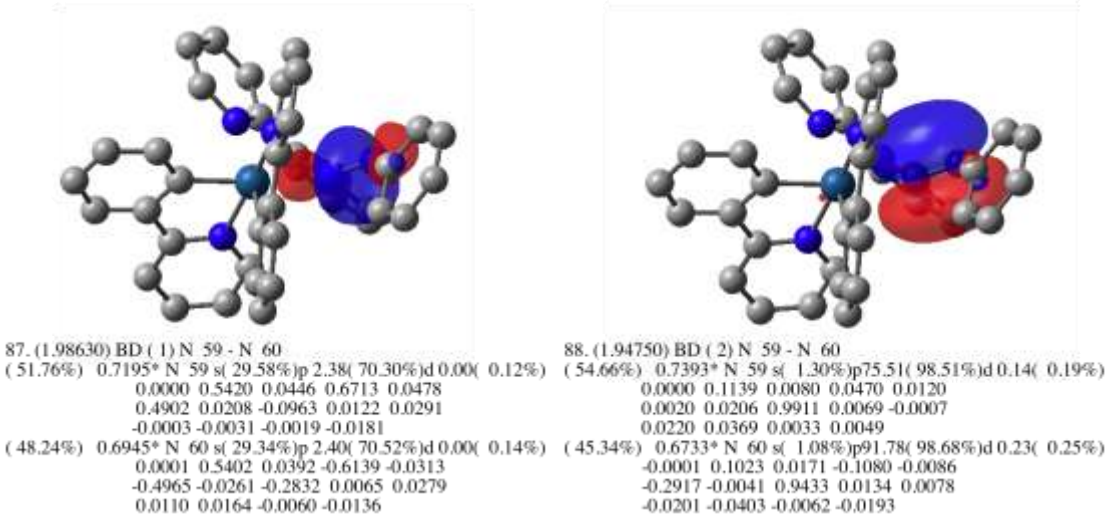


Figura S7. Natural orbitals and participation of atomic orbitals on the N-N bond of compound **$[Ir(ppy)_2(1)]^+$.**

Table S1. Total electronic energies[a] (E, in a.u.), zero point correction of energy[b] (ZPCE, in a. u.) and values of frontier orbitals[c] (in a. u.) of compounds discussed in the main text.

Structure	E	ZPCE	HOMO[c]	LUMO[c]
$[Ir(ppy)_2(1)]^+$	-1881.930266	0.587008	-0.29241	-0.18831
2	-819.858772	0.260522	-0.22390	-0.08011
3	-819.859102	0.260457	-0.27100	-0.05036
4	-1050.917057	0.341510	-0.26304	-0.04903
A2	-1881.505137	0.572463	-0.18941	-0.08344
A3	-1881.503501	0.572308	-0.18681	-0.08795
B2	- 2278.444243	0.540027	-0.20841	-0.07749

B3	-2278.442867	0.539831	-0.20738	-0.08659
A4	-2112 .556771	0.653369	-0.18573	-0.08922
B4	-2509.4 96044	0.620888	-0.20628	-0.08664

[a]Computed at the B3LYP/6-31G*&LANL2DZ level of theory. [b]Computed at 298.15 K at the B3LYP/6-31G*&LANL2DZ level of theory. [c]Computed at the B3LYP(PCM=acetonitrile)/6-31G*&LANL2DZ level of theory

Table S2. Final one electron symbolic density matrix of compound **[Ir(ppy)$_2$(1)]$^+$** obtained from the CASSCF(4,4) calculations:

	1	2	3	4
1	0.200000D+01			
2	0.683622D-08	0.200000D+01		
3	0.651247D-08	0.414147D-07	0.103500D-07	
4	0.172330D-07	0.303788D-07	-0.812606D-09	0.135145D-08

Molecular Orbital coefficients of frontier orbitals of compounds discussed in the main text.

A2

		156	157	158	159	160
		O	O	V	V	V
	Eigenvalues --	-0.18973	-0.17924	-0.06868	-0.05330	-0.05014
1	1 Ir 1S	0.00759	0.00813	0.00140	0.00232	-0.00797
2	2S	-0.01099	-0.01160	-0.00191	-0.00326	0.01141
3	3S	0.04615	0.06302	0.02352	0.00034	-0.00486
4	4PX	-0.05040	0.06576	0.00083	0.00236	-0.00278
5	4PY	0.01465	-0.00458	-0.00181	-0.00524	-0.01231
6	4PZ	-0.00792	0.00675	-0.00600	-0.01431	0.00649
7	5PX	0.03260	-0.02701	0.01041	0.00648	0.01781
8	5PY	-0.00222	-0.00706	0.03743	0.01480	0.09366
9	5PZ	0.01118	-0.00435	0.03303	0.11810	-0.04463
10	6PX	-0.02266	0.03742	-0.01477	-0.00733	-0.00667
11	6PY	0.02252	0.01825	-0.00619	-0.00096	-0.02662
12	6PZ	0.01710	-0.00200	-0.02368	-0.03361	0.00556
13	7D 0	0.15790	0.21588	0.02520	-0.02836	-0.13310
14	7D+1	0.30396	0.35346	0.07245	0.02487	0.14665

15		7D-1	0.02611	-0.15497	-0.00721	-0.00913	0.02130
16		7D+2	0.09968	-0.17667	0.01014	-0.01214	-0.09036
17		7D-2	0.33397	-0.27459	0.05869	0.05388	0.00705
18		8D 0	0.04750	0.06931	0.00213	-0.01020	-0.04902
19		8D+1	0.10752	0.12121	0.02121	0.01593	0.06185
20		8D-1	0.00761	-0.06536	-0.00985	0.00391	-0.00244
21		8D+2	0.04409	-0.06215	0.00641	0.00006	-0.04170
22		8D-2	0.12085	-0.10142	0.01510	0.02552	0.00343
23	2 C	1S	0.00010	0.00131	-0.00043	0.00174	-0.00355
24		2S	-0.00213	-0.00289	-0.00403	-0.00669	0.00852
25		2PX	-0.06036	0.04025	-0.01964	-0.01060	-0.00025
26		2PY	0.01150	-0.00702	0.00461	0.01518	0.00373
27		2PZ	-0.01478	0.01309	-0.00523	-0.00904	-0.01729
28		3S	0.00161	-0.01283	0.01836	-0.00464	0.02196
29		3PX	-0.05636	0.02568	-0.02988	0.00479	-0.00552
30		3PY	0.00674	-0.00578	0.00979	-0.00151	0.00112
31		3PZ	-0.00959	0.00785	-0.01331	-0.03704	-0.02458
32		4D 0	0.00038	0.00186	-0.00073	-0.00253	0.00026
33		4D+1	0.00187	0.00513	-0.00115	-0.00504	0.00107
34		4D-1	-0.00129	-0.00079	0.00005	0.00130	-0.00138
35		4D+2	-0.00045	-0.00067	0.00056	-0.00010	-0.00013
36		4D-2	0.00004	0.00164	0.00039	-0.00208	0.00105
37	3 C	1S	-0.00081	-0.00112	-0.00053	-0.00061	0.00281
38		2S	0.00095	0.00246	-0.00077	-0.00188	-0.01097
39		2PX	-0.07652	0.01044	-0.01579	-0.06718	0.02113
40		2PY	0.00822	-0.00870	0.00092	0.01045	0.00738
41		2PZ	-0.01516	0.00477	-0.00270	-0.01335	0.00097
42		3S	-0.00063	-0.00151	0.00674	0.00987	-0.01181
43		3PX	-0.06132	0.00384	-0.01704	-0.06957	0.01920
44		3PY	0.00911	-0.01198	0.00356	0.01602	-0.00224
45		3PZ	-0.01012	0.01349	0.00570	-0.01855	0.00875
46		4D 0	-0.00048	-0.00385	0.00015	0.00145	-0.00052
47		4D+1	-0.00177	-0.00857	-0.00017	0.00181	-0.00099
48		4D-1	0.00000	0.00164	-0.00082	-0.00165	0.00006
49		4D+2	0.00131	0.00269	-0.00051	-0.00112	0.00025
50		4D-2	0.00071	0.00010	-0.00186	-0.00236	0.00007
51	4 C	1S	0.00074	-0.00035	0.00039	-0.00087	0.00169
52		2S	-0.00099	0.00038	-0.00042	0.00061	-0.00464
53		2PX	0.02446	0.06953	0.00052	-0.05165	0.01836
54		2PY	-0.00203	-0.01478	0.00142	0.00822	0.00121
55		2PZ	0.00763	0.01568	0.00126	-0.01344	0.00828
56		3S	-0.00459	0.00502	-0.00797	0.02381	-0.00343
57		3PX	0.02008	0.06407	0.00152	-0.06683	0.02408

58			3PY	0.00028	-0.01413	0.00004	0.00403	-0.00265
59			3PZ	0.00609	0.01331	0.00805	-0.02021	0.00436
60			4D 0	0.00040	-0.00021	0.00017	0.00065	0.00095
61			4D+1	0.00098	-0.00047	0.00028	-0.00043	0.00007
62			4D-1	0.00089	-0.00048	0.00039	0.00103	0.00019
63			4D+2	0.00178	-0.00094	0.00085	0.00175	0.00008
64			4D-2	0.00438	-0.00241	0.00168	0.00288	-0.00039
65	5	H	1S	0.00064	-0.00057	-0.00108	0.00001	0.00455
66			2S	-0.00851	0.00174	0.00170	0.01095	0.00385
67	6	C	1S	0.00102	0.00082	0.00055	0.00103	-0.00067
68			2S	-0.00173	-0.00147	-0.00092	-0.00268	0.00103
69			2PX	0.00302	-0.06997	-0.01391	0.01273	-0.01137
70			2PY	0.00350	0.01670	0.00463	0.00066	0.00176
71			2PZ	0.00300	-0.01512	-0.00172	0.00507	-0.00303
72			3S	-0.00748	-0.00381	-0.01076	-0.00576	0.00567
73			3PX	0.00094	-0.05768	-0.01445	0.01210	-0.01165
74			3PY	0.00351	0.01534	0.01044	-0.00045	0.00503
75			3PZ	0.00153	-0.01485	-0.00428	0.00910	-0.00692
76			4D 0	0.00153	-0.00094	0.00048	0.00164	0.00003
77			4D+1	0.00453	-0.00169	0.00161	0.00458	-0.00106
78			4D-1	-0.00052	0.00031	-0.00028	-0.00045	0.00009
79			4D+2	-0.00025	0.00036	-0.00023	-0.00034	0.00025
80			4D-2	0.00265	-0.00006	0.00059	0.00269	-0.00080
81	7	C	1S	0.00029	0.00032	0.00011	0.00127	0.00032
82			2S	-0.00044	-0.00027	-0.00095	-0.00297	-0.00080
83			2PX	0.07483	-0.02588	0.02414	0.05616	-0.00778
84			2PY	-0.01575	0.00534	-0.00465	-0.00788	0.00336
85			2PZ	0.01834	-0.00575	0.00579	0.01193	-0.00357
86			3S	-0.00237	-0.00153	0.00714	-0.00904	-0.00019
87			3PX	0.06294	-0.02683	0.02648	0.06652	-0.01049
88			3PY	-0.01273	0.00693	-0.00963	-0.01181	0.00311
89			3PZ	0.01402	-0.00584	0.00286	0.01575	-0.00309
90			4D 0	0.00022	0.00154	0.00035	-0.00074	0.00057
91			4D+1	0.00052	0.00365	0.00068	-0.00112	0.00074
92			4D-1	-0.00034	-0.00150	-0.00016	0.00110	-0.00035
93			4D+2	-0.00025	-0.00208	-0.00025	0.00116	-0.00049
94			4D-2	-0.00033	-0.00251	0.00017	0.00247	-0.00085
95	8	H	1S	0.00076	-0.00044	0.00063	0.00286	0.00377
96			2S	0.00046	-0.00079	-0.00032	0.00509	0.01226
97	9	H	1S	0.00226	0.00150	0.00083	0.00142	-0.00164
98			2S	0.00283	0.00057	0.00035	0.00545	-0.00638
99	10	H	1S	-0.00074	0.00000	-0.00008	0.00119	-0.00012
100			2S	-0.00094	-0.00058	0.00187	0.00551	0.00048

101	11	C	1S	-0.01206	0.01713	0.00133	0.00337	-0.00014
102			2S	0.02035	-0.03149	-0.00185	-0.00722	0.00255
103			2PX	-0.07716	0.11597	0.00268	-0.01233	0.04287
104			2PY	0.00543	0.01558	-0.00615	-0.05403	0.08121
105			2PZ	-0.02526	-0.04885	0.00080	0.04652	-0.08319
106			3S	0.05404	-0.03373	-0.00922	-0.01090	-0.00639
107			3PX	-0.05713	0.14649	0.01245	0.00194	0.03458
108			3PY	0.01126	0.01596	0.00136	-0.05930	0.07883
109			3PZ	-0.00605	-0.00319	0.01747	0.03304	-0.07835
110			4D 0	-0.00140	-0.00158	-0.00051	0.00228	-0.00591
111			4D+1	-0.00727	-0.00901	-0.00198	-0.00117	-0.00185
112			4D-1	0.00042	0.00536	0.00043	-0.00041	0.00225
113			4D+2	-0.00371	0.00600	-0.00085	-0.00081	-0.00006
114			4D-2	-0.00590	0.00580	-0.00110	-0.00272	0.00225
115	12	C	1S	-0.00404	-0.00552	-0.00190	-0.00140	-0.00115
116			2S	0.00736	0.01349	0.00236	0.00308	0.00208
117			2PX	-0.00043	0.02021	-0.00095	0.01111	-0.02330
118			2PY	0.01181	0.10445	0.00946	0.03445	-0.04197
119			2PZ	0.02262	-0.05803	0.00482	-0.01919	0.05314
120			3S	0.03895	0.00157	0.02150	-0.00166	0.01034
121			3PX	0.02221	-0.01565	-0.00518	0.00694	-0.02620
122			3PY	0.00106	0.06407	0.00734	0.02294	-0.04534
123			3PZ	0.01746	-0.08729	0.00277	-0.03610	0.05780
124			4D 0	-0.00146	0.00034	0.00064	0.00809	-0.01360
125			4D+1	-0.00173	0.00347	-0.00010	0.00213	-0.00298
126			4D-1	-0.00122	0.00053	0.00017	-0.00194	0.00385
127			4D+2	0.00075	-0.00346	0.00001	0.00069	-0.00112
128			4D-2	-0.00231	0.00262	0.00022	-0.00430	0.00958
129	13	C	1S	0.01142	-0.00242	0.00194	0.00157	0.00063
130			2S	-0.02592	0.01091	-0.00329	-0.00482	0.00040
131			2PX	0.04817	0.01294	0.00607	-0.00345	0.01774
132			2PY	0.01164	0.06931	0.00383	-0.01587	0.03655
133			2PZ	0.04140	-0.07867	0.00219	0.01926	-0.03445
134			3S	-0.02612	-0.06365	-0.02440	-0.00807	-0.00343
135			3PX	0.03083	0.03184	0.00903	-0.01799	0.02860
136			3PY	0.00039	0.09091	0.00595	-0.02144	0.04537
137			3PZ	0.01934	-0.02642	0.00198	0.02600	-0.05033
138			4D 0	-0.00199	0.00449	-0.00027	-0.00330	0.00556
139			4D+1	0.00030	-0.00082	-0.00019	-0.00322	0.00567
140			4D-1	-0.00164	0.00135	0.00007	0.00191	-0.00296
141			4D+2	0.00279	-0.00361	0.00006	0.00195	-0.00355
142			4D-2	-0.00167	-0.00129	-0.00017	0.00360	-0.00718
143	14	C	1S	-0.00035	0.00409	0.00088	0.00099	0.00063

144		2S	0.00265	-0.01215	-0.00220	-0.00374	-0.00027
145		2PX	-0.01124	0.01126	0.00281	-0.02103	0.04752
146		2PY	0.00108	-0.03452	-0.00113	-0.05243	0.09462
147		2PZ	-0.00575	0.02385	-0.00006	0.05022	-0.09419
148		3S	-0.02887	0.02234	-0.00447	0.00319	-0.00730
149		3PX	0.00325	-0.00597	0.00176	-0.02105	0.04673
150		3PY	-0.01239	0.00394	0.00131	-0.04306	0.09361
151		3PZ	-0.01141	0.04173	-0.00077	0.06003	-0.09301
152		4D 0	-0.00030	0.00390	0.00014	0.00104	-0.00204
153		4D+1	-0.00106	0.00274	-0.00026	0.00089	-0.00266
154		4D-1	-0.00001	-0.00133	0.00006	-0.00058	0.00163
155		4D+2	-0.00027	-0.00346	-0.00026	-0.00124	0.00164
156		4D-2	-0.00004	-0.00646	-0.00055	-0.00207	0.00257
157	15 C	1S	-0.00584	0.00389	-0.00069	-0.00035	-0.00018
158		2S	0.01519	-0.01130	0.00107	0.00049	0.00029
159		2PX	-0.03107	0.01210	-0.00147	0.02702	-0.05157
160		2PY	0.00989	-0.03144	0.00137	0.05760	-0.10623
161		2PZ	-0.01032	0.02455	-0.00109	-0.05820	0.10712
162		3S	0.00250	0.01513	0.00647	0.00931	-0.00191
163		3PX	-0.00541	-0.00904	-0.00180	0.02648	-0.05473
164		3PY	0.01526	-0.04277	0.00017	0.06457	-0.11736
165		3PZ	0.00885	-0.01019	-0.00167	-0.06579	0.11989
166		4D 0	-0.00019	-0.00259	-0.00015	-0.00100	0.00180
167		4D+1	-0.00239	0.00571	0.00002	-0.00071	0.00161
168		4D-1	-0.00014	-0.00143	0.00004	0.00058	-0.00105
169		4D+2	-0.00079	-0.00477	-0.00025	0.00039	-0.00119
170		4D-2	-0.00119	-0.00178	-0.00017	0.00101	-0.00211
171	16 H	1S	-0.00324	0.01306	0.00055	0.00059	0.00171
172		2S	-0.00961	-0.00070	0.00824	0.00418	0.00660
173	17 C	1S	-0.00042	0.00125	0.00023	0.00050	0.00022
174		2S	-0.00124	-0.00016	-0.00061	-0.00100	-0.00038
175		2PX	0.00769	-0.04352	-0.00066	-0.00159	0.00370
176		2PY	0.00870	-0.08492	-0.00204	-0.00478	0.00726
177		2PZ	0.00136	0.08992	0.00348	0.00652	-0.00699
178		3S	0.02594	-0.05237	-0.00189	-0.01149	-0.00037
179		3PX	-0.01265	-0.01041	-0.00106	-0.00042	0.00680
180		3PY	0.01303	-0.08340	-0.00385	-0.01000	0.01741
181		3PZ	-0.00231	0.07326	0.00277	0.01364	-0.01713
182		4D 0	-0.00075	0.00046	-0.00008	-0.00571	0.01065
183		4D+1	-0.00039	-0.00027	-0.00002	0.00054	-0.00125
184		4D-1	-0.00016	0.00027	0.00002	0.00043	-0.00076
185		4D+2	0.00044	-0.00068	-0.00005	-0.00250	0.00450
186		4D-2	-0.00106	0.00091	-0.00008	0.00214	-0.00433

187	18	H	1S	0.00180	0.01191	0.00212	0.00267	0.00164
188			2S	0.00026	0.03369	0.00643	0.01170	0.00500
189	19	H	1S	-0.01663	0.00816	-0.00089	0.00002	-0.00069
190			2S	-0.03390	0.02533	-0.00172	0.00046	-0.00152
191	20	H	1S	0.00609	-0.00573	0.00020	0.00019	0.00012
192			2S	0.01374	-0.01426	0.00084	0.00071	0.00136
193	21	C	1S	-0.00215	-0.00090	0.00003	0.00012	0.00062
194			2S	0.00614	0.00033	0.00031	-0.00130	0.00106
195			2PX	-0.00267	0.02892	-0.00061	0.01452	0.00015
196			2PY	0.00244	-0.01395	0.03054	-0.17265	-0.08687
197			2PZ	-0.00904	0.00738	0.03670	-0.19716	-0.10260
198			3S	-0.01195	0.02843	-0.00627	-0.00043	-0.01101
199			3PX	0.00335	0.04382	0.00432	0.00883	0.00587
200			3PY	-0.00979	0.00613	0.03686	-0.17186	-0.08241
201			3PZ	0.00472	-0.01181	0.03557	-0.19913	-0.10232
202			4D 0	-0.00664	-0.00145	-0.00384	0.00261	0.00053
203			4D+1	-0.00296	-0.00148	0.00074	0.01267	0.00558
204			4D-1	0.00120	-0.00020	0.00066	0.00029	0.00054
205			4D+2	-0.00406	-0.00013	-0.00228	0.00024	-0.00047
206			4D-2	-0.00307	0.00036	0.00013	0.00936	0.00792
207	22	C	1S	0.00064	0.00325	-0.00007	0.00104	-0.00098
208			2S	-0.00099	-0.00958	0.00013	-0.00235	0.00182
209			2PX	-0.00660	0.02483	0.00060	-0.00662	0.02342
210			2PY	0.01838	-0.01845	-0.01808	-0.05110	-0.04037
211			2PZ	0.02127	0.01443	-0.02162	-0.06004	-0.03546
212			3S	-0.00807	-0.01239	-0.00242	-0.01568	0.01999
213			3PX	-0.00252	0.03088	0.00132	-0.01536	0.03764
214			3PY	0.01678	-0.02606	-0.02157	-0.03760	-0.05262
215			3PZ	0.00900	0.02165	-0.02693	-0.05605	-0.03852
216			4D 0	0.00457	0.00062	0.00285	-0.01955	-0.00935
217			4D+1	0.00051	-0.00048	-0.00011	-0.00233	-0.00217
218			4D-1	-0.00087	-0.00020	-0.00045	0.00351	0.00082
219			4D+2	0.00210	0.00035	0.00185	-0.01010	-0.00704
220			4D-2	0.00104	0.00140	0.00009	-0.00311	-0.00239
221	23	C	1S	0.00051	-0.00037	0.00023	0.00093	-0.00187
222			2S	-0.00083	0.00022	-0.00069	-0.00252	0.00446
223			2PX	0.00303	-0.00099	0.00234	-0.00259	0.00371
224			2PY	-0.04404	-0.00194	-0.02690	0.00481	-0.00438
225			2PZ	-0.04864	-0.00917	-0.03074	0.01027	-0.01514
226			3S	-0.00448	0.01278	0.00308	-0.00479	0.01301
227			3PX	-0.00023	0.00061	0.00733	0.00005	-0.00018
228			3PY	-0.03864	0.00583	-0.03608	-0.00198	-0.00763
229			3PZ	-0.04310	-0.01384	-0.04890	0.00470	-0.02594

230			4D 0	-0.00024	-0.00028	-0.00136	0.01878	0.01069
231			4D+1	-0.00055	-0.00057	0.00092	-0.00061	0.00034
232			4D-1	-0.00011	0.00046	0.00023	-0.00316	-0.00192
233			4D+2	-0.00039	0.00104	-0.00083	0.01132	0.00534
234			4D-2	-0.00058	0.00060	0.00081	0.00112	0.00047
235	24	C	1S	-0.00052	-0.00164	0.00004	0.00043	-0.00101
236			2S	0.00071	0.00361	-0.00053	-0.00086	0.00301
237			2PX	-0.00128	0.00030	-0.00173	0.00714	0.00625
238			2PY	0.04565	0.01256	0.02954	-0.12576	-0.05827
239			2PZ	0.05044	0.00221	0.03474	-0.14463	-0.07192
240			3S	0.00927	0.00223	0.00378	-0.00064	0.00232
241			3PX	-0.00041	-0.00734	-0.00328	0.01080	0.00793
242			3PY	0.04215	0.00682	0.03498	-0.15728	-0.07483
243			3PZ	0.04315	0.00502	0.03886	-0.18315	-0.08617
244			4D 0	-0.00060	-0.00025	0.00115	0.00367	0.00186
245			4D+1	0.00102	-0.00077	-0.00023	-0.01046	-0.00701
246			4D-1	0.00005	0.00062	-0.00029	-0.00171	-0.00002
247			4D+2	-0.00064	0.00085	0.00067	0.00280	0.00282
248			4D-2	0.00064	0.00072	-0.00020	-0.00935	-0.00452
249	25	H	1S	-0.00282	0.00226	0.00019	0.00207	-0.00433
250			2S	0.00157	-0.03110	0.00337	0.02917	-0.04941
251	26	C	1S	0.00016	0.00006	0.00012	0.00083	-0.00186
252			2S	0.00015	-0.00093	-0.00022	-0.00240	0.00379
253			2PX	-0.00162	0.00663	-0.00017	-0.01154	-0.00214
254			2PY	-0.00556	-0.00087	-0.00094	0.15586	0.09018
255			2PZ	-0.00782	0.00655	-0.00112	0.18178	0.10400
256			3S	-0.00078	0.00131	-0.00171	-0.00472	0.01723
257			3PX	-0.00182	-0.00040	-0.00293	-0.01188	-0.00571
258			3PY	-0.00818	0.00281	0.00073	0.19072	0.10949
259			3PZ	-0.00757	0.00123	0.00273	0.22003	0.12771
260			4D 0	0.00217	0.00029	0.00151	0.00032	0.00105
261			4D+1	0.00310	0.00024	0.00248	-0.00823	-0.00343
262			4D-1	-0.00012	-0.00015	-0.00011	-0.00065	-0.00022
263			4D+2	0.00088	0.00014	0.00055	0.00114	0.00090
264			4D-2	0.00288	0.00062	0.00225	-0.00682	-0.00327
265	27	H	1S	-0.00037	0.00430	0.00023	0.00180	-0.00323
266			2S	-0.00242	0.01053	0.00495	0.00513	-0.01155
267	28	H	1S	0.00053	-0.00677	0.00034	0.00278	-0.00539
268			2S	0.00073	-0.01045	0.00154	0.00755	-0.01725
269	29	H	1S	0.00013	0.00144	0.00012	0.00038	-0.00129
270			2S	-0.00074	0.00342	-0.00020	0.00402	-0.00830
271	30	C	1S	0.01238	-0.01752	-0.00070	-0.00298	0.00158
272			2S	-0.02157	0.02613	0.00280	0.00564	-0.00171

273		2PX	-0.07629	0.09700	0.00009	0.01182	-0.00924
274		2PY	0.11935	-0.01083	0.10358	0.08777	0.04580
275		2PZ	0.12096	0.04187	0.11804	0.09617	0.05380
276		3S	-0.03198	0.10581	0.00402	0.01517	-0.00960
277		3PX	-0.09569	0.08028	-0.00864	0.01670	-0.01158
278		3PY	0.10278	0.00504	0.09205	0.08582	0.03856
279		3PZ	0.06484	0.01701	0.10898	0.08339	0.06099
280		4D 0	-0.00168	-0.00079	0.00256	-0.00466	-0.00366
281		4D+1	-0.01080	-0.00906	-0.00247	-0.00081	-0.00306
282		4D-1	-0.00161	0.00266	-0.00091	-0.00004	0.00037
283		4D+2	-0.00028	0.00124	0.00188	-0.00276	-0.00058
284		4D-2	-0.01086	0.00558	-0.00202	-0.00253	0.00036
285	31 C	1S	-0.00408	0.01044	0.00025	-0.00125	0.00175
286		2S	0.01373	-0.02422	0.00048	0.00367	-0.00277
287		2PX	0.01695	-0.03378	0.00138	0.00203	-0.00357
288		2PY	0.08284	0.06436	-0.02203	0.02923	0.02319
289		2PZ	0.12283	-0.02539	-0.02470	0.03413	0.02000
290		3S	-0.04316	-0.01316	-0.00356	0.00614	-0.00798
291		3PX	0.01475	-0.03780	0.00213	-0.00102	-0.00389
292		3PY	0.09880	0.04747	-0.02520	0.04921	0.02374
293		3PZ	0.07489	-0.01527	-0.03692	0.04461	0.03166
294		4D 0	0.00680	-0.00107	0.00580	0.00565	0.00297
295		4D+1	0.00205	0.00136	0.00706	0.00749	0.00404
296		4D-1	-0.00181	0.00128	-0.00053	-0.00058	-0.00065
297		4D+2	0.00045	0.00423	0.00315	0.00310	0.00188
298		4D-2	0.00486	-0.00078	0.00632	0.00632	0.00383
299	32 C	1S	-0.00268	-0.00342	-0.00005	0.00035	-0.00130
300		2S	0.00770	0.00537	0.00134	-0.00134	0.00265
301		2PX	0.01181	0.00273	-0.00042	-0.00128	0.00475
302		2PY	0.10965	0.03010	0.02927	-0.05848	-0.01435
303		2PZ	0.10577	0.00640	0.03274	-0.05431	-0.03679
304		3S	-0.01302	0.04084	-0.00754	0.00641	0.00396
305		3PX	0.03662	-0.02909	-0.00369	0.00140	-0.00095
306		3PY	0.06460	0.02920	0.02848	-0.05264	-0.02486
307		3PZ	0.10839	0.00367	0.04175	-0.06263	-0.03219
308		4D 0	-0.00279	-0.00218	-0.00252	-0.01463	-0.00724
309		4D+1	0.00577	-0.00064	0.01087	-0.00502	-0.00215
310		4D-1	-0.00076	0.00243	0.00074	0.00229	0.00067
311		4D+2	-0.00506	0.00272	-0.00195	-0.00705	-0.00471
312		4D-2	0.00343	0.00196	0.00970	-0.00460	-0.00282
313	33 C	1S	0.00342	-0.00591	-0.00031	-0.00008	-0.00036
314		2S	-0.01053	0.01643	0.00073	0.00012	0.00113
315		2PX	-0.01989	0.03211	0.00180	0.00366	0.00277

316		2PY	-0.04927	-0.01366	-0.08686	-0.10360	-0.05983
317		2PZ	-0.06131	0.00107	-0.09760	-0.11788	-0.06743
318		3S	0.01958	-0.01196	0.00243	0.00014	-0.00163
319		3PX	-0.00160	0.00347	0.00235	0.00191	0.00360
320		3PY	-0.06362	0.00679	-0.07954	-0.11780	-0.06324
321		3PZ	-0.02960	-0.01591	-0.08767	-0.13034	-0.07727
322		4D 0	-0.00503	-0.00065	0.00075	0.00165	0.00086
323		4D+1	0.00904	-0.00085	-0.00423	0.00180	0.00118
324		4D-1	0.00023	0.00127	-0.00015	-0.00011	-0.00005
325		4D+2	-0.00313	-0.00042	0.00052	0.00087	0.00032
326		4D-2	0.00626	0.00362	-0.00368	0.00179	0.00122
327	34 H	1S	0.00812	0.00002	0.00002	-0.00111	0.00155
328		2S	0.00030	-0.02765	-0.00796	-0.01500	0.00994
329	35 C	1S	0.00256	-0.00148	0.00010	-0.00105	0.00077
330		2S	-0.00847	0.00552	-0.00074	0.00353	-0.00176
331		2PX	-0.01510	0.01365	0.00400	0.00151	-0.00454
332		2PY	-0.05670	-0.00945	-0.12659	0.09349	0.04705
333		2PZ	-0.06288	-0.00379	-0.14083	0.10561	0.05411
334		3S	0.02861	-0.03081	0.00168	0.00209	-0.00384
335		3PX	0.01397	-0.01361	0.00314	-0.00300	-0.00748
336		3PY	-0.02670	-0.01882	-0.14512	0.08757	0.04931
337		3PZ	-0.06282	0.00588	-0.16411	0.10469	0.04553
338		4D 0	0.00637	0.00121	-0.00129	-0.00260	-0.00145
339		4D+1	0.00612	0.00070	0.00014	-0.00328	-0.00228
340		4D-1	-0.00117	0.00036	0.00023	0.00032	0.00010
341		4D+2	0.00389	0.00024	-0.00078	-0.00149	-0.00054
342		4D-2	0.00714	0.00144	0.00006	-0.00366	-0.00092
343	36 C	1S	0.00050	-0.00113	-0.00005	-0.00021	0.00055
344		2S	0.00106	0.00019	0.00025	0.00093	-0.00108
345		2PX	0.00297	0.00389	-0.00161	0.00045	-0.00128
346		2PY	-0.14176	-0.01402	0.03913	0.01316	0.00685
347		2PZ	-0.16168	-0.03079	0.04361	0.01545	0.00479
348		3S	-0.03811	0.03095	-0.00261	-0.00047	-0.00583
349		3PX	-0.02265	0.02818	-0.00220	0.00002	0.00082
350		3PY	-0.10289	-0.01082	0.05369	0.02500	0.01843
351		3PZ	-0.11331	-0.02091	0.06023	0.03099	0.01076
352		4D 0	0.00050	-0.00044	-0.00690	0.01102	0.00580
353		4D+1	-0.00348	-0.00044	-0.01739	-0.00066	-0.00114
354		4D-1	-0.00021	0.00021	0.00054	-0.00156	-0.00086
355		4D+2	-0.00065	0.00097	-0.00306	0.00633	0.00351
356		4D-2	-0.00287	0.00003	-0.01509	-0.00047	-0.00056
357	37 H	1S	0.00703	0.00002	-0.00017	-0.00184	0.00319
358		2S	0.01945	-0.00539	-0.00270	-0.00696	0.00730

359	38	C	1S	0.00112	0.00257	-0.00180	-0.00228	-0.00133
360			2S	-0.00602	-0.00460	0.00600	0.00528	0.00327
361			2PX	-0.04547	0.00474	-0.01540	-0.00365	-0.04025
362			2PY	-0.00097	0.01088	0.01662	0.03742	-0.05655
363			2PZ	-0.01463	-0.02310	-0.01131	-0.03094	0.05698
364			3S	0.00832	-0.02520	0.00598	0.02342	0.01465
365			3PX	-0.04491	-0.00135	-0.01441	-0.02429	-0.04911
366			3PY	-0.00802	0.01085	-0.00007	0.02760	-0.06083
367			3PZ	-0.02851	-0.01048	-0.04029	-0.03013	0.05022
368			4D 0	-0.00081	0.00351	0.00010	0.01070	-0.01848
369			4D+1	-0.00047	-0.00020	0.00071	0.00055	-0.00115
370			4D-1	0.00017	-0.00019	-0.00069	-0.00210	0.00434
371			4D+2	-0.00041	-0.00014	-0.00009	0.00276	-0.00430
372			4D-2	-0.00102	-0.00202	-0.00037	-0.00502	0.01077
373	39	C	1S	-0.00206	-0.00459	-0.00070	0.00003	-0.00072
374			2S	0.00308	0.01053	0.00091	0.00287	0.00255
375			2PX	-0.03345	-0.00094	0.00048	0.04864	-0.08404
376			2PY	0.00490	0.01127	0.00546	0.09731	-0.17196
377			2PZ	-0.00924	0.00536	-0.00427	-0.09278	0.16818
378			3S	0.03709	0.00547	0.01481	-0.01306	0.00264
379			3PX	-0.04010	-0.02683	-0.01655	0.04270	-0.07833
380			3PY	0.01834	0.00717	0.01109	0.09742	-0.17146
381			3PZ	0.00479	-0.01187	-0.00112	-0.09776	0.16502
382			4D 0	0.00011	-0.00484	0.00031	-0.00105	0.00136
383			4D+1	-0.00090	-0.00220	-0.00123	-0.00575	0.00901
384			4D-1	0.00059	0.00126	0.00030	0.00278	-0.00448
385			4D+2	-0.00025	0.00017	0.00070	0.00367	-0.00939
386			4D-2	-0.00114	0.00408	-0.00009	0.00386	-0.00842
387	40	C	1S	-0.00095	-0.00170	0.00079	0.00017	-0.00009
388			2S	0.00248	0.00299	-0.00017	-0.00035	0.00079
389			2PX	0.00247	0.01552	-0.00004	0.03415	-0.05894
390			2PY	-0.00181	0.03815	-0.00425	0.07028	-0.12259
391			2PZ	0.00843	-0.02729	0.00058	-0.06886	0.11696
392			3S	-0.00997	0.01763	-0.02524	-0.00281	-0.00464
393			3PX	0.00240	0.01557	-0.00337	0.04597	-0.07250
394			3PY	-0.00804	0.03613	-0.01212	0.08897	-0.15459
395			3PZ	0.00210	-0.02307	-0.00578	-0.08542	0.14412
396			4D 0	-0.00054	-0.00072	-0.00098	-0.00277	0.00409
397			4D+1	-0.00164	0.00065	-0.00021	0.00385	-0.00939
398			4D-1	-0.00034	-0.00017	-0.00052	-0.00199	0.00327
399			4D+2	0.00013	-0.00100	-0.00075	-0.00533	0.01016
400			4D-2	-0.00140	-0.00041	-0.00100	-0.00336	0.00443
401	41	H	1S	0.00681	-0.00293	0.00201	-0.00134	-0.00157

402		2S	-0.03592	-0.00216	-0.01604	-0.04339	-0.02585
403	42 C	1S	-0.00025	0.00129	-0.00032	-0.00109	-0.00045
404		2S	0.00034	-0.00290	0.00138	0.00233	0.00138
405		2PX	0.00530	-0.01502	0.00295	-0.00392	-0.00236
406		2PY	0.00629	-0.03568	0.00869	-0.00418	-0.00197
407		2PZ	-0.00147	0.02882	-0.00660	0.00937	0.00373
408		3S	0.00442	-0.00568	-0.00083	0.00884	0.00032
409		3PX	0.00900	-0.00552	0.01414	-0.00153	-0.00717
410		3PY	0.00841	-0.03040	0.01119	-0.00175	-0.01103
411		3PZ	0.00342	0.02797	-0.00298	0.00813	0.01163
412		4D 0	-0.00047	-0.00065	-0.00071	-0.01008	0.01900
413		4D+1	-0.00073	-0.00032	-0.00010	0.00099	-0.00103
414		4D-1	-0.00036	0.00033	0.00009	0.00149	-0.00293
415		4D+2	0.00023	-0.00005	-0.00022	-0.00382	0.00660
416		4D-2	-0.00112	0.00075	0.00055	0.00494	-0.00859
417	43 C	1S	-0.00080	0.00009	-0.00130	-0.00146	-0.00074
418		2S	0.00054	0.00032	0.00250	0.00344	0.00198
419		2PX	-0.00967	-0.00339	-0.00846	-0.04547	0.07753
420		2PY	0.00475	-0.00921	-0.00708	-0.08592	0.16696
421		2PZ	-0.00619	0.00907	0.00873	0.08435	-0.15934
422		3S	0.01071	0.00157	0.01803	0.00755	0.00312
423		3PX	-0.00270	-0.00160	-0.00590	-0.05287	0.09477
424		3PY	0.00686	-0.01244	-0.00646	-0.10706	0.20160
425		3PZ	0.00022	0.00893	0.01362	0.09880	-0.19405
426		4D 0	-0.00026	0.00144	-0.00046	-0.00026	0.00129
427		4D+1	-0.00027	0.00156	0.00002	0.00368	-0.00572
428		4D-1	0.00020	-0.00116	0.00001	-0.00193	0.00242
429		4D+2	0.00022	-0.00134	0.00025	-0.00346	0.00632
430		4D-2	0.00011	-0.00227	0.00054	-0.00247	0.00412
431	44 H	1S	-0.00921	-0.00166	-0.00354	-0.00377	-0.00250
432		2S	-0.01402	-0.00255	-0.01030	-0.00886	-0.00692
433	45 H	1S	0.00507	0.00096	-0.00036	-0.00147	-0.00063
434		2S	0.00988	-0.00143	-0.00450	-0.00585	-0.00092
435	46 H	1S	0.00007	0.00016	-0.00152	-0.00157	-0.00068
436		2S	0.00148	-0.00110	-0.00494	-0.00800	-0.00373
437	47 C	1S	0.00091	0.00239	0.00008	-0.00378	0.00503
438		2S	-0.00071	-0.00509	0.00175	0.00628	-0.00945
439		2PX	0.00337	0.13047	0.00735	0.03395	-0.01168
440		2PY	0.00008	-0.01447	-0.00308	-0.01935	0.01180
441		2PZ	0.00207	0.02705	0.00156	0.01041	-0.01253
442		3S	-0.00751	0.00397	-0.00553	0.03811	-0.05403
443		3PX	0.00614	0.09906	0.01358	0.02004	0.00419
444		3PY	-0.00452	0.00333	-0.00131	-0.03044	0.04191

445		3PZ	-0.01596	-0.00570	-0.02005	0.01217	0.00097
446		4D 0	0.00098	-0.00477	0.00054	0.00174	0.00275
447		4D+1	0.00445	-0.00724	0.00005	-0.00251	-0.00023
448		4D-1	-0.00053	0.00581	-0.00023	-0.00150	0.00056
449		4D+2	-0.00128	0.00715	0.00037	0.00091	0.00329
450		4D-2	-0.00002	0.01325	0.00030	-0.00036	-0.00040
451	48 C	1S	0.00093	0.00114	-0.00005	-0.00239	-0.00314
452		2S	-0.00049	0.00028	0.00213	0.00798	0.00469
453		2PX	-0.05304	0.14712	-0.00016	0.01014	-0.00354
454		2PY	0.01070	-0.02883	0.00034	-0.00574	0.00167
455		2PZ	-0.01653	0.03124	0.00189	0.00965	0.01245
456		3S	-0.02086	-0.03217	-0.01765	0.00683	0.02740
457		3PX	-0.03723	0.12391	0.00175	0.02743	-0.01625
458		3PY	0.00662	-0.03444	-0.00410	0.00345	-0.02582
459		3PZ	-0.01570	0.01062	-0.01010	0.00073	0.02476
460		4D 0	0.00017	0.00192	0.00004	0.00150	-0.00075
461		4D+1	0.00096	0.00544	0.00055	0.00268	-0.00101
462		4D-1	-0.00048	-0.00068	-0.00004	-0.00040	0.00019
463		4D+2	-0.00060	-0.00131	0.00002	-0.00088	0.00021
464		4D-2	-0.00086	0.00002	-0.00016	-0.00181	0.00081
465	49 C	1S	-0.00090	-0.00126	0.00025	0.00220	0.00276
466		2S	0.00047	0.00381	-0.00095	-0.00502	-0.00995
467		2PX	0.00382	0.16217	-0.00091	-0.01784	0.01182
468		2PY	-0.00379	-0.03956	0.00204	0.01366	0.00937
469		2PZ	0.00047	0.03465	0.00112	0.00180	0.00787
470		3S	0.01200	-0.00430	0.00547	-0.00875	-0.01653
471		3PX	0.00093	0.12689	-0.00235	-0.02205	0.01347
472		3PY	-0.01129	-0.03058	-0.00619	0.00893	0.01966
473		3PZ	0.00346	0.04985	0.00632	-0.00957	0.01399
474		4D 0	-0.00141	-0.00006	-0.00051	-0.00238	0.00027
475		4D+1	-0.00272	-0.00095	-0.00078	-0.00426	0.00137
476		4D-1	0.00081	-0.00094	0.00000	0.00054	-0.00064
477		4D+2	0.00124	-0.00150	-0.00005	0.00064	-0.00008
478		4D-2	0.00070	-0.00547	-0.00039	-0.00018	0.00034
479	50 C	1S	-0.00042	0.00010	0.00013	0.00108	0.00040
480		2S	0.00024	-0.00045	-0.00069	-0.00183	-0.00233
481		2PX	-0.03687	-0.04751	-0.00578	-0.04504	0.01579
482		2PY	0.00617	0.01021	0.00141	0.01160	-0.00163
483		2PZ	-0.00747	-0.01105	-0.00161	-0.01236	0.00154
484		3S	0.00675	0.00938	0.00404	-0.01519	0.01808
485		3PX	-0.03181	-0.03519	-0.00664	-0.05057	0.01476
486		3PY	0.00486	0.01070	0.00407	0.01569	-0.01180
487		3PZ	-0.00332	0.00126	0.00419	-0.01402	0.00956

488		4D 0	-0.00024	0.00017	0.00013	0.00032	0.00051
489		4D+1	-0.00015	-0.00015	0.00005	0.00066	-0.00051
490		4D-1	0.00072	-0.00270	-0.00007	-0.00029	-0.00048
491		4D+2	0.00105	-0.00457	-0.00003	-0.00026	0.00016
492		4D-2	0.00274	-0.01075	0.00007	-0.00023	-0.00020
493	51 H	1S	0.00007	0.00153	0.00005	0.00073	-0.00038
494		2S	0.00507	-0.00651	-0.00564	0.00117	-0.02314
495	52 C	1S	0.00039	0.00084	-0.00016	-0.00117	-0.00097
496		2S	-0.00088	-0.00223	0.00027	0.00303	0.00168
497		2PX	0.05469	-0.05598	0.00489	0.04008	-0.01220
498		2PY	-0.00944	0.01448	-0.00153	-0.01150	0.00061
499		2PZ	0.01228	-0.01432	0.00130	0.01126	-0.00192
500		3S	0.00345	0.00875	0.00616	0.00293	0.00505
501		3PX	0.04070	-0.04330	0.00230	0.04141	-0.01113
502		3PY	-0.00919	0.00030	-0.00351	-0.00684	0.00430
503		3PZ	0.00957	-0.01629	0.00255	0.01599	-0.00628
504		4D 0	-0.00056	0.00377	-0.00001	0.00009	0.00066
505		4D+1	-0.00114	0.00942	-0.00026	-0.00099	0.00042
506		4D-1	0.00028	-0.00306	0.00001	0.00011	-0.00034
507		4D+2	0.00025	-0.00486	0.00011	0.00091	0.00001
508		4D-2	-0.00005	-0.00476	0.00000	0.00053	-0.00051
509	53 C	1S	0.00005	0.00028	0.00002	-0.00049	0.00018
510		2S	0.00027	0.00027	0.00037	0.00120	-0.00059
511		2PX	0.03113	-0.18700	0.00122	0.00299	-0.00589
512		2PY	-0.00631	0.03580	-0.00016	-0.00113	0.00319
513		2PZ	0.00701	-0.04473	0.00062	0.00160	0.00088
514		3S	-0.00305	-0.01497	-0.00445	0.00556	-0.00249
515		3PX	0.02740	-0.15105	0.00329	0.00628	-0.00638
516		3PY	-0.00276	0.03675	0.00351	-0.00200	0.00176
517		3PZ	0.00477	-0.03960	0.00072	0.00324	-0.00475
518		4D 0	0.00101	-0.00038	0.00019	0.00137	-0.00023
519		4D+1	0.00260	-0.00053	0.00037	0.00282	-0.00089
520		4D-1	-0.00017	0.00028	-0.00007	-0.00015	-0.00007
521		4D+2	-0.00004	0.00037	0.00008	0.00020	-0.00002
522		4D-2	0.00151	0.00015	0.00021	0.00189	-0.00068
523	54 H	1S	-0.00080	-0.00010	0.00039	0.00060	0.00287
524		2S	-0.00017	0.00191	0.00256	0.00263	0.00742
525	55 H	1S	0.00069	0.00240	-0.00042	-0.00257	-0.00227
526		2S	0.00099	0.00728	-0.00040	-0.00923	-0.00632
527	56 H	1S	-0.00005	-0.00065	-0.00009	-0.00046	0.00012
528		2S	-0.00109	-0.00310	-0.00129	-0.00190	0.00023
529	57 N	1S	0.00134	-0.00254	0.00098	0.00517	-0.01071
530		2S	-0.00263	0.00566	-0.00236	-0.01174	0.02203

531		2PX	0.00456	-0.00700	-0.00031	-0.02157	0.01220
532		2PY	-0.04593	0.00733	-0.02057	0.15952	0.13025
533		2PZ	-0.05020	-0.02513	-0.01915	0.21403	0.09440
534		3S	-0.01106	0.01005	-0.00714	-0.03667	0.08492
535		3PX	0.00418	0.02600	0.00106	-0.02620	0.01493
536		3PY	-0.03841	-0.00960	-0.01917	0.16114	0.14166
537		3PZ	-0.04430	-0.00413	-0.01620	0.22083	0.10851
538		4D 0	-0.00088	-0.00324	-0.00225	0.00378	0.00206
539		4D+1	0.00189	-0.00192	-0.00249	0.00461	0.00290
540		4D-1	0.00039	0.00423	0.00023	-0.00008	0.00085
541		4D+2	-0.00053	0.00387	-0.00107	0.00069	0.00296
542		4D-2	0.00147	0.00370	-0.00195	0.00550	0.00051
543	58 N	1S	0.00425	0.00199	0.00368	0.00650	0.00405
544		2S	-0.00979	-0.00426	-0.00752	-0.01159	-0.00734
545		2PX	-0.03090	-0.06976	0.02925	0.06645	-0.01237
546		2PY	0.02193	0.02083	0.00362	0.00287	0.01206
547		2PZ	0.00155	-0.01509	0.01250	0.02477	0.00904
548		3S	-0.02319	-0.01373	-0.03529	-0.07339	-0.04492
549		3PX	-0.02621	-0.06568	0.02971	0.06119	-0.01202
550		3PY	0.01828	0.00959	0.00338	0.01834	0.01661
551		3PZ	0.00546	-0.00922	0.01209	0.01817	0.00109
552		4D 0	-0.00436	-0.00112	-0.00146	-0.00036	0.00331
553		4D+1	-0.00701	0.00141	-0.00070	0.00169	-0.00161
554		4D-1	-0.00083	-0.00094	-0.00020	-0.00082	0.00212
555		4D+2	-0.00192	-0.00153	0.00091	-0.00051	0.00286
556		4D-2	-0.00944	-0.00158	-0.00120	-0.00204	-0.00143
557	59 N	1S	-0.00338	0.00082	-0.00359	-0.00700	-0.00331
558		2S	0.00554	-0.00111	0.00570	0.01390	0.00697
559		2PX	0.01539	-0.01513	-0.00714	-0.05075	0.08827
560		2PY	0.01181	-0.03381	-0.00142	-0.08019	0.19927
561		2PZ	0.02036	0.03900	0.01799	0.11071	-0.17342
562		3S	0.02488	-0.01405	0.03775	0.06581	0.03229
563		3PX	-0.02420	-0.03202	-0.03248	-0.05152	0.09081
564		3PY	0.01769	-0.02292	0.00621	-0.07049	0.20880
565		3PZ	0.00780	0.03035	0.01852	0.10781	-0.18192
566		4D 0	-0.00421	-0.00139	-0.00016	-0.00128	0.00289
567		4D+1	-0.00490	-0.00029	-0.00028	-0.00197	0.00361
568		4D-1	-0.00235	-0.00152	-0.00106	0.00161	-0.00192
569		4D+2	0.00049	-0.00117	0.00032	0.00333	-0.00152
570		4D-2	-0.00567	-0.00313	-0.00108	0.00186	-0.00567
571	60 N	1S	0.00108	-0.00122	0.00019	-0.00001	-0.00007
572		2S	-0.00214	0.00214	-0.00041	-0.00021	-0.00010
573		2PX	-0.00485	0.00335	-0.00848	-0.00007	0.00055

574		2PY	0.03655	0.00411	0.22975	-0.00334	0.00625
575		2PZ	0.04510	0.00252	0.26797	-0.00429	0.00820
576		3S	-0.01324	0.01791	-0.00123	0.00170	0.00252
577		3PX	-0.00372	0.00297	-0.00743	0.00047	0.00060
578		3PY	0.02802	-0.00108	0.21024	-0.01146	0.00006
579		3PZ	0.03052	0.00486	0.24546	-0.01273	0.00377
580		4D 0	0.00653	0.00083	-0.00019	0.00097	0.00056
581		4D+1	-0.00928	-0.00150	0.01296	0.00033	0.00046
582		4D-1	-0.00160	-0.00011	0.00051	-0.00013	-0.00012
583		4D+2	0.00456	0.00065	-0.00084	0.00049	0.00035
584		4D-2	-0.00760	-0.00118	0.01114	0.00039	0.00041
585	61 N	1S	0.00074	-0.00027	-0.00017	-0.00028	0.00021
586		2S	-0.00160	0.00069	0.00032	0.00068	-0.00039
587		2PX	-0.00517	-0.00025	0.00753	0.00071	-0.00005
588		2PY	0.11598	0.01445	-0.21324	-0.00565	-0.00813
589		2PZ	0.12767	0.02200	-0.24963	-0.00503	-0.01081
590		3S	-0.00192	-0.00174	0.00119	0.00141	-0.00253
591		3PX	-0.00329	-0.00249	0.00727	-0.00125	-0.00045
592		3PY	0.08932	0.00966	-0.19777	0.00307	-0.00381
593		3PZ	0.09804	0.01849	-0.23151	0.00494	-0.00436
594		4D 0	-0.00768	-0.00104	-0.00120	0.00045	0.00006
595		4D+1	0.00165	0.00008	0.01448	0.00080	0.00106
596		4D-1	0.00118	0.00043	0.00070	0.00002	0.00003
597		4D+2	-0.00461	-0.00053	-0.00162	0.00015	0.00001
598		4D-2	0.00086	-0.00003	0.01218	0.00073	0.00078
599	62 C	1S	-0.00025	0.00010	0.00012	0.00014	-0.00012
600		2S	0.00066	-0.00031	0.00005	-0.00035	0.00027
601		2PX	0.00340	-0.00023	0.00236	-0.00060	0.00071
602		2PY	-0.05654	-0.00612	-0.06676	-0.00210	-0.00455
603		2PZ	-0.06626	-0.00788	-0.08093	-0.00271	-0.00542
604		3S	0.00027	0.00030	-0.00297	-0.00111	0.00093
605		3PX	0.00208	-0.00117	0.00393	-0.00130	0.00057
606		3PY	-0.03249	-0.00264	-0.07686	-0.00604	-0.00681
607		3PZ	-0.04096	-0.00519	-0.09242	-0.00707	-0.00839
608		4D 0	0.00107	0.00021	-0.00572	0.00001	-0.00023
609		4D+1	0.00822	0.00133	-0.01650	-0.00060	-0.00088
610		4D-1	0.00014	-0.00002	0.00053	-0.00003	0.00002
611		4D+2	0.00019	-0.00002	-0.00223	0.00001	-0.00006
612		4D-2	0.00732	0.00096	-0.01426	-0.00057	-0.00069
613	63 C	1S	-0.00031	0.00011	0.00025	0.00003	0.00000
614		2S	0.00060	-0.00020	-0.00062	-0.00004	0.00003
615		2PX	0.00345	0.00005	-0.00456	-0.00018	-0.00018
616		2PY	-0.06050	-0.00868	0.09438	0.00305	0.00465

617		2PZ	-0.07404	-0.01015	0.11421	0.00371	0.00563
618		3S	0.00271	-0.00055	-0.00099	-0.00059	0.00000
619		3PX	0.00271	0.00025	-0.00309	-0.00001	-0.00043
620		3PY	-0.05039	-0.00731	0.08871	0.00425	0.00537
621		3PZ	-0.06208	-0.00864	0.10507	0.00591	0.00646
622		4D 0	0.00261	0.00031	0.00222	0.00005	0.00016
623		4D+1	-0.00204	-0.00019	-0.00624	-0.00004	-0.00032
624		4D-1	-0.00065	-0.00006	-0.00074	-0.00002	-0.00003
625		4D+2	0.00162	0.00023	0.00175	0.00003	0.00013
626		4D-2	-0.00151	-0.00017	-0.00508	-0.00005	-0.00025
627	64 C	1S	0.00039	-0.00017	-0.00011	-0.00007	0.00001
628		2S	-0.00075	0.00036	0.00033	0.00015	-0.00001
629		2PX	0.00119	0.00080	-0.00398	0.00007	-0.00020
630		2PY	-0.05839	-0.00851	0.10378	0.00204	0.00510
631		2PZ	-0.07266	-0.00964	0.12699	0.00288	0.00576
632		3S	-0.00294	-0.00012	0.00090	0.00025	-0.00019
633		3PX	0.00144	0.00123	-0.00503	0.00041	-0.00008
634		3PY	-0.04724	-0.00560	0.11892	0.00317	0.00659
635		3PZ	-0.05817	-0.00918	0.14693	0.00368	0.00715
636		4D 0	-0.00316	-0.00037	-0.00312	-0.00006	-0.00022
637		4D+1	-0.00138	-0.00017	-0.00213	-0.00021	-0.00020
638		4D-1	0.00066	0.00007	0.00059	0.00000	0.00004
639		4D+2	-0.00167	-0.00023	-0.00166	-0.00005	-0.00011
640		4D-2	-0.00127	-0.00012	-0.00187	-0.00015	-0.00019
641	65 C	1S	0.00011	-0.00004	-0.00009	0.00000	-0.00001
642		2S	-0.00022	0.00010	0.00018	-0.00002	0.00003
643		2PX	-0.00125	0.00006	-0.00116	-0.00003	-0.00004
644		2PY	0.02018	0.00220	0.03837	0.00022	0.00202
645		2PZ	0.02452	0.00259	0.04629	0.00024	0.00245
646		3S	-0.00084	0.00040	0.00078	0.00036	-0.00003
647		3PX	-0.00097	0.00002	-0.00151	0.00008	-0.00018
648		3PY	0.01452	0.00159	0.05106	0.00022	0.00253
649		3PZ	0.01802	0.00175	0.06266	-0.00012	0.00306
650		4D 0	-0.00364	-0.00049	0.00727	0.00023	0.00040
651		4D+1	-0.00455	-0.00062	0.00836	0.00024	0.00042
652		4D-1	0.00061	0.00008	-0.00123	-0.00004	-0.00007
653		4D+2	-0.00180	-0.00025	0.00363	0.00012	0.00020
654		4D-2	-0.00386	-0.00055	0.00718	0.00021	0.00036
655	66 H	1S	-0.00007	-0.00001	-0.00013	0.00005	-0.00004
656		2S	-0.00049	0.00026	0.00117	-0.00016	-0.00001
657	67 C	1S	-0.00018	0.00006	0.00005	0.00005	-0.00002
658		2S	0.00038	-0.00021	-0.00013	-0.00011	0.00002
659		2PX	-0.00001	-0.00042	-0.00034	-0.00023	-0.00001

660		2PY	0.01988	0.00243	0.00633	0.00168	0.00138
661		2PZ	0.02448	0.00277	0.00749	0.00201	0.00167
662		3S	0.00109	0.00057	-0.00050	0.00010	0.00023
663		3PX	0.00020	-0.00005	-0.00053	-0.00006	0.00010
664		3PY	0.01377	0.00088	0.00917	0.00169	0.00154
665		3PZ	0.01655	0.00249	0.01058	0.00239	0.00193
666		4D 0	0.00230	0.00030	-0.00466	-0.00017	-0.00028
667		4D+1	-0.00515	-0.00068	0.01005	0.00025	0.00049
668		4D-1	-0.00069	-0.00011	0.00140	0.00004	0.00008
669		4D+2	0.00169	0.00023	-0.00335	-0.00011	-0.00019
670		4D-2	-0.00408	-0.00059	0.00806	0.00017	0.00041
671	68 H	1S	-0.00005	0.00009	-0.00006	0.00005	-0.00002
672		2S	0.00058	-0.00164	0.00132	-0.00021	-0.00049
673	69 C	1S	-0.00002	0.00001	0.00005	0.00001	-0.00002
674		2S	0.00003	0.00003	-0.00014	-0.00001	0.00004
675		2PX	-0.00293	-0.00039	0.00458	0.00013	0.00027
676		2PY	0.07451	0.00987	-0.11790	-0.00339	-0.00613
677		2PZ	0.08965	0.01193	-0.14200	-0.00407	-0.00744
678		3S	0.00042	-0.00075	0.00031	-0.00039	0.00009
679		3PX	-0.00233	-0.00069	0.00518	-0.00004	0.00025
680		3PY	0.06081	0.00822	-0.12761	-0.00361	-0.00685
681		3PZ	0.07334	0.01002	-0.15353	-0.00446	-0.00839
682		4D 0	0.00004	0.00000	0.00196	-0.00007	0.00006
683		4D+1	0.00024	0.00002	0.00233	0.00009	0.00015
684		4D-1	0.00001	0.00000	-0.00033	0.00002	-0.00001
685		4D+2	0.00002	-0.00001	0.00099	-0.00005	0.00002
686		4D-2	0.00024	-0.00001	0.00198	0.00007	0.00013
687	70 H	1S	0.00021	-0.00006	-0.00013	0.00002	-0.00002
688		2S	0.00029	-0.00012	-0.00049	0.00011	-0.00009
689	71 H	1S	-0.00043	0.00015	0.00023	0.00008	-0.00006
690		2S	-0.00079	0.00060	0.00044	0.00031	-0.00013
691	72 H	1S	0.00003	-0.00002	0.00007	-0.00001	-0.00001
692		2S	0.00002	-0.00011	0.00027	-0.00004	-0.00008
693	73 H	1S	0.00841	-0.01904	-0.00018	-0.00061	-0.00073
694		2S	0.02232	-0.03742	-0.00129	-0.00104	-0.00260

A3

	156	157	158	159	160

			O	O	V	V	V
	Eigenvalues --		-0.19127	-0.17541	-0.07475	-0.04673	-0.04061
1	1 Ir	1S	-0.00998	0.00870	0.00000	0.00796	-0.00361
2		2S	0.01459	-0.01236	-0.00009	-0.01137	0.00532
3		3S	-0.05216	0.06291	-0.00822	0.00574	0.00201
4		4PX	0.06920	0.06574	-0.00085	-0.00710	0.01005
5		4PY	-0.02162	-0.03576	-0.00257	-0.01327	-0.00225
6		4PZ	0.00807	0.00762	-0.00699	0.01082	0.00452
7		5PX	-0.03964	-0.02642	-0.01420	0.06589	0.07590
8		5PY	0.01557	0.02328	0.00712	0.08197	-0.05885
9		5PZ	0.00132	0.00277	0.03176	-0.06882	-0.02003
10		6PX	0.02090	0.02219	0.00626	-0.01866	-0.03314
11		6PY	0.00537	-0.03537	0.00214	-0.02017	0.02322
12		6PZ	0.02190	0.00232	0.01439	0.01800	0.02350
13		7D 0	-0.01800	0.01197	0.04018	0.06571	-0.03883
14		7D+1	0.50986	-0.25009	0.04238	-0.00016	0.09187
15		7D-1	-0.12977	0.06316	-0.05757	-0.13785	0.01531
16		7D+2	0.06388	0.34865	0.02140	-0.03711	0.08797
17		7D-2	0.17549	0.34089	0.01103	-0.03007	0.12828
18		8D 0	0.00065	-0.00513	0.02154	0.03200	-0.01852
19		8D+1	0.18071	-0.08316	0.01956	0.00465	0.03790
20		8D-1	-0.04352	0.01653	-0.03294	-0.04951	0.00327
21		8D+2	0.02814	0.12655	0.00961	-0.01205	0.04995
22		8D-2	0.07051	0.12642	0.00853	-0.02430	0.06139
23	2 C	1S	-0.00076	0.00122	-0.00035	0.00380	-0.00096
24		2S	0.00348	-0.00282	0.00047	-0.01088	0.00072
25		2PX	0.06334	0.04351	0.00407	-0.00950	-0.08540
26		2PY	-0.02496	-0.01664	0.00706	0.00334	0.02904
27		2PZ	0.00429	-0.00202	-0.00341	-0.01162	-0.00034
28		3S	0.00290	-0.01160	0.00770	-0.01835	0.01352
29		3PX	0.05531	0.02938	-0.00446	-0.00138	-0.09006
30		3PY	-0.02804	-0.01087	0.01193	0.00025	0.03006
31		3PZ	0.00334	0.00070	-0.00920	0.00491	0.01012
32		4D 0	0.00084	-0.00050	0.00034	0.00129	0.00121
33		4D+1	0.00300	-0.00519	-0.00122	0.00569	0.02319
34		4D-1	-0.00096	0.00211	0.00036	-0.00094	-0.00883
35		4D+2	-0.00101	0.00065	-0.00008	-0.00014	-0.00328
36		4D-2	-0.00120	0.00045	-0.00035	-0.00049	-0.00246
37	3 C	1S	0.00116	-0.00095	-0.00047	-0.00275	0.00062
38		2S	-0.00272	0.00217	0.00536	0.00846	-0.00237
39		2PX	0.08383	0.02106	0.00993	-0.05764	-0.26282
40		2PY	-0.04163	-0.00175	-0.00239	0.03349	0.09478
41		2PZ	0.00261	0.00097	0.00126	-0.00086	-0.00710

42			3S	0.00306	-0.00159	-0.01154	0.01350	-0.00350
43			3PX	0.06459	0.01884	0.01160	-0.06630	-0.26030
44			3PY	-0.03195	0.00711	-0.01636	0.02040	0.09292
45			3PZ	0.00722	-0.00614	-0.00378	0.00145	-0.00886
46			4D 0	0.00002	0.00014	0.00034	0.00010	-0.00005
47			4D+1	-0.00240	0.00795	0.00054	-0.00151	-0.00190
48			4D-1	0.00157	-0.00339	0.00039	0.00026	0.00133
49			4D+2	0.00167	-0.00304	-0.00013	0.00239	0.01171
50			4D-2	0.00220	-0.00335	-0.00021	0.00238	0.01334
51	4	C	1S	-0.00030	-0.00033	-0.00033	-0.00197	0.00022
52			2S	0.00024	0.00030	0.00097	0.00432	-0.00036
53			2PX	-0.03791	0.06546	0.01147	-0.04789	-0.18473
54			2PY	0.01556	-0.02424	-0.00404	0.02186	0.06947
55			2PZ	-0.00015	0.00287	0.00119	0.00429	-0.00624
56			3S	0.00058	0.00507	-0.00244	0.01800	0.00099
57			3PX	-0.03002	0.06103	0.01619	-0.06055	-0.23229
58			3PY	0.01386	-0.02212	-0.00585	0.03041	0.09089
59			3PZ	-0.00034	0.00395	0.00060	0.00258	-0.00700
60			4D 0	0.00016	0.00007	-0.00040	-0.00029	0.00005
61			4D+1	0.00266	0.00149	0.00029	-0.00056	-0.00456
62			4D-1	-0.00087	-0.00042	0.00025	0.00017	0.00112
63			4D+2	0.00300	0.00172	0.00011	-0.00202	-0.01075
64			4D-2	0.00362	0.00201	0.00046	-0.00227	-0.01248
65	5	H	1S	0.00027	-0.00073	-0.00195	-0.00417	0.00068
66			2S	0.00783	0.00239	-0.00682	0.00206	0.00067
67	6	C	1S	-0.00097	0.00071	-0.00060	0.00105	-0.00033
68			2S	0.00162	-0.00125	0.00126	-0.00221	0.00056
69			2PX	0.00591	-0.06773	-0.00791	0.01244	-0.01001
70			2PY	0.00071	0.02394	0.00420	-0.00615	0.00382
71			2PZ	0.00310	-0.00392	0.00170	-0.00160	0.00048
72			3S	0.00662	-0.00315	0.00201	-0.00795	0.00109
73			3PX	0.00764	-0.05694	-0.00835	0.01474	-0.02401
74			3PY	-0.00006	0.01799	0.00757	-0.00176	0.00735
75			3PZ	0.00262	-0.00195	-0.00262	-0.00610	-0.00049
76			4D 0	0.00069	-0.00004	0.00008	-0.00063	-0.00102
77			4D+1	0.00587	0.00225	0.00069	-0.00479	-0.02308
78			4D-1	-0.00239	-0.00078	-0.00028	0.00218	0.00858
79			4D+2	0.00046	-0.00058	0.00001	-0.00040	-0.00001
80			4D-2	0.00051	-0.00049	0.00015	-0.00022	-0.00110
81	7	C	1S	-0.00033	0.00031	-0.00065	0.00038	-0.00008
82			2S	0.00047	-0.00028	0.00141	-0.00091	-0.00058
83			2PX	-0.08433	-0.03127	-0.00667	0.04892	0.25029
84			2PY	0.03082	0.01173	0.00450	-0.01876	-0.09537

85		2PZ	-0.00175	-0.00129	-0.00038	0.00081	0.00762
86		3S	0.00291	-0.00141	0.00148	-0.00432	0.00485
87		3PX	-0.06923	-0.03228	-0.00723	0.06030	0.30945
88		3PY	0.02643	0.01111	0.00572	-0.02225	-0.11538
89		3PZ	-0.00185	-0.00209	-0.00209	0.00116	0.01013
90		4D 0	0.00015	-0.00021	-0.00006	-0.00013	-0.00003
91		4D+1	0.00075	-0.00255	-0.00032	0.00052	-0.00135
92		4D-1	-0.00030	0.00114	0.00007	0.00003	0.00020
93		4D+2	-0.00094	0.00301	0.00052	-0.00220	-0.00707
94		4D-2	-0.00104	0.00329	0.00062	-0.00229	-0.00806
95	8 H	1S	0.00002	-0.00034	-0.00206	-0.00151	0.00132
96		2S	0.00054	-0.00064	-0.00392	-0.00761	0.00243
97	9 H	1S	-0.00246	0.00130	-0.00018	0.00196	-0.00058
98		2S	-0.00312	0.00043	0.00098	0.00797	-0.00231
99	10 H	1S	0.00044	0.00006	-0.00027	0.00074	-0.00014
100		2S	0.00069	-0.00046	-0.00159	0.00265	0.00058
101	11 C	1S	0.01651	0.01916	-0.00083	0.00262	0.01337
102		2S	-0.02728	-0.03516	0.00103	-0.00752	-0.02311
103		2PX	0.10783	0.08080	-0.00442	0.04867	0.04324
104		2PY	-0.02484	-0.08790	-0.00522	0.12285	-0.03242
105		2PZ	-0.01227	0.05634	-0.00148	-0.05320	0.02036
106		3S	-0.07049	-0.03729	-0.00042	-0.00423	-0.08794
107		3PX	0.09028	0.12315	-0.01685	0.05769	0.06848
108		3PY	-0.02425	-0.09833	0.00124	0.11379	-0.04743
109		3PZ	0.00147	0.01852	-0.00631	-0.03843	0.03675
110		4D 0	-0.00289	0.00306	-0.00068	0.00327	-0.00077
111		4D+1	-0.00991	0.00508	-0.00164	-0.00334	0.00004
112		4D-1	0.00360	-0.00289	0.00030	-0.00332	0.00082
113		4D+2	0.00060	-0.00655	-0.00025	0.00332	-0.00171
114		4D-2	-0.00401	-0.00952	-0.00075	0.00321	-0.00199
115	12 C	1S	0.00369	-0.00565	0.00127	0.00020	-0.00035
116		2S	-0.00704	0.01381	-0.00334	-0.00077	-0.00278
117		2PX	0.00014	-0.05460	0.00254	-0.02526	0.00361
118		2PY	0.02178	-0.10311	0.00453	-0.07273	0.00754
119		2PZ	0.01440	0.01162	0.00741	0.03272	-0.01105
120		3S	-0.03971	-0.00126	-0.00157	-0.00781	-0.00370
121		3PX	-0.03563	-0.08092	0.00863	-0.02782	-0.00359
122		3PY	0.03117	-0.05636	-0.00145	-0.07205	0.01929
123		3PZ	0.00705	0.05000	-0.00651	0.04856	0.00633
124		4D 0	0.00224	0.00014	-0.00027	0.00863	-0.00116
125		4D+1	-0.00353	-0.00361	0.00069	-0.00857	0.00001
126		4D-1	0.00172	0.00391	0.00008	-0.00826	0.00226
127		4D+2	-0.00180	-0.00217	-0.00029	0.01158	-0.00359

128		4D-2	-0.00107	0.00147	-0.00009	0.00647	-0.00191
129	13 C	1S	-0.01381	-0.00334	-0.00172	0.00009	-0.00342
130		2S	0.03222	0.01334	0.00374	-0.00251	0.00703
131		2PX	-0.05625	-0.05465	-0.00450	0.01813	-0.01532
132		2PY	0.04681	-0.07630	0.00186	0.04863	-0.00932
133		2PZ	0.03217	0.04557	0.00216	-0.02074	0.01738
134		3S	0.01694	-0.06991	0.01312	-0.00093	-0.00232
135		3PX	-0.03136	-0.02752	-0.00244	0.01468	-0.03627
136		3PY	0.02319	-0.09474	0.00001	0.07149	-0.01039
137		3PZ	0.00038	-0.01166	0.00778	-0.03494	-0.00205
138		4D 0	0.00338	0.00527	0.00019	-0.00203	0.00217
139		4D+1	-0.00064	-0.00080	-0.00040	0.00552	-0.00012
140		4D-1	0.00213	0.00025	0.00009	0.00017	0.00060
141		4D+2	-0.00379	-0.00084	0.00011	-0.00843	0.00057
142		4D-2	0.00147	0.00366	0.00034	-0.00859	0.00235
143	14 C	1S	0.00098	0.00444	-0.00051	-0.00013	0.00156
144		2S	-0.00526	-0.01333	0.00182	-0.00140	-0.00505
145		2PX	0.01647	0.03589	-0.00334	0.04733	-0.00271
146		2PY	-0.01078	0.02389	-0.00482	0.13773	-0.03238
147		2PZ	0.00038	-0.00455	0.00120	-0.05952	0.01436
148		3S	0.04277	0.02880	-0.00390	0.00870	0.00566
149		3PX	-0.00841	0.00645	-0.00154	0.04909	-0.00482
150		3PY	-0.01167	0.00749	-0.00301	0.13234	-0.03810
151		3PZ	-0.02237	-0.04364	0.01015	-0.06736	-0.00132
152		4D 0	-0.00008	0.00239	-0.00022	0.00059	0.00037
153		4D+1	-0.00005	-0.00142	-0.00046	-0.00218	0.00092
154		4D-1	0.00058	0.00012	-0.00002	0.00009	0.00014
155		4D+2	-0.00028	0.00545	-0.00015	0.00348	-0.00021
156		4D-2	-0.00117	0.00613	-0.00026	0.00410	-0.00028
157	15 C	1S	0.00746	0.00454	0.00046	0.00002	0.00194
158		2S	-0.01985	-0.01317	-0.00085	-0.00027	-0.00725
159		2PX	0.04074	0.03602	0.00351	-0.05369	0.01992
160		2PY	-0.01863	0.01976	0.00502	-0.15634	0.02899
161		2PZ	0.00512	-0.00508	-0.00230	0.06926	-0.01151
162		3S	0.00208	0.01831	-0.00652	0.00726	0.01956
163		3PX	0.00748	0.00828	0.00429	-0.06511	0.00134
164		3PY	0.00419	0.03556	0.00477	-0.17290	0.04147
165		3PZ	0.02735	0.03090	-0.00507	0.07820	-0.00317
166		4D 0	-0.00007	-0.00341	-0.00005	-0.00076	-0.00054
167		4D+1	-0.00251	-0.00184	-0.00010	0.00156	-0.00126
168		4D-1	0.00068	0.00512	-0.00003	0.00037	0.00067
169		4D+2	0.00018	0.00211	0.00006	-0.00228	0.00119
170		4D-2	-0.00239	0.00445	-0.00004	-0.00253	0.00020

171	16	H	1S	0.00705	0.01457	-0.00025	-0.00091	0.00569
172			2S	0.01312	0.00191	0.00170	-0.00258	0.00009
173	17	C	1S	0.00067	0.00133	-0.00031	0.00026	0.00105
174			2S	0.00149	0.00002	0.00054	-0.00057	-0.00156
175			2PX	-0.01110	0.03567	-0.00081	0.00548	0.00221
176			2PY	-0.00906	0.10880	0.00036	0.01378	0.00440
177			2PZ	0.01266	-0.05130	0.00098	-0.00673	-0.00046
178			3S	-0.04049	-0.06020	0.00852	-0.00883	-0.02582
179			3PX	0.01923	0.06041	-0.00323	0.01454	0.01274
180			3PY	-0.01391	0.08514	0.00067	0.02715	-0.00213
181			3PZ	0.01583	-0.03025	0.00020	-0.01543	-0.00042
182			4D 0	0.00058	0.00059	0.00027	-0.00837	0.00184
183			4D+1	-0.00135	-0.00045	-0.00027	0.00453	-0.00114
184			4D-1	0.00057	0.00030	-0.00024	0.00851	-0.00169
185			4D+2	-0.00111	-0.00120	0.00016	-0.00594	0.00123
186			4D-2	0.00019	0.00026	-0.00006	0.00030	0.00009
187	18	H	1S	0.00021	0.01252	-0.00200	0.00043	0.00328
188			2S	0.00648	0.03661	-0.00871	0.00246	0.01538
189	19	H	1S	0.02099	0.00966	0.00066	0.00079	0.00522
190			2S	0.04450	0.02974	0.00081	0.00230	0.02131
191	20	H	1S	-0.00848	-0.00663	-0.00032	0.00012	-0.00086
192			2S	-0.01925	-0.01677	-0.00072	-0.00021	-0.00173
193	21	C	1S	0.00378	-0.00009	-0.00016	-0.00040	0.00070
194			2S	-0.00974	-0.00155	-0.00027	-0.00158	-0.00184
195			2PX	0.00708	0.03196	-0.00860	0.00870	0.01131
196			2PY	0.00249	-0.00180	-0.04541	0.00466	0.01012
197			2PZ	-0.01638	0.00361	-0.13990	0.02168	0.02911
198			3S	0.00908	0.02764	0.00738	0.00808	-0.00274
199			3PX	-0.01719	0.02369	-0.00665	0.00291	-0.00051
200			3PY	-0.00531	-0.02856	-0.05315	0.01049	0.00317
201			3PZ	-0.00695	0.01513	-0.14450	0.02162	0.02644
202			4D 0	0.00266	-0.00069	-0.00217	-0.00085	-0.00270
203			4D+1	-0.00953	0.00110	0.01220	-0.00101	-0.00240
204			4D-1	-0.00331	-0.00048	0.00083	0.00158	0.00457
205			4D+2	0.00114	-0.00094	0.00015	0.00221	-0.00200
206			4D-2	-0.00396	-0.00030	0.00428	0.00070	-0.00018
207	22	C	1S	-0.00130	0.00308	-0.00034	0.00131	0.00086
208			2S	0.00291	-0.00943	0.00077	-0.00269	-0.00153
209			2PX	0.00206	0.03055	-0.00150	-0.02088	0.01339
210			2PY	0.00575	0.00436	-0.00438	0.01157	0.01789
211			2PZ	0.03468	0.00059	-0.01028	0.00798	0.05702
212			3S	0.00957	-0.01108	0.00261	-0.02476	0.00426
213			3PX	0.00377	0.04233	0.00002	-0.03996	0.01309

214		3PY	0.01265	0.00801	-0.00066	0.01004	0.02759
215		3PZ	0.01969	-0.00211	-0.00069	-0.00395	0.06535
216		4D 0	-0.00276	0.00011	0.00585	-0.00129	-0.00142
217		4D+1	0.00476	-0.00043	-0.00875	0.00160	0.00354
218		4D-1	0.00357	-0.00048	-0.00762	0.00161	0.00092
219		4D+2	-0.00026	-0.00118	0.00236	0.00021	-0.00066
220		4D-2	0.00113	-0.00049	-0.00346	-0.00156	0.00186
221	23 C	1S	-0.00057	-0.00054	-0.00024	0.00218	-0.00038
222		2S	0.00102	0.00070	0.00067	-0.00536	0.00073
223		2PX	-0.00637	-0.00376	0.00491	0.00145	0.00230
224		2PY	-0.02596	-0.00140	0.02415	0.00796	0.01395
225		2PZ	-0.07901	0.00523	0.07761	-0.00197	0.04800
226		3S	0.00380	0.01184	0.00362	-0.01415	0.00431
227		3PX	-0.00049	-0.00638	0.00567	0.00894	0.00630
228		3PY	-0.02322	-0.00792	0.02422	0.00782	0.01639
229		3PZ	-0.06675	0.00639	0.07924	-0.00154	0.06306
230		4D 0	-0.00021	0.00007	-0.00508	0.00073	0.00196
231		4D+1	-0.00091	0.00032	0.00589	-0.00080	-0.00336
232		4D-1	0.00048	-0.00030	0.00683	-0.00148	-0.00243
233		4D+2	-0.00014	-0.00037	-0.00214	0.00014	0.00048
234		4D-2	-0.00068	-0.00134	0.00248	-0.00139	-0.00177
235	24 C	1S	0.00108	-0.00153	0.00001	0.00126	-0.00064
236		2S	-0.00189	0.00339	-0.00037	-0.00344	0.00212
237		2PX	0.00581	-0.00408	-0.00834	0.00066	0.00069
238		2PY	0.03152	-0.00765	-0.04361	0.00911	0.00053
239		2PZ	0.08067	-0.00322	-0.13401	0.01427	0.00884
240		3S	-0.01356	0.00118	0.00078	-0.00355	-0.00338
241		3PX	0.00529	-0.00677	-0.01082	-0.00136	0.00576
242		3PY	0.02971	0.00172	-0.05101	0.00925	0.00580
243		3PZ	0.07035	-0.00521	-0.15662	0.02339	0.01170
244		4D 0	0.00078	0.00028	-0.00151	0.00041	0.00285
245		4D+1	0.00046	0.00047	-0.00367	0.00009	0.00232
246		4D-1	-0.00133	-0.00030	0.00313	-0.00118	-0.00462
247		4D+2	0.00053	-0.00055	-0.00134	0.00117	0.00166
248		4D-2	-0.00003	-0.00109	-0.00096	0.00155	-0.00021
249	25 H	1S	0.00414	0.00187	-0.00005	0.00541	-0.00083
250		2S	0.00375	-0.03042	-0.00163	0.05799	-0.00628
251	26 C	1S	-0.00006	0.00019	0.00014	0.00203	-0.00004
252		2S	-0.00038	-0.00127	0.00000	-0.00452	-0.00030
253		2PX	0.00138	0.00774	0.00598	-0.00370	-0.00196
254		2PY	-0.00326	-0.00141	0.02985	-0.00458	-0.02288
255		2PZ	-0.00852	-0.00504	0.09126	-0.02262	-0.06968
256		3S	-0.00118	-0.00011	-0.00267	-0.01807	0.00148

257			3PX	0.00080	-0.00102	0.00758	-0.00293	-0.00365
258			3PY	-0.00643	-0.00244	0.03683	-0.00868	-0.03026
259			3PZ	-0.01092	-0.00288	0.10970	-0.02727	-0.08654
260			4D 0	-0.00021	-0.00006	-0.00081	0.00013	0.00102
261			4D+1	0.00582	-0.00036	-0.00884	0.00059	-0.00203
262			4D-1	-0.00089	-0.00013	0.00299	-0.00077	-0.00122
263			4D+2	0.00081	-0.00031	-0.00161	-0.00003	0.00029
264			4D-2	0.00189	-0.00013	-0.00263	0.00005	-0.00077
265	27	H	1S	0.00046	0.00422	0.00018	0.00399	0.00090
266			2S	0.00278	0.01002	0.00062	0.01474	0.00314
267	28	H	1S	0.00066	-0.00607	-0.00010	0.00601	-0.00208
268			2S	0.00160	-0.00942	0.00038	0.01950	-0.00837
269	29	H	1S	-0.00045	0.00153	0.00029	0.00120	0.00024
270			2S	0.00057	0.00406	0.00039	0.00926	0.00095
271	30	C	1S	-0.01699	-0.02004	0.00019	-0.00355	-0.01308
272			2S	0.03088	0.03113	0.00000	0.00559	0.02412
273			2PX	0.09441	0.10759	0.00549	0.01137	0.04462
274			2PY	-0.00683	-0.04387	0.03848	-0.01517	-0.03224
275			2PZ	0.15339	-0.00235	0.10094	-0.00575	-0.00620
276			3S	0.02532	0.10638	-0.00175	0.02041	0.08366
277			3PX	0.13572	0.08371	0.01034	0.00735	0.06166
278			3PY	-0.00548	-0.05381	0.04110	-0.02379	-0.03157
279			3PZ	0.10223	0.00748	0.09906	0.00498	0.00805
280			4D 0	-0.00322	0.00297	0.00559	0.00046	-0.00005
281			4D+1	-0.01131	0.00373	-0.00878	-0.00183	-0.00156
282			4D-1	0.00972	-0.00257	-0.00551	0.00037	-0.00115
283			4D+2	-0.00375	-0.00854	0.00168	0.00226	-0.00140
284			4D-2	-0.00402	-0.00381	-0.00354	0.00127	-0.00113
285	31	C	1S	0.00462	0.01150	0.00059	-0.00209	0.00178
286			2S	-0.01605	-0.02821	-0.00299	0.00433	-0.00448
287			2PX	-0.02589	-0.06935	0.00889	0.00618	-0.01243
288			2PY	0.03962	-0.02734	0.05205	0.00549	-0.00402
289			2PZ	0.10062	0.00233	0.14131	0.01536	0.03011
290			3S	0.06922	0.00361	0.00588	0.00950	0.02507
291			3PX	0.01674	-0.05952	0.01064	-0.00305	-0.02382
292			3PY	0.07379	-0.00360	0.05440	-0.00267	-0.00479
293			3PZ	0.06273	-0.00463	0.13179	0.01475	0.01691
294			4D 0	-0.00267	-0.00115	-0.00132	0.00026	-0.00073
295			4D+1	0.00759	0.00079	0.00995	-0.00048	-0.00097
296			4D-1	0.00238	0.00061	0.00047	0.00042	0.00114
297			4D+2	0.00421	0.00385	0.00046	0.00030	0.00196
298			4D-2	-0.00075	-0.00445	0.00373	-0.00017	-0.00160
299	32	C	1S	0.00523	-0.00273	0.00018	0.00123	0.00046

300		2S	-0.01312	0.00388	0.00002	-0.00287	0.00018
301		2PX	0.00132	-0.01008	-0.00725	0.00595	-0.00010
302		2PY	0.09672	-0.01437	-0.05338	0.01354	-0.00005
303		2PZ	0.16363	-0.01035	-0.14657	-0.00880	-0.00671
304		3S	0.00444	0.03868	-0.00242	0.00110	-0.00160
305		3PX	-0.05101	-0.03849	-0.01262	0.00177	-0.01142
306		3PY	0.05757	-0.00627	-0.04631	-0.00106	-0.00492
307		3PZ	0.14336	-0.01129	-0.14194	-0.00475	-0.00440
308		4D 0	0.00300	-0.00009	0.00491	-0.00063	-0.00093
309		4D+1	0.00224	0.00188	-0.00875	0.00114	0.00193
310		4D-1	-0.00456	0.00056	-0.00555	0.00068	0.00121
311		4D+2	0.00151	-0.00106	0.00169	-0.00054	-0.00101
312		4D-2	-0.00466	-0.00478	-0.00342	-0.00098	-0.00178
313	33 C	1S	-0.00477	-0.00717	0.00021	0.00020	-0.00204
314		2S	0.01442	0.01934	0.00011	-0.00032	0.00664
315		2PX	0.01964	0.03318	-0.00735	-0.00018	0.00706
316		2PY	-0.04888	-0.01641	-0.04438	0.00125	-0.00130
317		2PZ	-0.07763	0.00943	-0.12276	0.00412	0.01359
318		3S	-0.02048	-0.01218	-0.00700	-0.00319	-0.01221
319		3PX	-0.03345	-0.02036	-0.01190	0.00208	-0.00631
320		3PY	-0.05350	-0.00927	-0.05120	0.00371	0.00724
321		3PZ	-0.04032	0.00802	-0.12590	0.00305	0.01411
322		4D 0	0.00620	0.00073	-0.00717	-0.00036	0.00011
323		4D+1	0.00329	0.00047	0.01563	0.00161	0.00294
324		4D-1	-0.00767	0.00049	0.00697	0.00030	0.00028
325		4D+2	0.00265	-0.00312	-0.00256	-0.00006	-0.00154
326		4D-2	-0.00014	-0.00160	0.00664	0.00052	0.00045
327	34 H	1S	-0.01500	-0.00539	-0.00087	-0.00215	-0.00444
328		2S	-0.00398	-0.03209	0.00436	-0.01814	-0.03687
329	35 C	1S	-0.00430	-0.00247	0.00023	-0.00140	-0.00191
330		2S	0.01343	0.00787	-0.00069	0.00350	0.00508
331		2PX	0.01881	0.01536	0.00265	0.00348	0.00541
332		2PY	-0.02995	-0.00685	0.02127	-0.00522	-0.00890
333		2PZ	-0.02988	0.00486	0.05648	-0.00527	-0.01426
334		3S	-0.03644	-0.03093	-0.00714	0.00791	0.00321
335		3PX	0.01326	0.00810	0.00302	0.00789	0.00528
336		3PY	0.02007	0.02242	0.02369	0.00255	0.00368
337		3PZ	-0.03962	-0.00537	0.05355	-0.00751	-0.01196
338		4D 0	0.00010	0.00056	0.00070	0.00006	0.00018
339		4D+1	0.01199	-0.00087	-0.01081	-0.00030	-0.00011
340		4D-1	-0.00015	0.00052	0.00079	0.00040	0.00046
341		4D+2	0.00296	-0.00009	-0.00089	0.00089	0.00047
342		4D-2	0.00484	-0.00048	-0.00385	0.00037	0.00028

343	36	C	1S	-0.00057	-0.00057	-0.00040	-0.00075	-0.00077
344			2S	-0.00147	-0.00100	0.00020	0.00166	0.00186
345			2PX	-0.01096	-0.00256	0.00663	0.00201	0.00054
346			2PY	-0.06115	0.00258	0.03787	0.00177	-0.00089
347			2PZ	-0.18411	0.01600	0.10788	0.00301	0.00419
348			3S	0.05433	0.02970	0.00922	0.00812	0.00830
349			3PX	0.02339	0.02535	0.01196	0.00216	0.00475
350			3PY	-0.06849	-0.00797	0.04262	0.00260	-0.00310
351			3PZ	-0.14039	0.01506	0.12963	0.00275	0.00186
352			4D 0	-0.00179	-0.00026	-0.00394	0.00026	0.00072
353			4D+1	-0.00030	0.00039	0.00337	-0.00022	-0.00052
354			4D-1	0.00175	-0.00014	0.00475	-0.00020	-0.00062
355			4D+2	-0.00006	0.00025	-0.00187	0.00027	0.00034
356			4D-2	-0.00137	-0.00111	0.00166	0.00003	-0.00026
357	37	H	1S	-0.01253	-0.00305	-0.00004	-0.00374	-0.00281
358			2S	-0.03410	-0.01258	-0.00067	-0.01339	-0.01491
359	38	H	1S	0.00695	0.00456	-0.00041	-0.00037	-0.00014
360			2S	0.02036	0.01760	0.00186	-0.00243	0.00024
361	39	C	1S	-0.00238	0.00282	0.00262	-0.00014	-0.00230
362			2S	0.00907	-0.00474	-0.00339	0.00102	0.00834
363			2PX	0.03847	-0.00567	0.01835	-0.02959	0.01209
364			2PY	-0.02401	-0.01666	-0.00499	-0.08209	0.02022
365			2PZ	-0.00947	0.01699	0.00436	0.03366	-0.01630
366			3S	0.00115	-0.02848	-0.03123	-0.00241	0.00830
367			3PX	0.04060	-0.00553	0.03126	-0.03047	0.00598
368			3PY	-0.02323	-0.01188	-0.02443	-0.07847	0.03159
369			3PZ	-0.01998	0.00228	0.01113	0.03061	-0.00872
370			4D 0	-0.00021	0.00268	-0.00074	0.01266	-0.00313
371			4D+1	-0.00098	-0.00117	0.00040	-0.01009	0.00214
372			4D-1	0.00015	-0.00152	0.00076	-0.01367	0.00274
373			4D+2	-0.00094	0.00159	-0.00018	0.01345	-0.00315
374			4D-2	-0.00082	0.00140	0.00041	0.00480	-0.00135
375	40	C	1S	0.00146	-0.00461	0.00088	0.00092	0.00100
376			2S	-0.00174	0.01084	-0.00347	-0.00144	-0.00466
377			2PX	0.03599	-0.00151	0.00511	-0.08794	0.03300
378			2PY	-0.02026	-0.00934	0.00831	-0.25504	0.05080
379			2PZ	-0.00092	-0.00977	-0.00194	0.10734	-0.02227
380			3S	-0.04116	0.00190	0.00571	-0.01138	-0.00761
381			3PX	0.03850	-0.02691	0.00799	-0.09803	0.01556
382			3PY	-0.01164	0.00653	0.00738	-0.25238	0.05360
383			3PZ	0.02594	0.00659	-0.00754	0.10631	-0.02038
384			4D 0	-0.00033	-0.00247	-0.00027	0.00260	-0.00084
385			4D+1	-0.00170	0.00270	-0.00080	0.00527	-0.00023

386		4D-1	-0.00021	0.00152	-0.00024	-0.00540	0.00145
387		4D+2	0.00027	-0.00449	0.00037	-0.00920	0.00174
388		4D-2	0.00034	-0.00263	-0.00044	-0.01346	0.00385
389	41 C	1S	0.00131	-0.00179	-0.00001	0.00019	0.00099
390		2S	-0.00296	0.00320	0.00046	-0.00066	-0.00175
391		2PX	-0.00248	-0.01587	0.00335	-0.06495	0.01393
392		2PY	0.00699	-0.04247	0.01020	-0.18254	0.03767
393		2PZ	0.00436	0.00991	-0.00597	0.07542	-0.01297
394		3S	0.00475	0.02014	-0.00217	0.00151	-0.00955
395		3PX	-0.00473	-0.01380	0.00131	-0.08133	0.02172
396		3PY	0.00275	-0.04060	0.01828	-0.23187	0.04685
397		3PZ	-0.00208	0.00648	-0.00627	0.09349	-0.01544
398		4D 0	-0.00012	-0.00057	0.00020	-0.00641	0.00175
399		4D+1	-0.00178	0.00001	-0.00090	-0.00170	0.00024
400		4D-1	0.00111	0.00096	0.00017	0.00927	-0.00241
401		4D+2	-0.00043	0.00020	-0.00031	0.00490	-0.00124
402		4D-2	-0.00041	0.00083	-0.00039	0.01188	-0.00305
403	42 H	1S	-0.00592	-0.00403	0.00094	0.00045	0.00186
404		2S	0.03308	0.00122	0.04574	-0.00157	-0.01192
405	43 C	1S	0.00013	0.00138	0.00075	-0.00034	-0.00076
406		2S	0.00001	-0.00309	-0.00131	0.00047	0.00177
407		2PX	-0.00402	0.01467	-0.00248	0.00146	0.00264
408		2PY	0.00168	0.04095	-0.00829	0.00268	0.00928
409		2PZ	0.00319	-0.01233	0.00548	-0.00256	-0.00621
410		3S	-0.00765	-0.00729	-0.00575	0.00527	0.00357
411		3PX	-0.00388	0.02001	-0.00277	0.00084	0.01208
412		3PY	0.00427	0.03150	-0.00916	-0.01056	0.01121
413		3PZ	0.00836	-0.01169	0.00602	0.00055	-0.01073
414		4D 0	0.00019	-0.00025	0.00036	-0.01374	0.00331
415		4D+1	-0.00129	0.00025	-0.00006	0.00875	-0.00293
416		4D-1	0.00095	0.00048	-0.00048	0.01525	-0.00321
417		4D+2	-0.00083	-0.00092	0.00022	-0.01166	0.00236
418		4D-2	-0.00021	-0.00045	-0.00006	-0.00152	0.00042
419	44 C	1S	0.00034	0.00015	0.00120	-0.00024	-0.00051
420		2S	0.00036	0.00032	-0.00255	0.00027	0.00145
421		2PX	0.01299	0.00634	0.00201	0.08492	-0.01993
422		2PY	0.00130	0.01096	-0.00486	0.23797	-0.05967
423		2PZ	-0.00407	-0.00503	0.00285	-0.09846	0.02335
424		3S	-0.00578	0.00119	-0.00436	0.00352	0.00512
425		3PX	0.00572	0.00873	0.00021	0.10529	-0.02262
426		3PY	0.00456	0.01282	-0.00670	0.29183	-0.07442
427		3PZ	0.00102	-0.00289	0.00084	-0.11963	0.03012
428		4D 0	-0.00010	0.00030	0.00018	-0.00313	0.00081

429		4D+1	-0.00018	-0.00108	0.00055	-0.00231	-0.00004
430		4D-1	0.00000	-0.00006	-0.00003	0.00492	-0.00126
431		4D+2	-0.00023	0.00211	-0.00057	0.00471	-0.00067
432		4D-2	-0.00016	0.00243	-0.00054	0.00868	-0.00155
433	45 H	1S	0.00917	-0.00098	0.00322	0.00001	0.00077
434		2S	0.01367	-0.00175	0.00554	0.00045	0.00367
435	46 H	1S	-0.00611	0.00034	0.00032	-0.00080	-0.00287
436		2S	-0.01302	-0.00281	0.00101	-0.00494	-0.01043
437	47 H	1S	-0.00075	0.00023	0.00128	-0.00041	-0.00061
438		2S	-0.00267	-0.00114	0.00506	-0.00179	-0.00355
439	48 C	1S	-0.00194	0.00196	0.00040	-0.00531	0.00118
440		2S	0.00339	-0.00438	0.00008	0.01005	-0.00096
441		2PX	-0.01500	0.11686	-0.00749	0.04212	0.12403
442		2PY	0.01157	-0.05451	-0.00029	-0.00272	-0.05211
443		2PZ	0.00379	0.00271	-0.00433	-0.00097	0.00599
444		3S	0.00662	0.00697	-0.00709	0.06221	-0.01534
445		3PX	-0.00763	0.07217	-0.00445	0.03632	0.11603
446		3PY	0.01654	-0.05787	-0.00532	0.02933	-0.05447
447		3PZ	-0.01791	0.01819	-0.00388	0.02068	0.00210
448		4D 0	0.00104	-0.00018	-0.00073	-0.00117	0.00124
449		4D+1	0.00366	0.00366	0.00046	0.00146	0.00638
450		4D-1	-0.00357	-0.00061	0.00175	-0.00015	-0.00396
451		4D+2	-0.00067	-0.01254	-0.00032	-0.00163	-0.00258
452		4D-2	-0.00017	-0.01381	0.00036	0.00225	-0.00273
453	49 C	1S	-0.00178	0.00107	0.00187	0.00110	-0.00129
454		2S	0.00278	0.00023	-0.00590	0.00109	0.00355
455		2PX	0.05129	0.14696	-0.00284	0.00910	0.06646
456		2PY	-0.01602	-0.05752	-0.00364	-0.00286	-0.02313
457		2PZ	-0.00539	0.00763	0.00449	0.00672	-0.00343
458		3S	0.02694	-0.03059	-0.00274	-0.02113	0.00673
459		3PX	0.03624	0.12273	-0.00900	0.00651	0.08634
460		3PY	-0.01319	-0.04388	0.00299	-0.04054	-0.02280
461		3PZ	-0.01076	0.02424	0.00213	0.01603	0.00078
462		4D 0	0.00031	-0.00033	-0.00019	0.00055	-0.00032
463		4D+1	0.00101	-0.00469	0.00038	-0.00196	-0.00707
464		4D-1	-0.00077	0.00235	-0.00026	0.00095	0.00330
465		4D+2	-0.00137	0.00177	-0.00061	0.00263	0.00663
466		4D-2	-0.00135	0.00134	-0.00038	0.00170	0.00716
467	50 C	1S	0.00179	-0.00116	-0.00161	-0.00128	0.00089
468		2S	-0.00291	0.00380	0.00616	0.00632	-0.00211
469		2PX	-0.02408	0.16080	0.00207	-0.02052	-0.06621
470		2PY	0.00197	-0.05567	0.00521	0.01234	0.02244
471		2PZ	-0.00657	0.01019	0.00620	0.00270	-0.00481

472		3S	-0.01254	-0.00575	0.00115	0.00847	-0.00607
473		3PX	-0.02412	0.13388	0.00890	-0.02100	-0.06996
474		3PY	-0.00607	-0.03937	0.00692	0.02263	0.02376
475		3PZ	0.00204	-0.01181	0.00004	0.01503	-0.00478
476		4D 0	-0.00011	0.00037	0.00036	0.00054	0.00094
477		4D+1	-0.00321	0.00242	-0.00072	0.00424	0.01690
478		4D-1	0.00128	-0.00094	0.00012	-0.00144	-0.00666
479		4D+2	0.00118	0.00360	0.00036	-0.00120	-0.00491
480		4D-2	0.00173	0.00351	0.00039	-0.00091	-0.00452
481	51 C	1S	0.00051	0.00005	-0.00054	0.00048	0.00034
482		2S	-0.00047	-0.00025	0.00132	0.00027	-0.00110
483		2PX	0.04710	-0.04172	0.01146	-0.04346	-0.16019
484		2PY	-0.01949	0.01540	-0.00221	0.01555	0.05983
485		2PZ	0.00311	-0.00194	-0.00036	-0.00231	-0.00504
486		3S	-0.00923	0.00966	0.00352	-0.02347	0.00398
487		3PX	0.03761	-0.02820	0.01292	-0.05407	-0.17566
488		3PY	-0.01730	0.01078	-0.00490	0.00701	0.06867
489		3PZ	0.00667	-0.01109	-0.00011	-0.00291	-0.00880
490		4D 0	0.00015	0.00024	-0.00003	-0.00016	-0.00003
491		4D+1	0.00042	0.00391	0.00013	-0.00044	-0.00214
492		4D-1	-0.00034	-0.00107	0.00017	0.00077	0.00061
493		4D+2	0.00169	0.00764	0.00001	0.00024	0.00274
494		4D-2	0.00174	0.00886	-0.00009	0.00016	0.00299
495	52 H	1S	-0.00083	0.00113	-0.00061	0.00115	0.00076
496		2S	-0.00291	-0.00730	-0.00228	0.01940	-0.00997
497	53 C	1S	-0.00085	0.00076	0.00057	0.00032	-0.00034
498		2S	0.00206	-0.00196	-0.00154	-0.00035	0.00085
499		2PX	-0.05575	-0.05941	-0.01097	0.03679	0.14551
500		2PY	0.02499	0.01924	0.00214	-0.01431	-0.05507
501		2PZ	-0.00128	-0.00209	-0.00064	0.00133	0.00484
502		3S	-0.00466	0.00875	0.00337	-0.00015	0.00241
503		3PX	-0.04237	-0.04214	-0.01055	0.03949	0.14469
504		3PY	0.01445	0.02166	0.00753	-0.00997	-0.05530
505		3PZ	-0.00496	0.00701	0.00319	-0.00262	0.00414
506		4D 0	0.00003	-0.00052	-0.00011	-0.00005	0.00022
507		4D+1	-0.00076	-0.00719	0.00013	0.00085	0.00209
508		4D-1	-0.00015	0.00352	0.00035	-0.00022	-0.00110
509		4D+2	-0.00016	0.00674	-0.00016	-0.00105	-0.00261
510		4D-2	-0.00033	0.00743	0.00015	-0.00097	-0.00283
511	54 C	1S	-0.00015	0.00023	0.00021	-0.00033	0.00009
512		2S	-0.00023	0.00048	-0.00040	0.00111	-0.00007
513		2PX	-0.01757	-0.18366	0.00038	0.00786	0.00035
514		2PY	0.00638	0.07042	-0.00043	-0.00167	-0.00046

515		2PZ	-0.00203	-0.00528	0.00095	0.00240	-0.00099
516		3S	0.00720	-0.01494	-0.00423	0.00181	-0.00190
517		3PX	-0.01420	-0.15389	-0.00046	0.01163	0.01385
518		3PY	0.01024	0.05024	-0.00135	-0.00417	-0.00661
519		3PZ	-0.00188	-0.00444	-0.00011	-0.00278	0.00011
520		4D 0	0.00028	0.00000	-0.00004	-0.00015	-0.00070
521		4D+1	0.00344	0.00082	0.00083	-0.00322	-0.01270
522		4D-1	-0.00145	-0.00024	-0.00017	0.00124	0.00472
523		4D+2	0.00016	-0.00025	0.00002	-0.00028	-0.00094
524		4D-2	0.00044	-0.00047	0.00014	-0.00064	-0.00172
525	55 H	1S	0.00146	-0.00013	-0.00096	-0.00166	0.00110
526		2S	0.00101	0.00179	-0.00254	-0.00269	0.00391
527	56 H	1S	-0.00225	0.00205	0.00175	0.00091	-0.00070
528		2S	-0.00484	0.00656	0.00654	0.00225	-0.00191
529	57 H	1S	0.00023	-0.00055	0.00024	-0.00047	-0.00004
530		2S	0.00171	-0.00295	0.00072	-0.00171	-0.00009
531	58 N	1S	-0.00078	-0.00248	0.00018	0.01180	-0.00239
532		2S	0.00123	0.00544	0.00013	-0.02542	0.00440
533		2PX	-0.00568	-0.01781	0.00978	0.00658	-0.00722
534		2PY	-0.02022	-0.00790	0.04478	0.03909	-0.02963
535		2PZ	-0.08076	0.01318	0.14054	-0.03141	-0.06495
536		3S	0.01227	0.01210	-0.00563	-0.08882	0.02358
537		3PX	-0.00813	0.02203	0.01175	0.00409	-0.01211
538		3PY	-0.01463	-0.00754	0.04291	0.04506	-0.03223
539		3PZ	-0.07032	0.00728	0.14568	-0.02258	-0.07186
540		4D 0	0.00145	0.00003	-0.00121	-0.00055	-0.00015
541		4D+1	0.00103	0.00243	0.00621	-0.00047	0.00232
542		4D-1	-0.00314	0.00129	0.00033	0.00011	-0.00036
543		4D+2	0.00119	-0.00245	0.00022	-0.00307	-0.00015
544		4D-2	0.00168	-0.00605	0.00227	0.00145	-0.00141
545	59 N	1S	-0.00337	0.00190	-0.00410	-0.00003	0.00094
546		2S	0.00798	-0.00406	0.00778	0.00029	-0.00158
547		2PX	0.05433	-0.06787	-0.00706	0.05745	0.28718
548		2PY	-0.00976	0.02027	0.00908	-0.02411	-0.10932
549		2PZ	0.01114	-0.00556	0.01152	0.00680	0.00559
550		3S	0.01786	-0.01356	0.04457	-0.00190	-0.01460
551		3PX	0.04140	-0.05813	0.00054	0.05465	0.29487
552		3PY	-0.01041	0.02746	0.00130	-0.02794	-0.12021
553		3PZ	0.01266	-0.00491	0.01437	0.00251	0.00837
554		4D 0	0.00106	-0.00132	-0.00049	-0.00382	0.00037
555		4D+1	-0.01261	-0.00065	-0.00031	-0.00052	-0.00510
556		4D-1	0.00325	0.00125	0.00033	0.00209	0.00134
557		4D+2	-0.00466	0.00108	-0.00167	-0.00003	0.00559

558		4D-2	-0.00606	0.00151	0.00033	0.00278	0.00474
559	60 N	1S	0.00266	0.00082	0.00381	-0.00137	-0.00159
560		2S	-0.00427	-0.00092	-0.00780	0.00254	0.00327
561		2PX	-0.02145	0.01670	0.00135	0.09542	-0.02922
562		2PY	0.00231	0.04211	0.00390	0.26860	-0.06508
563		2PZ	0.02188	-0.02216	0.01530	-0.11534	0.02123
564		3S	-0.01800	-0.01552	-0.03551	0.01069	0.01179
565		3PX	0.02016	-0.00212	0.00543	0.09625	-0.03630
566		3PY	-0.01344	0.04068	0.01178	0.27711	-0.07031
567		3PZ	0.01783	-0.02233	0.00788	-0.12130	0.01905
568		4D 0	0.00307	-0.00121	0.00035	-0.00071	0.00088
569		4D+1	-0.00813	0.00148	-0.00082	0.00247	-0.00398
570		4D-1	0.00299	-0.00027	0.00087	-0.00027	0.00121
571		4D+2	-0.00263	0.00184	-0.00088	-0.00604	0.00017
572		4D-2	-0.00272	0.00225	0.00102	-0.00615	0.00018
573	61 N	1S	0.00246	0.00437	-0.00037	-0.00003	0.00171
574		2S	-0.00358	-0.00930	0.00108	-0.00010	-0.00412
575		2PX	-0.00795	-0.01891	-0.01284	-0.00125	-0.00798
576		2PY	0.01015	-0.00882	-0.10335	-0.00979	-0.01826
577		2PZ	0.03119	0.00299	-0.26113	-0.02451	-0.03801
578		3S	-0.03558	-0.03479	0.00004	0.00250	-0.01079
579		3PX	-0.00793	-0.01119	-0.01324	-0.00120	-0.00337
580		3PY	0.00132	-0.01223	-0.09524	-0.00831	-0.01844
581		3PZ	0.02635	0.00424	-0.23978	-0.02393	-0.03759
582		4D 0	-0.00014	-0.00049	0.00460	0.00032	0.00025
583		4D+1	-0.00451	0.00075	-0.01621	-0.00059	-0.00056
584		4D-1	0.00073	0.00047	-0.00373	-0.00034	-0.00040
585		4D+2	0.00041	0.00150	0.00090	0.00017	0.00092
586		4D-2	-0.00273	-0.00162	-0.00656	-0.00024	-0.00070
587	62 N	1S	-0.00126	-0.00284	0.00029	-0.00001	-0.00089
588		2S	0.00280	0.00652	-0.00069	0.00012	0.00205
589		2PX	0.01009	0.01172	0.01390	0.00088	0.00459
590		2PY	0.02178	-0.00010	0.11197	0.00727	0.00945
591		2PZ	0.06004	-0.00363	0.28384	0.01812	0.02672
592		3S	0.01287	0.02073	-0.00227	-0.00130	0.00865
593		3PX	0.00472	0.00362	0.01313	0.00083	0.00118
594		3PY	0.01247	-0.00194	0.10226	0.00755	0.00803
595		3PZ	0.04119	-0.00122	0.25811	0.01698	0.02650
596		4D 0	0.00198	0.00026	0.00486	0.00028	0.00047
597		4D+1	0.00203	0.00033	-0.01383	-0.00145	-0.00228
598		4D-1	-0.00272	0.00008	-0.00413	-0.00009	-0.00016
599		4D+2	0.00093	-0.00094	0.00144	-0.00002	-0.00045
600		4D-2	0.00008	-0.00076	-0.00579	-0.00059	-0.00112

601	63	C	1S	0.00068	0.00165	-0.00011	0.00000	0.00052
602			2S	-0.00146	-0.00368	-0.00007	-0.00013	-0.00133
603			2PX	-0.00567	-0.00902	0.00341	0.00038	-0.00168
604			2PY	-0.01390	-0.00306	0.03014	0.00419	0.00632
605			2PZ	-0.03057	0.00275	0.07262	0.01031	0.01842
606			3S	-0.00446	-0.01164	0.00280	0.00119	-0.00382
607			3PX	-0.00542	-0.00473	0.00414	0.00102	-0.00142
608			3PY	-0.01162	-0.00671	0.03630	0.00450	0.00326
609			3PZ	-0.01418	0.00328	0.08834	0.01163	0.02204
610			4D 0	-0.00142	0.00009	-0.00869	-0.00070	-0.00110
611			4D+1	0.00363	-0.00001	0.01547	0.00100	0.00151
612			4D-1	0.00138	0.00002	0.00864	0.00069	0.00115
613			4D+2	-0.00042	0.00010	-0.00344	-0.00028	-0.00038
614			4D-2	0.00123	-0.00043	0.00674	0.00048	0.00057
615	64	C	1S	-0.00041	-0.00059	-0.00021	-0.00001	-0.00024
616			2S	0.00090	0.00111	0.00048	0.00001	0.00043
617			2PX	0.00079	0.00345	-0.00491	-0.00035	0.00036
618			2PY	-0.01425	-0.00070	-0.05151	-0.00366	-0.00602
619			2PZ	-0.03281	0.00168	-0.12602	-0.00899	-0.01339
620			3S	0.00115	0.00461	0.00123	0.00035	0.00257
621			3PX	0.00219	0.00490	-0.00617	-0.00060	0.00146
622			3PY	-0.01118	-0.00112	-0.04758	-0.00357	-0.00568
623			3PZ	-0.02898	0.00170	-0.11730	-0.00855	-0.01292
624			4D 0	-0.00036	0.00002	-0.00083	-0.00004	-0.00005
625			4D+1	-0.00132	0.00014	0.00621	0.00081	0.00144
626			4D-1	0.00056	-0.00013	0.00034	-0.00005	-0.00014
627			4D+2	-0.00044	-0.00024	0.00003	0.00004	0.00000
628			4D-2	-0.00065	-0.00018	0.00255	0.00033	0.00051
629	65	C	1S	0.00003	-0.00005	0.00016	0.00002	0.00006
630			2S	0.00005	0.00016	-0.00035	-0.00005	-0.00008
631			2PX	-0.00087	0.00064	-0.00598	-0.00056	-0.00090
632			2PY	-0.01371	0.00149	-0.05612	-0.00466	-0.00756
633			2PZ	-0.03282	0.00092	-0.13433	-0.01139	-0.01834
634			3S	-0.00149	-0.00084	-0.00136	-0.00031	-0.00271
635			3PX	-0.00012	-0.00093	-0.00643	-0.00055	0.00014
636			3PY	-0.01405	-0.00119	-0.06341	-0.00637	-0.01180
637			3PZ	-0.02537	0.00188	-0.15202	-0.01383	-0.02215
638			4D 0	0.00097	-0.00007	-0.00195	-0.00031	-0.00056
639			4D+1	0.00001	0.00011	0.00102	0.00009	0.00017
640			4D-1	-0.00113	0.00005	0.00217	0.00037	0.00067
641			4D+2	0.00062	0.00004	-0.00103	-0.00017	-0.00028
642			4D-2	-0.00022	-0.00029	0.00057	0.00005	-0.00002
643	66	C	1S	0.00024	0.00043	0.00008	0.00001	0.00018

644		2S	-0.00059	-0.00093	-0.00014	-0.00002	-0.00037
645		2PX	-0.00076	-0.00214	-0.00218	-0.00031	-0.00100
646		2PY	0.00453	-0.00089	-0.01746	-0.00249	-0.00471
647		2PZ	0.01222	0.00002	-0.04231	-0.00603	-0.01061
648		3S	0.00059	-0.00144	-0.00109	-0.00023	-0.00063
649		3PX	0.00077	-0.00081	-0.00303	-0.00041	-0.00069
650		3PY	0.00409	0.00039	-0.02447	-0.00346	-0.00591
651		3PZ	0.00897	-0.00047	-0.05779	-0.00794	-0.01421
652		4D 0	0.00146	-0.00010	0.00675	0.00059	0.00094
653		4D+1	-0.00130	0.00009	-0.00585	-0.00043	-0.00064
654		4D-1	-0.00159	0.00010	-0.00727	-0.00065	-0.00103
655		4D+2	0.00083	0.00010	0.00337	0.00030	0.00054
656		4D-2	-0.00071	-0.00009	-0.00288	-0.00022	-0.00037
657	67 H	1S	0.00020	0.00059	0.00014	0.00004	0.00027
658		2S	0.00025	0.00202	-0.00082	-0.00007	0.00055
659	68 C	1S	0.00009	0.00024	-0.00007	0.00000	0.00005
660		2S	-0.00013	-0.00041	0.00016	-0.00003	-0.00017
661		2PX	-0.00020	-0.00131	-0.00007	-0.00006	-0.00032
662		2PY	0.00412	-0.00067	-0.00202	-0.00055	-0.00102
663		2PZ	0.01048	0.00002	-0.00533	-0.00133	-0.00231
664		3S	0.00001	-0.00194	0.00051	0.00002	0.00064
665		3PX	-0.00145	-0.00252	-0.00007	-0.00029	-0.00096
666		3PY	0.00362	-0.00021	-0.00362	-0.00029	0.00004
667		3PZ	0.00678	0.00000	-0.00926	-0.00173	-0.00319
668		4D 0	0.00012	0.00000	0.00056	0.00003	0.00003
669		4D+1	-0.00253	0.00010	-0.01156	-0.00105	-0.00172
670		4D-1	0.00012	-0.00005	0.00062	0.00008	0.00011
671		4D+2	-0.00018	-0.00009	-0.00068	-0.00008	-0.00015
672		4D-2	-0.00106	0.00005	-0.00475	-0.00042	-0.00068
673	69 H	1S	0.00076	0.00097	0.00005	0.00001	0.00030
674		2S	-0.00142	0.00096	-0.00032	-0.00045	-0.00118
675	70 C	1S	0.00003	0.00012	-0.00004	0.00000	0.00005
676		2S	0.00000	-0.00025	0.00009	0.00000	-0.00006
677		2PX	0.00209	0.00004	0.00687	0.00058	0.00096
678		2PY	0.01660	-0.00078	0.06176	0.00542	0.00872
679		2PZ	0.04093	-0.00149	0.15074	0.01320	0.02143
680		3S	-0.00110	-0.00072	0.00004	-0.00036	-0.00120
681		3PX	0.00069	-0.00042	0.00734	0.00058	0.00051
682		3PY	0.01404	0.00036	0.06561	0.00624	0.01054
683		3PZ	0.03292	-0.00163	0.16063	0.01519	0.02497
684		4D 0	-0.00007	0.00000	0.00168	0.00021	0.00037
685		4D+1	0.00011	0.00003	-0.00147	-0.00015	-0.00025
686		4D-1	0.00008	-0.00001	-0.00180	-0.00023	-0.00041

687		4D+2	-0.00005	-0.00003	0.00084	0.00010	0.00018
688		4D-2	0.00000	-0.00006	-0.00074	-0.00008	-0.00013
689	71 H	1S	0.00063	0.00099	0.00011	0.00001	0.00028
690		2S	0.00115	0.00171	0.00038	0.00009	0.00096
691	72 H	1S	0.00010	0.00052	-0.00019	0.00001	0.00011
692		2S	0.00045	0.00103	-0.00045	0.00023	0.00082
693	73 H	1S	-0.00024	-0.00030	-0.00006	0.00000	-0.00004
694		2S	-0.00045	-0.00025	-0.00018	0.00000	-0.00002

B2

			O	O	O	V	V
Eigenvalues --			-0.21581	-0.19854	-0.19358	-0.07062	-0.05731
1	1 Ir	1S	0.00149	-0.00519	0.01118	-0.00139	-0.00226
2		2S	-0.00198	0.00765	-0.01593	0.00189	0.00320
3		3S	0.00827	-0.03299	0.07154	-0.02237	-0.00078
4		4PX	-0.05766	-0.05449	-0.06605	0.00079	0.00226
5		4PY	-0.01965	-0.01541	-0.00561	0.00093	0.00222
6		4PZ	-0.01715	-0.00733	-0.00753	-0.00725	-0.01608
7		5PX	0.01229	0.03428	0.03104	0.00924	0.00648
8		5PY	0.00060	-0.00321	-0.00703	-0.03207	0.00334
9		5PZ	0.01589	0.01407	0.00469	0.04301	0.11867
10		6PX	0.01443	-0.02540	-0.03379	-0.01371	-0.00791
11		6PY	-0.00010	-0.01586	0.02031	0.00293	-0.00723
12		6PZ	-0.01046	0.01971	-0.00491	-0.02960	-0.03147
13		7D 0	-0.07506	-0.12934	0.18768	-0.01983	0.02939
14		7D+1	-0.00548	-0.30860	0.32977	-0.07834	-0.03683
15		7D-1	-0.04117	-0.00185	0.19362	-0.01442	0.00251
16		7D+2	-0.00136	-0.10344	-0.19829	-0.00652	0.01255
17		7D-2	-0.04734	0.30962	0.30288	0.04480	0.04655
18		8D 0	-0.03274	-0.03872	0.05546	0.00135	0.00822
19		8D+1	-0.00034	-0.10871	0.11409	-0.02243	-0.02196
20		8D-1	-0.01310	-0.00024	0.07702	-0.00990	0.00658
21		8D+2	0.00707	-0.04226	-0.07111	-0.00364	-0.00159
22		8D-2	-0.00256	0.11398	0.11395	0.01113	0.02070
23	2 C	1S	-0.00140	0.00035	0.00131	0.00036	-0.00201
24		2S	0.00203	0.00129	-0.00344	0.00456	0.00685
25		2PX	-0.01362	-0.05888	-0.04004	-0.01878	-0.01025
26		2PY	-0.00412	-0.01392	-0.00880	-0.00590	-0.01726

27			2PZ	0.00392	-0.01569	-0.01223	-0.00462	-0.00612
28			3S	0.01173	-0.00514	-0.00995	-0.01961	0.00825
29			3PX	-0.00966	-0.05465	-0.02500	-0.02936	0.00663
30			3PY	-0.00139	-0.00846	-0.00654	-0.01241	-0.00691
31			3PZ	0.00152	-0.01112	-0.00633	-0.01427	-0.03717
32			4D 0	-0.00051	0.00012	0.00167	0.00072	0.00216
33			4D+1	-0.00061	-0.00128	0.00515	0.00102	0.00513
34			4D-1	0.00046	-0.00121	0.00123	0.00023	0.00187
35			4D+2	0.00037	0.00060	-0.00095	-0.00062	-0.00034
36			4D-2	-0.00045	-0.00025	-0.00069	0.00063	-0.00120
37	3	C	1S	0.00107	0.00051	-0.00110	0.00050	0.00037
38			2S	-0.00355	-0.00023	0.00240	0.00092	0.00262
39			2PX	-0.01478	-0.06616	0.00714	-0.01523	-0.06358
40			2PY	-0.00016	-0.01034	-0.00569	-0.00137	-0.01252
41			2PZ	-0.00276	-0.01406	0.00075	-0.00271	-0.01191
42			3S	0.00201	0.00146	-0.00288	-0.00749	-0.00741
43			3PX	-0.01165	-0.05439	0.01042	-0.01710	-0.06755
44			3PY	0.00025	-0.01185	-0.00930	-0.00150	-0.01619
45			3PZ	0.00252	-0.00840	-0.00982	0.00568	-0.01682
46			4D 0	0.00022	0.00012	-0.00364	0.00008	-0.00097
47			4D+1	0.00005	0.00055	-0.00825	0.00047	-0.00135
48			4D-1	0.00068	-0.00041	-0.00222	-0.00082	-0.00187
49			4D+2	-0.00034	-0.00094	0.00332	0.00071	0.00142
50			4D-2	0.00056	0.00088	-0.00151	-0.00182	-0.00252
51	4	C	1S	0.00101	-0.00091	-0.00025	-0.00032	0.00081
52			2S	-0.00212	0.00122	0.00038	0.00034	-0.00050
53			2PX	0.00497	0.01608	-0.07065	0.00047	-0.04967
54			2PY	0.00401	0.00086	-0.01737	-0.00102	-0.00995
55			2PZ	-0.00301	0.00665	-0.01500	0.00143	-0.01265
56			3S	-0.00659	0.00614	0.00339	0.00699	-0.02417
57			3PX	0.00241	0.01256	-0.06331	0.00136	-0.06506
58			3PY	0.00291	-0.00077	-0.01594	0.00233	-0.00673
59			3PZ	-0.00248	0.00599	-0.01333	0.00802	-0.02075
60			4D 0	0.00000	-0.00069	-0.00037	-0.00031	-0.00094
61			4D+1	-0.00043	-0.00168	-0.00095	-0.00057	-0.00014
62			4D-1	0.00023	0.00046	0.00020	0.00020	0.00048
63			4D+2	-0.00025	-0.00184	-0.00078	-0.00089	-0.00186
64			4D-2	0.00085	0.00400	0.00202	0.00157	0.00284
65	5	H	1S	0.00156	-0.00087	-0.00077	0.00123	-0.00045
66			2S	-0.00135	0.00800	0.00043	-0.00264	-0.01408
67	6	C	1S	0.00007	-0.00089	0.00086	-0.00054	-0.00111
68			2S	-0.00026	0.00138	-0.00139	0.00094	0.00292
69			2PX	0.00410	0.01230	0.07148	-0.01351	0.01351

70		2PY	0.00108	-0.00050	0.02061	-0.00479	0.00098
71		2PZ	-0.00040	0.00579	0.01375	-0.00111	0.00561
72		3S	0.00028	0.00779	-0.00647	0.01042	0.00406
73		3PX	0.00203	0.00725	0.05479	-0.01409	0.01094
74		3PY	-0.00046	-0.00276	0.01896	-0.01101	0.00318
75		3PZ	-0.00113	0.00361	0.01315	-0.00290	0.00880
76		4D 0	-0.00028	-0.00145	-0.00065	-0.00045	-0.00164
77		4D+1	-0.00093	-0.00449	-0.00087	-0.00163	-0.00474
78		4D-1	-0.00009	-0.00091	-0.00047	-0.00036	-0.00085
79		4D+2	0.00014	0.00055	0.00059	0.00032	0.00058
80		4D-2	0.00031	0.00142	-0.00082	0.00030	0.00168
81	7 C	1S	-0.00009	-0.00022	0.00036	-0.00014	-0.00130
82		2S	0.00021	0.00031	-0.00047	0.00102	0.00284
83		2PX	0.01518	0.07064	0.01883	0.02333	0.05409
84		2PY	0.00356	0.01795	0.00455	0.00534	0.00947
85		2PZ	0.00424	0.01579	0.00370	0.00523	0.01110
86		3S	-0.00055	0.00107	-0.00016	-0.00775	0.00997
87		3PX	0.01265	0.05962	0.02113	0.02580	0.06482
88		3PY	0.00251	0.01512	0.00631	0.00997	0.01396
89		3PZ	0.00305	0.01171	0.00501	0.00153	0.01562
90		4D 0	0.00007	0.00004	0.00125	-0.00031	0.00046
91		4D+1	0.00001	0.00004	0.00317	-0.00066	0.00066
92		4D-1	0.00014	-0.00018	0.00166	-0.00020	0.00116
93		4D+2	0.00010	0.00005	-0.00249	0.00031	-0.00137
94		4D-2	-0.00008	-0.00011	0.00307	0.00004	0.00251
95	8 H	1S	0.00166	-0.00115	-0.00029	-0.00071	-0.00296
96		2S	0.00247	-0.00087	-0.00101	0.00027	-0.00545
97	9 H	1S	-0.00036	-0.00195	0.00175	-0.00080	-0.00133
98		2S	-0.00020	-0.00138	0.00039	-0.00045	-0.00589
99	10 H	1S	-0.00079	0.00090	-0.00014	0.00001	-0.00132
100		2S	-0.00110	0.00098	-0.00057	-0.00206	-0.00539
101	11 C	1S	0.01527	0.01336	0.01720	-0.00147	-0.00353
102		2S	-0.02586	-0.02359	-0.03227	0.00211	0.00748
103		2PX	-0.06827	-0.08287	-0.11030	0.00200	-0.01239
104		2PY	-0.07389	-0.00651	0.01455	0.00727	0.05814
105		2PZ	-0.03138	-0.01574	0.03766	0.00136	0.03485
106		3S	-0.04782	-0.05070	-0.02921	0.01319	0.01502
107		3PX	-0.10308	-0.07490	-0.14703	0.00930	0.00108
108		3PY	-0.04911	-0.01364	0.01276	0.00137	0.06279
109		3PZ	-0.05064	-0.00001	-0.01521	0.02083	0.02267
110		4D 0	-0.00068	0.00125	-0.00075	0.00043	-0.00145
111		4D+1	0.00227	0.00693	-0.00841	0.00211	0.00175
112		4D-1	-0.00114	0.00081	-0.00473	0.00060	-0.00071

113		4D+2	-0.00285	0.00439	0.00691	0.00068	0.00089
114		4D-2	0.00166	-0.00508	-0.00648	-0.00080	-0.00223
115	12 C	1S	-0.00471	0.00299	-0.00637	0.00177	0.00137
116		2S	0.00963	-0.00472	0.01546	-0.00212	-0.00314
117		2PX	0.03778	-0.00601	-0.02146	-0.00015	0.01057
118		2PY	-0.03441	0.00739	0.11026	-0.00880	-0.03299
119		2PZ	-0.05276	0.02901	0.03439	0.00581	-0.00992
120		3S	0.00821	-0.04343	0.00283	-0.02110	0.00185
121		3PX	0.06838	0.02119	0.02296	-0.00517	0.00503
122		3PY	-0.02975	0.00966	0.07934	-0.01009	-0.02592
123		3PZ	-0.01231	0.03103	0.06956	0.00732	-0.02620
124		4D 0	0.00416	0.00151	0.00088	-0.00087	-0.00702
125		4D+1	0.00187	0.00197	0.00353	-0.00004	-0.00124
126		4D-1	-0.00005	-0.00101	-0.00132	-0.00009	-0.00428
127		4D+2	-0.00022	-0.00089	-0.00251	-0.00013	-0.00033
128		4D-2	-0.00195	-0.00209	-0.00302	0.00028	-0.00416
129	13 C	1S	-0.00452	-0.01140	-0.00162	-0.00190	-0.00164
130		2S	0.01319	0.02698	0.00917	0.00342	0.00512
131		2PX	0.02754	0.03835	-0.01896	0.00571	0.00041
132		2PY	-0.00561	0.00599	0.07876	-0.00311	0.00911
133		2PZ	0.00787	0.04503	0.05854	0.00296	0.00892
134		3S	-0.04792	0.00807	-0.07658	0.02336	0.00665
135		3PX	0.00987	0.02829	-0.03442	0.00922	-0.01245
136		3PY	0.01339	0.01560	0.09212	-0.00441	0.01430
137		3PZ	-0.02695	0.01736	-0.00040	0.00165	0.01135
138		4D 0	0.00091	0.00308	0.00437	0.00034	0.00261
139		4D+1	-0.00258	-0.00109	-0.00200	0.00021	0.00240
140		4D-1	-0.00361	-0.00192	-0.00092	0.00017	0.00247
141		4D+2	-0.00213	-0.00328	-0.00302	-0.00020	-0.00257
142		4D-2	-0.00298	-0.00113	0.00072	-0.00005	0.00392
143	14 C	1S	0.00529	0.00205	0.00621	-0.00113	-0.00143
144		2S	-0.01572	-0.00669	-0.01749	0.00279	0.00468
145		2PX	-0.01474	-0.00816	-0.01033	0.00202	-0.02317
146		2PY	-0.01274	-0.00447	-0.02388	-0.00014	0.05708
147		2PZ	-0.01183	-0.00296	-0.02056	0.00231	0.04226
148		3S	0.02610	0.02494	0.02542	0.00501	-0.00376
149		3PX	0.01246	0.00927	0.01345	-0.00085	-0.01989
150		3PY	0.00814	0.01115	0.01080	-0.00084	0.04087
151		3PZ	-0.01886	-0.01060	-0.02695	-0.00170	0.04188
152		4D 0	-0.00126	0.00111	0.00470	-0.00019	-0.00198
153		4D+1	-0.00289	0.00112	0.00099	0.00039	0.00028
154		4D-1	-0.00338	0.00034	0.00202	0.00018	-0.00086
155		4D+2	0.00128	-0.00046	-0.00366	0.00033	0.00047

156		4D-2	-0.00205	0.00116	0.00765	-0.00065	-0.00224
157	15 C	1S	0.00584	0.00788	0.00516	0.00058	0.00011
158		2S	-0.01636	-0.02040	-0.01456	-0.00096	-0.00007
159		2PX	-0.03671	-0.02225	-0.00662	-0.00103	0.02771
160		2PY	0.02542	-0.02190	-0.03153	-0.00358	-0.06823
161		2PZ	0.02812	0.00000	-0.01397	-0.00084	-0.04632
162		3S	0.01102	-0.00111	0.01606	-0.00433	-0.00676
163		3PX	-0.00310	0.00839	0.00949	-0.00024	0.02256
164		3PY	0.00977	-0.00983	-0.02715	-0.00184	-0.06114
165		3PZ	0.03227	0.01109	0.02092	-0.00067	-0.04074
166		4D 0	0.00291	0.00000	-0.00326	0.00008	-0.00069
167		4D+1	0.00038	0.00326	0.00581	-0.00005	-0.00001
168		4D-1	0.00010	-0.00062	-0.00083	0.00008	-0.00018
169		4D+2	0.00229	-0.00017	-0.00570	0.00025	-0.00021
170		4D-2	-0.00029	-0.00044	0.00256	-0.00018	-0.00022
171	16 H	1S	0.01317	0.00823	0.01355	-0.00022	-0.00042
172		2S	0.01288	0.01478	-0.00073	-0.00914	-0.00437
173	17 C	1S	-0.00097	-0.00112	-0.00045	-0.00013	-0.00027
174		2S	0.00335	0.00377	0.00272	0.00050	0.00063
175		2PX	-0.01702	0.01160	0.04454	-0.00090	-0.00193
176		2PY	0.04575	-0.01803	-0.09977	0.00307	0.00633
177		2PZ	0.02879	-0.01341	-0.07107	0.00205	0.00451
178		3S	-0.01907	-0.01052	-0.03475	-0.00135	0.00798
179		3PX	-0.03255	-0.00799	0.01482	-0.00271	-0.00221
180		3PY	0.02843	-0.02285	-0.09922	0.00408	0.01125
181		3PZ	0.02509	-0.01252	-0.05815	0.00140	0.01033
182		4D 0	-0.00104	0.00056	0.00021	0.00020	0.00529
183		4D+1	0.00086	-0.00005	-0.00039	-0.00011	-0.00128
184		4D-1	-0.00068	-0.00011	-0.00019	0.00003	0.00242
185		4D+2	-0.00132	-0.00013	0.00038	-0.00003	0.00214
186		4D-2	-0.00040	-0.00047	-0.00091	-0.00007	0.00176
187	18 H	1S	-0.00227	-0.00300	-0.00166	-0.00064	-0.00111
188		2S	-0.01067	-0.01245	-0.01149	-0.00189	-0.00253
189	19 C	1S	-0.00392	0.00181	-0.00028	0.00009	0.00006
190		2S	0.00654	-0.00548	-0.00053	-0.00069	0.00070
191		2PX	0.01478	-0.00572	-0.02686	-0.00136	0.01753
192		2PY	0.01955	-0.00505	-0.01704	-0.02300	0.13833
193		2PZ	0.00630	-0.00941	-0.00455	0.03994	-0.23359
194		3S	0.02330	0.01433	0.02152	0.00726	-0.00019
195		3PX	0.03312	-0.00104	-0.03983	0.00331	0.01120
196		3PY	-0.00108	0.00970	0.00711	-0.02959	0.14043
197		3PZ	-0.00352	0.00324	0.01041	0.04122	-0.23729
198		4D 0	-0.00022	0.00581	-0.00217	0.00338	-0.00332

199		4D+1	0.00010	0.00296	-0.00168	-0.00136	-0.01447
200		4D-1	0.00014	0.00385	-0.00072	0.00228	-0.00073
201		4D+2	-0.00158	0.00356	-0.00058	0.00213	-0.00024
202		4D-2	0.00036	-0.00245	-0.00032	0.00025	0.00718
203	20 C	1S	-0.00248	-0.00012	0.00334	0.00009	-0.00086
204		2S	0.00750	-0.00046	-0.01010	-0.00014	0.00230
205		2PX	0.01021	-0.00906	-0.01960	0.00093	-0.00448
206		2PY	0.01808	-0.01753	-0.01822	0.01677	0.03809
207		2PZ	-0.00120	0.02385	-0.01333	-0.02982	-0.06613
208		3S	0.00580	0.00679	-0.01099	0.00227	0.01249
209		3PX	0.00706	-0.00590	-0.02615	0.00168	-0.01283
210		3PY	0.01227	-0.01886	-0.02471	0.01889	0.02603
211		3PZ	-0.00007	0.01082	-0.01636	-0.03674	-0.06087
212		4D 0	0.00035	-0.00395	0.00100	-0.00231	0.01809
213		4D+1	0.00014	-0.00058	-0.00019	0.00030	0.00228
214		4D-1	-0.00007	-0.00250	0.00078	-0.00152	0.01165
215		4D+2	0.00043	-0.00181	0.00053	-0.00159	0.00920
216		4D-2	0.00069	0.00064	-0.00151	-0.00002	-0.00273
217	21 C	1S	-0.00057	-0.00054	-0.00047	-0.00033	-0.00093
218		2S	0.00110	0.00084	0.00038	0.00087	0.00251
219		2PX	0.00658	0.00412	0.00017	0.00308	-0.00322
220		2PY	-0.00849	0.03440	-0.00343	0.02243	-0.00480
221		2PZ	0.00634	-0.05467	0.01629	-0.03731	0.01457
222		3S	0.00192	0.00522	0.01399	-0.00210	0.00592
223		3PX	0.01197	0.00109	-0.00323	0.00943	-0.00129
224		3PY	-0.03188	0.03006	0.00466	0.02888	0.00111
225		3PZ	-0.00800	-0.04858	0.01812	-0.05929	0.00837
226		4D 0	-0.00029	0.00024	-0.00018	0.00091	-0.01724
227		4D+1	0.00016	0.00062	-0.00051	-0.00120	0.00104
228		4D-1	-0.00023	-0.00002	-0.00032	0.00061	-0.01124
229		4D+2	-0.00024	0.00052	0.00111	0.00062	-0.01047
230		4D-2	0.00041	-0.00056	-0.00061	0.00072	0.00113
231	22 C	1S	0.00058	0.00021	-0.00161	-0.00007	-0.00041
232		2S	-0.00153	-0.00001	0.00347	0.00063	0.00083
233		2PX	0.00337	-0.00213	-0.00029	-0.00219	0.00946
234		2PY	-0.00221	-0.03368	0.01613	-0.02236	0.10160
235		2PZ	-0.00796	0.05704	-0.01159	0.03892	-0.17166
236		3S	-0.00439	-0.00882	0.00334	-0.00451	0.00102
237		3PX	0.00050	-0.00002	0.00752	-0.00379	0.01447
238		3PY	0.00396	-0.03242	0.00986	-0.02736	0.12792
239		3PZ	-0.00411	0.04869	-0.01199	0.04403	-0.21859
240		4D 0	-0.00020	0.00058	-0.00012	-0.00116	-0.00248
241		4D+1	0.00066	-0.00121	-0.00043	0.00067	0.01242

242		4D-1	0.00006	0.00033	-0.00050	-0.00092	-0.00324
243		4D+2	-0.00065	0.00076	0.00076	-0.00072	-0.00250
244		4D-2	0.00010	0.00038	-0.00076	-0.00037	-0.00741
245	23 H	1S	-0.00037	0.00274	0.00145	-0.00019	-0.00205
246		2S	0.00479	-0.00581	-0.02849	-0.00415	-0.02672
247	24 C	1S	0.00035	-0.00009	0.00028	-0.00009	-0.00070
248		2S	0.00022	-0.00035	-0.00137	0.00016	0.00217
249		2PX	0.00046	-0.00208	-0.00560	-0.00057	-0.01412
250		2PY	-0.00294	0.00393	-0.00277	-0.00225	-0.12304
251		2PZ	0.00806	-0.00993	-0.00587	0.00348	0.21138
252		3S	-0.01588	0.00024	-0.00101	0.00150	0.00328
253		3PX	-0.01106	-0.00188	0.00092	-0.00400	-0.01489
254		3PY	-0.00683	0.00702	0.00146	-0.00378	-0.15231
255		3PZ	0.00326	-0.00924	-0.00119	0.00888	0.25832
256		4D 0	0.00028	-0.00211	0.00048	-0.00162	0.00051
257		4D+1	0.00052	-0.00348	0.00073	-0.00288	0.00985
258		4D-1	-0.00017	-0.00093	0.00038	-0.00075	-0.00077
259		4D+2	0.00037	-0.00076	0.00017	-0.00054	-0.00100
260		4D-2	-0.00002	0.00219	-0.00089	0.00181	-0.00559
261	25 H	1S	0.00242	0.00105	0.00411	-0.00017	-0.00173
262		2S	-0.02098	0.00290	0.01079	-0.00640	-0.00440
263	26 H	1S	0.00320	-0.00137	-0.00609	-0.00046	-0.00246
264		2S	0.00614	-0.00200	-0.00887	-0.00189	-0.00663
265	27 H	1S	-0.00213	0.00011	0.00185	-0.00010	-0.00017
266		2S	-0.00143	0.00137	0.00410	0.00038	-0.00340
267	28 C	1S	-0.01107	-0.01306	-0.01700	0.00067	0.00272
268		2S	0.01375	0.02227	0.02581	-0.00276	-0.00522
269		2PX	-0.10937	-0.08612	-0.09659	-0.00204	0.00989
270		2PY	0.02737	-0.10366	-0.00741	-0.08268	-0.07138
271		2PZ	-0.02107	0.14252	-0.06188	0.13548	0.11171
272		3S	0.06308	0.03689	0.09687	-0.00483	-0.01261
273		3PX	-0.07624	-0.09911	-0.07827	-0.00995	0.01453
274		3PY	-0.01024	-0.09080	0.00475	-0.07424	-0.07188
275		3PZ	-0.02915	0.08442	-0.03550	0.12667	0.10000
276		4D 0	0.00003	0.00223	-0.00043	-0.00227	0.00466
277		4D+1	0.00042	0.01135	-0.00931	0.00250	0.00112
278		4D-1	-0.00081	-0.00142	-0.00258	-0.00211	0.00194
279		4D+2	0.00029	0.00064	0.00189	-0.00179	0.00265
280		4D-2	0.00270	-0.00953	-0.00607	-0.00146	-0.00229
281	29 C	1S	0.00259	0.00523	0.01079	0.00000	0.00116
282		2S	-0.00985	-0.01624	-0.02521	-0.00094	-0.00350
283		2PX	0.02010	0.01889	0.03733	0.00132	0.00156
284		2PY	0.01517	-0.05297	0.07478	0.02153	-0.02298

285		2PZ	-0.00901	0.13529	-0.00042	-0.03405	0.03847
286		3S	0.01036	0.03980	-0.01010	0.00090	-0.00588
287		3PX	0.00788	0.01700	0.03538	0.00143	-0.00198
288		3PY	0.00680	-0.07649	0.05154	0.02253	-0.04075
289		3PZ	-0.01149	0.09069	-0.00683	-0.04847	0.05324
290		4D 0	-0.00051	-0.00644	-0.00007	-0.00566	-0.00557
291		4D+1	0.00289	-0.00315	0.00198	-0.00811	-0.00865
292		4D-1	-0.00100	-0.00400	-0.00050	-0.00277	-0.00279
293		4D+2	0.00446	0.00034	0.00498	-0.00284	-0.00282
294		4D-2	0.00215	0.00483	0.00067	0.00513	0.00520
295	30 C	1S	0.01134	0.00222	-0.00334	-0.00003	-0.00033
296		2S	-0.02317	-0.00682	0.00573	-0.00094	0.00133
297		2PX	0.00810	0.01002	-0.00154	-0.00018	-0.00064
298		2PY	-0.02997	-0.08430	0.03730	-0.02129	0.05011
299		2PZ	-0.03596	0.12232	-0.02683	0.03561	-0.06850
300		3S	-0.08541	0.01724	0.03767	0.00653	-0.00715
301		3PX	-0.00132	0.03603	0.03195	-0.00421	0.00341
302		3PY	-0.02747	-0.04162	0.03466	-0.01928	0.04373
303		3PZ	-0.03013	0.11553	-0.02063	0.04550	-0.07629
304		4D 0	-0.00098	0.00277	-0.00196	0.00205	0.01363
305		4D+1	0.00347	-0.00667	0.00063	-0.01278	0.00572
306		4D-1	-0.00131	0.00092	-0.00291	0.00185	0.00814
307		4D+2	0.00187	0.00556	0.00295	0.00196	0.00645
308		4D-2	0.00272	0.00263	-0.00249	0.00771	-0.00397
309	31 C	1S	0.00476	-0.00374	-0.00620	-0.00026	0.00012
310		2S	-0.01227	0.01125	0.01707	0.00070	-0.00041
311		2PX	-0.04996	-0.02245	-0.03451	0.00441	0.00495
312		2PY	-0.00281	0.04109	-0.02062	0.06749	0.08441
313		2PZ	0.01619	-0.07620	0.01067	-0.11019	-0.13695
314		3S	-0.02144	-0.02126	-0.01175	0.00129	0.00119
315		3PX	-0.03547	-0.00193	-0.00582	0.00236	0.00381
316		3PY	-0.05610	0.05880	0.00540	0.06398	0.09638
317		3PZ	-0.01955	-0.04599	0.02346	-0.09836	-0.15395
318		4D 0	0.00017	0.00462	-0.00078	-0.00072	-0.00168
319		4D+1	0.00210	-0.01003	0.00093	0.00547	-0.00205
320		4D-1	0.00173	0.00226	-0.00194	-0.00062	-0.00077
321		4D+2	-0.00402	0.00299	-0.00047	-0.00073	-0.00084
322		4D-2	0.00114	0.00436	-0.00426	-0.00332	0.00144
323	32 H	1S	-0.01577	-0.00806	-0.00151	0.00016	0.00089
324		2S	-0.02382	-0.00454	-0.02767	0.00874	0.01412
325	33 C	1S	-0.01222	-0.00279	-0.00148	0.00014	0.00104
326		2S	0.02151	0.00896	0.00547	0.00017	-0.00330
327		2PX	-0.00699	-0.01554	-0.01469	0.00423	0.00025

328		2PY	0.07730	0.04947	-0.01558	0.09859	-0.07672
329		2PZ	0.06954	-0.07537	0.01499	-0.16203	0.12582
330		3S	0.12990	-0.02837	-0.03235	-0.00426	-0.00383
331		3PX	-0.03064	0.01505	0.01447	0.00311	-0.00414
332		3PY	0.14394	0.02200	-0.02459	0.11317	-0.07216
333		3PZ	0.10442	-0.06720	0.00537	-0.19301	0.12370
334		4D 0	0.00153	-0.00585	0.00205	0.00149	0.00266
335		4D+1	0.00148	-0.00718	0.00185	0.00004	0.00418
336		4D-1	0.00155	-0.00365	0.00044	0.00091	0.00145
337		4D+2	-0.00151	-0.00353	0.00067	0.00091	0.00142
338		4D-2	0.00075	0.00571	-0.00184	-0.00012	-0.00315
339	34 C	1S	0.02920	0.00030	-0.00103	-0.00019	0.00013
340		2S	-0.06795	-0.00273	-0.00014	-0.00043	-0.00073
341		2PX	-0.15380	-0.00030	-0.00375	-0.00173	-0.00014
342		2PY	-0.06278	0.11243	-0.02251	-0.03589	-0.01182
343		2PZ	-0.00668	-0.18347	0.05479	0.05906	0.01932
344		3S	-0.16356	0.03323	0.03207	0.00944	0.00033
345		3PX	0.08230	-0.02178	-0.02981	-0.00301	0.00002
346		3PY	0.03823	0.08322	-0.01614	-0.04932	-0.02267
347		3PZ	0.04992	-0.12670	0.03774	0.07619	0.03706
348		4D 0	0.00149	-0.00035	-0.00045	0.00684	-0.01041
349		4D+1	0.00604	0.00478	-0.00111	0.01940	0.00077
350		4D-1	0.00126	-0.00021	-0.00023	0.00309	-0.00603
351		4D+2	-0.00322	0.00068	0.00119	0.00292	-0.00605
352		4D-2	0.01247	-0.00239	0.00026	-0.01250	-0.00018
353	35 H	1S	-0.02852	-0.00692	-0.00015	0.00029	0.00129
354		2S	0.07363	-0.01512	-0.00637	0.00110	0.00675
355	36 C	1S	0.00079	-0.00025	0.00270	0.00198	0.00249
356		2S	-0.00125	0.00436	-0.00550	-0.00637	-0.00566
357		2PX	0.00562	-0.04462	-0.00198	-0.01493	-0.00499
358		2PY	-0.01278	-0.00112	0.01704	-0.01999	-0.03917
359		2PZ	-0.00354	-0.01131	0.02438	-0.00871	-0.02107
360		3S	-0.00285	-0.01439	-0.02097	-0.00698	-0.02525
361		3PX	0.00818	-0.04289	0.00329	-0.01404	-0.02530
362		3PY	-0.00639	0.00241	0.01391	-0.00956	-0.03000
363		3PZ	-0.00221	-0.02669	0.01327	-0.04095	-0.02185
364		4D 0	-0.00160	0.00119	0.00315	-0.00008	-0.00881
365		4D+1	-0.00015	0.00057	-0.00069	-0.00062	0.00050
366		4D-1	-0.00183	0.00068	0.00095	-0.00075	-0.00526
367		4D+2	-0.00099	0.00033	-0.00045	0.00027	-0.00188
368		4D-2	-0.00146	-0.00060	0.00185	-0.00054	-0.00445
369	37 C	1S	-0.00331	0.00200	-0.00509	0.00080	0.00024
370		2S	0.00836	-0.00289	0.01168	-0.00113	-0.00348

371		2PX	-0.01351	-0.02803	0.00463	0.00205	0.04556
372		2PY	0.02211	-0.00896	0.00527	-0.00813	-0.10147
373		2PZ	0.00318	-0.00971	-0.01232	-0.00399	-0.06527
374		3S	-0.00489	-0.04210	0.00785	-0.01794	0.01077
375		3PX	0.00508	-0.03320	0.02988	-0.01389	0.04152
376		3PY	0.00952	-0.01721	0.00341	-0.01242	-0.10367
377		3PZ	0.02342	0.00594	0.00921	-0.00010	-0.07268
378		4D 0	0.00293	-0.00095	-0.00418	-0.00036	0.00061
379		4D+1	0.00019	0.00101	-0.00147	0.00139	0.00461
380		4D-1	0.00208	0.00019	-0.00257	0.00011	0.00236
381		4D+2	-0.00079	0.00031	0.00047	-0.00085	-0.00367
382		4D-2	0.00244	-0.00161	-0.00411	0.00022	0.00445
383	38 C	1S	-0.00095	0.00076	-0.00200	-0.00072	-0.00006
384		2S	0.00208	-0.00207	0.00395	0.00006	0.00014
385		2PX	0.01361	0.00022	-0.01566	0.00039	0.03204
386		2PY	-0.02873	0.01037	0.04116	0.00350	-0.07460
387		2PZ	-0.02411	0.01110	0.01750	-0.00075	-0.05022
388		3S	0.00609	0.01200	0.01568	0.02533	0.00159
389		3PX	0.01005	-0.00037	-0.01418	-0.00298	0.04327
390		3PY	-0.02531	0.01382	0.03601	0.01018	-0.09510
391		3PZ	-0.01797	0.00355	0.01642	-0.00865	-0.06263
392		4D 0	0.00026	0.00058	-0.00087	0.00117	0.00285
393		4D+1	-0.00021	0.00186	0.00037	0.00033	-0.00277
394		4D-1	0.00017	-0.00019	-0.00025	-0.00006	-0.00009
395		4D+2	0.00019	-0.00013	-0.00106	0.00096	0.00510
396		4D-2	0.00007	-0.00106	0.00056	-0.00103	-0.00370
397	39 H	1S	-0.00246	-0.00665	-0.00309	-0.00153	0.00199
398		2S	-0.01017	0.03626	-0.00724	0.01840	0.04407
399	40 C	1S	0.00025	0.00062	0.00104	0.00044	0.00121
400		2S	-0.00037	-0.00117	-0.00220	-0.00173	-0.00271
401		2PX	-0.01140	0.00835	0.01374	0.00348	-0.00509
402		2PY	0.02656	-0.01212	-0.04046	-0.00991	0.00897
403		2PZ	0.01911	-0.00374	-0.02119	-0.00510	0.01028
404		3S	-0.01119	-0.00516	-0.01047	0.00138	-0.00720
405		3PX	-0.01790	0.01229	-0.00035	0.01586	-0.00123
406		3PY	0.01987	-0.01001	-0.03236	-0.01131	0.00466
407		3PZ	0.01163	-0.00049	-0.02342	-0.00118	0.00897
408		4D 0	-0.00047	0.00067	-0.00031	0.00081	0.00810
409		4D+1	0.00055	0.00071	-0.00046	-0.00004	-0.00178
410		4D-1	-0.00035	-0.00023	-0.00045	0.00043	0.00477
411		4D+2	-0.00079	-0.00006	0.00022	0.00027	0.00289
412		4D-2	-0.00019	-0.00093	-0.00074	0.00065	0.00431
413	41 C	1S	-0.00028	0.00088	-0.00009	0.00134	0.00152

414		2S	0.00043	-0.00071	0.00010	-0.00251	-0.00334
415		2PX	0.00070	-0.00989	0.00413	-0.00937	-0.04212
416		2PY	-0.00441	-0.00522	-0.00964	0.01050	0.08964
417		2PZ	-0.00384	-0.00463	-0.00661	0.00846	0.06030
418		3S	0.00748	-0.01103	0.00858	-0.01925	-0.00940
419		3PX	-0.00369	-0.00406	-0.00036	-0.00677	-0.04865
420		3PY	-0.00212	-0.00730	-0.01201	0.01084	0.11213
421		3PZ	-0.00459	0.00201	-0.00961	0.01423	0.07085
422		4D 0	-0.00086	0.00042	0.00104	0.00048	0.00043
423		4D+1	-0.00094	0.00040	0.00108	-0.00018	-0.00296
424		4D-1	-0.00094	0.00039	0.00132	0.00009	-0.00125
425		4D+2	0.00116	-0.00053	-0.00140	-0.00025	0.00342
426		4D-2	-0.00175	0.00053	0.00248	0.00053	-0.00298
427	42 H	1S	-0.00118	0.00897	-0.00289	0.00372	0.00396
428		2S	-0.00231	0.01362	-0.00517	0.01112	0.00977
429	43 H	1S	-0.00074	-0.00477	0.00124	0.00052	0.00164
430		2S	-0.00266	-0.00557	-0.00130	0.00647	0.00598
431	44 H	1S	-0.00007	0.00029	-0.00010	0.00167	0.00175
432		2S	-0.00031	-0.00126	-0.00084	0.00527	0.00830
433	45 C	1S	-0.00284	-0.00071	0.00210	0.00000	0.00333
434		2S	0.00612	0.00004	-0.00458	-0.00184	-0.00556
435		2PX	-0.01126	-0.00908	-0.11307	0.00768	0.03479
436		2PY	-0.01891	-0.00112	-0.01772	0.00334	0.01835
437		2PZ	-0.00338	-0.00197	-0.02412	0.00126	0.00729
438		3S	0.00260	0.01076	0.00623	0.00293	-0.03930
439		3PX	0.00148	-0.00223	-0.08764	0.01481	0.02257
440		3PY	-0.02080	0.00034	0.00200	-0.00278	0.02708
441		3PZ	-0.01714	-0.01845	0.00719	-0.01883	0.00791
442		4D 0	0.00081	-0.00181	-0.00325	-0.00055	-0.00128
443		4D+1	-0.00176	-0.00504	-0.00430	-0.00008	0.00226
444		4D-1	0.00112	-0.00165	-0.00596	-0.00054	-0.00207
445		4D+2	0.00075	0.00229	0.00840	-0.00031	-0.00063
446		4D-2	-0.00039	-0.00241	-0.01438	0.00027	0.00014
447	46 C	1S	-0.00090	-0.00042	0.00132	0.00012	0.00253
448		2S	0.00224	-0.00051	-0.00013	-0.00240	-0.00845
449		2PX	-0.02947	-0.07292	-0.13852	-0.00108	0.00306
450		2PY	-0.00551	-0.01788	-0.03164	-0.00023	0.00555
451		2PZ	-0.01187	-0.01760	-0.02708	0.00211	0.00762
452		3S	0.01575	0.01856	-0.03461	0.01854	-0.00486
453		3PX	-0.02174	-0.05561	-0.11517	0.00031	0.01839
454		3PY	0.00048	-0.01262	-0.03385	0.00318	-0.00218
455		3PZ	-0.01828	-0.01558	-0.00433	-0.01145	-0.00059
456		4D 0	0.00008	0.00012	0.00157	-0.00006	-0.00150

457		4D+1	0.00011	-0.00016	0.00457	-0.00055	-0.00228
458		4D-1	0.00063	-0.00040	0.00082	-0.00002	-0.00057
459		4D+2	0.00002	0.00066	-0.00101	-0.00002	0.00107
460		4D-2	-0.00081	-0.00130	0.00011	-0.00029	-0.00243
461	47 C	1S	0.00188	0.00041	-0.00131	-0.00033	-0.00210
462		2S	-0.00414	0.00076	0.00368	0.00096	0.00506
463		2PX	0.00030	-0.01093	-0.15969	-0.00187	-0.01591
464		2PY	0.01035	-0.00215	-0.04459	-0.00218	-0.01175
465		2PZ	-0.00688	-0.00140	-0.03142	0.00154	0.00388
466		3S	-0.00470	-0.01181	-0.00206	-0.00492	0.00878
467		3PX	-0.00205	-0.00857	-0.12081	-0.00276	-0.01869
468		3PY	0.01024	0.00825	-0.04161	0.00458	-0.01379
469		3PZ	0.00733	-0.00078	-0.04659	0.00516	-0.00494
470		4D 0	-0.00039	0.00113	-0.00070	0.00057	0.00246
471		4D+1	0.00034	0.00209	-0.00266	0.00083	0.00413
472		4D-1	0.00049	0.00092	0.00013	0.00014	0.00123
473		4D+2	-0.00109	-0.00136	-0.00056	0.00007	-0.00087
474		4D-2	0.00081	0.00127	0.00354	-0.00031	0.00039
475	48 C	1S	-0.00049	0.00034	0.00000	-0.00016	-0.00097
476		2S	0.00152	-0.00003	-0.00027	0.00077	0.00197
477		2PX	-0.01056	-0.03031	0.04618	-0.00585	-0.04695
478		2PY	-0.00481	-0.00637	0.01062	-0.00204	-0.01566
479		2PZ	-0.00332	-0.00643	0.01042	-0.00135	-0.01137
480		3S	-0.00441	-0.00738	0.01198	-0.00494	0.01121
481		3PX	-0.00851	-0.02217	0.02174	-0.00559	-0.04277
482		3PY	-0.00407	-0.00190	0.00735	-0.00232	-0.01522
483		3PZ	0.00325	-0.00311	-0.00531	0.00510	-0.00859
484		4D 0	0.00011	0.00021	-0.00123	-0.00002	0.00023
485		4D+1	0.00010	0.00026	-0.00360	0.00008	0.00047
486		4D-1	0.00059	0.00115	0.00196	-0.00008	-0.00004
487		4D+2	-0.00085	-0.00229	-0.00519	-0.00002	-0.00001
488		4D-2	0.00176	0.00452	0.01162	0.00012	-0.00002
489	49 H	1S	-0.00280	0.00042	0.00083	-0.00016	-0.00126
490		2S	0.00279	-0.00540	-0.00690	0.00662	-0.00115
491	50 C	1S	-0.00135	-0.00010	0.00095	0.00026	0.00141
492		2S	0.00363	0.00024	-0.00253	-0.00059	-0.00360
493		2PX	0.02562	0.05417	0.03828	0.00452	0.04137
494		2PY	0.00247	0.01221	0.01153	0.00128	0.01093
495		2PZ	0.00240	0.01174	0.01038	0.00153	0.01235
496		3S	-0.00513	-0.00376	0.01224	-0.00612	-0.00241
497		3PX	0.01263	0.02918	0.01688	0.00197	0.03539
498		3PY	0.00722	0.00780	-0.00493	0.00162	0.00555
499		3PZ	-0.00150	0.00734	0.00943	0.00186	0.01012

500		4D 0	0.00064	0.00120	0.00400	0.00004	0.00023
501		4D+1	0.00095	0.00305	0.01016	0.00031	0.00149
502		4D-1	0.00078	0.00071	0.00385	0.00002	-0.00018
503		4D+2	0.00028	-0.00072	-0.00600	-0.00015	-0.00087
504		4D-2	-0.00032	-0.00023	0.00588	0.00004	-0.00002
505	51 C	1S	0.00007	-0.00006	0.00013	-0.00004	0.00027
506		2S	-0.00063	-0.00011	0.00066	-0.00030	-0.00086
507		2PX	0.01998	0.05092	0.18671	0.00136	0.00365
508		2PY	0.00537	0.01211	0.04445	0.00032	0.00180
509		2PZ	0.00396	0.01153	0.04138	0.00052	0.00053
510		3S	0.00737	0.00079	-0.01443	0.00457	-0.00102
511		3PX	0.01803	0.04544	0.15813	0.00340	0.00747
512		3PY	-0.00040	0.00898	0.04760	-0.00288	0.00157
513		3PZ	0.00194	0.00897	0.03754	0.00031	0.00068
514		4D 0	-0.00046	-0.00102	-0.00024	-0.00017	-0.00141
515		4D+1	-0.00111	-0.00262	-0.00035	-0.00039	-0.00321
516		4D-1	-0.00019	-0.00049	-0.00047	-0.00008	-0.00033
517		4D+2	0.00009	0.00028	0.00095	-0.00007	-0.00015
518		4D-2	0.00019	0.00072	-0.00131	0.00016	0.00145
519	52 H	1S	0.00041	0.00009	-0.00039	0.00019	0.00108
520		2S	0.00240	0.00090	-0.00361	0.00146	0.00325
521	53 N	1S	0.00386	-0.00152	-0.00218	-0.00108	-0.00475
522		2S	-0.00945	0.00300	0.00492	0.00271	0.01113
523		2PX	-0.00417	0.00593	0.00647	-0.00056	-0.02481
524		2PY	-0.01757	0.03616	0.00670	0.01387	-0.12179
525		2PZ	-0.00967	-0.05226	0.02926	-0.01672	0.24284
526		3S	-0.00807	0.01208	0.00779	0.00742	0.03222
527		3PX	0.01311	0.00218	-0.02142	0.00018	-0.02947
528		3PY	-0.00741	0.02813	-0.01159	0.01222	-0.12515
529		3PZ	-0.00359	-0.04745	0.01144	-0.01335	0.25244
530		4D 0	0.00083	0.00028	-0.00190	0.00232	-0.00402
531		4D+1	0.00065	-0.00210	-0.00068	0.00296	-0.00588
532		4D-1	0.00186	0.00013	-0.00411	0.00117	-0.00158
533		4D+2	-0.00074	0.00099	0.00422	0.00103	-0.00079
534		4D-2	0.00190	0.00057	-0.00372	-0.00159	0.00494
535	54 N	1S	0.00155	-0.00425	0.00261	-0.00376	-0.00631
536		2S	-0.00395	0.00954	-0.00579	0.00756	0.01112
537		2PX	-0.01352	-0.02243	0.06609	0.02928	0.06278
538		2PY	0.00069	-0.01898	0.02441	-0.00154	0.00142
539		2PZ	-0.01152	0.00778	0.01046	0.01382	0.02579
540		3S	-0.00496	0.02498	-0.01675	0.03852	0.07423
541		3PX	-0.01033	-0.01761	0.06156	0.03053	0.05806
542		3PY	0.00211	-0.01690	0.01247	-0.00144	-0.01418

543		3PZ	-0.00393	0.01056	0.00819	0.01311	0.02201
544		4D 0	0.00174	0.00408	-0.00158	0.00150	0.00053
545		4D+1	0.00097	0.00811	0.00069	0.00069	-0.00131
546		4D-1	0.00008	0.00067	0.00053	0.00008	-0.00045
547		4D+2	0.00146	0.00102	-0.00199	-0.00103	0.00048
548		4D-2	-0.00094	-0.00725	0.00299	-0.00096	-0.00229
549	55 N	1S	-0.00081	0.00337	0.00002	0.00368	0.00698
550		2S	0.00158	-0.00536	0.00019	-0.00591	-0.01408
551		2PX	-0.00998	0.01662	0.01271	-0.00847	-0.04751
552		2PY	0.03411	-0.01471	-0.03467	0.00631	0.08691
553		2PZ	0.01124	0.01788	-0.03395	0.01941	0.08686
554		3S	0.00420	-0.02580	-0.00738	-0.03895	-0.06589
555		3PX	-0.00206	-0.02031	0.03197	-0.03414	-0.04818
556		3PY	0.03147	-0.02111	-0.02179	-0.00058	0.07794
557		3PZ	0.00848	0.00821	-0.02713	0.02078	0.08683
558		4D 0	0.00071	0.00426	-0.00223	0.00050	0.00091
559		4D+1	-0.00165	0.00529	-0.00115	0.00031	0.00124
560		4D-1	0.00068	-0.00118	0.00127	-0.00113	0.00116
561		4D+2	0.00212	-0.00088	-0.00139	-0.00028	-0.00351
562		4D-2	-0.00013	-0.00404	0.00377	-0.00093	0.00187
563	56 N	1S	-0.04408	-0.00250	-0.00119	0.00022	0.00002
564		2S	0.08296	0.00464	0.00216	-0.00034	-0.00012
565		2PX	0.12020	-0.00222	-0.00421	-0.00780	0.00028
566		2PY	0.31588	-0.02610	0.00807	-0.18635	0.00521
567		2PZ	0.18064	0.06411	-0.01221	0.29305	-0.00832
568		3S	0.19307	0.02182	0.01839	-0.00312	-0.00044
569		3PX	0.14578	-0.00004	-0.00351	-0.00713	0.00096
570		3PY	0.21742	-0.02125	0.00103	-0.17252	0.01186
571		3PZ	0.12540	0.04360	-0.01117	0.27355	-0.01913
572		4D 0	0.01095	-0.00594	0.00159	0.00026	-0.00085
573		4D+1	-0.00432	0.01026	-0.00286	-0.01494	-0.00042
574		4D-1	-0.00719	-0.00418	0.00091	0.00068	-0.00047
575		4D+2	-0.00862	-0.00453	0.00114	0.00090	-0.00049
576		4D-2	-0.00254	-0.00607	0.00172	0.00938	0.00029
577	57 N	1S	-0.04320	-0.00148	-0.00022	-0.00018	0.00007
578		2S	0.08046	0.00264	0.00064	0.00030	-0.00020
579		2PX	-0.12149	-0.00687	0.00090	0.00732	0.00024
580		2PY	-0.29356	-0.10249	0.02213	0.17556	0.00305
581		2PZ	-0.22038	0.13303	-0.03969	-0.27595	-0.00440
582		3S	0.18159	0.00471	-0.00237	0.00254	-0.00046
583		3PX	-0.14117	-0.00614	0.00314	0.00662	0.00004
584		3PY	-0.20658	-0.07827	0.01520	0.16628	-0.00481
585		3PZ	-0.15762	0.10105	-0.03159	-0.26004	0.00805

586		4D 0	0.00811	0.00758	-0.00185	0.00098	-0.00049
587		4D+1	-0.00232	-0.00245	0.00044	-0.01614	-0.00083
588		4D-1	-0.00887	0.00356	-0.00125	0.00129	-0.00022
589		4D+2	-0.00990	0.00426	-0.00095	0.00145	-0.00025
590		4D-2	-0.00420	0.00110	-0.00020	0.01027	0.00058
591	58 C	1S	0.02961	0.00091	0.00002	0.00008	-0.00002
592		2S	-0.06763	-0.00207	-0.00014	0.00017	0.00006
593		2PX	0.15601	0.00654	-0.00045	0.00231	-0.00005
594		2PY	0.03155	0.05420	-0.01212	0.05857	0.00123
595		2PZ	0.05257	-0.07993	0.01940	-0.08929	-0.00187
596		3S	-0.19622	-0.00572	0.00113	-0.00264	-0.00003
597		3PX	-0.09248	-0.00106	0.00131	0.00267	0.00036
598		3PY	-0.05993	0.03051	-0.00673	0.06618	0.00413
599		3PZ	-0.02350	-0.05099	0.01213	-0.10228	-0.00752
600		4D 0	0.00235	-0.00101	0.00032	0.00571	-0.00005
601		4D+1	0.00827	-0.00891	0.00253	0.01857	0.00060
602		4D-1	0.00172	-0.00012	0.00009	0.00224	-0.00006
603		4D+2	-0.00475	-0.00032	-0.00001	0.00232	-0.00007
604		4D-2	0.01000	0.00640	-0.00149	-0.01200	-0.00041
605	59 C	1S	0.00847	0.00036	0.00016	0.00021	0.00000
606		2S	-0.02366	-0.00088	-0.00025	-0.00048	0.00003
607		2PX	0.02114	0.00302	-0.00006	-0.00248	-0.00007
608		2PY	-0.01461	0.05312	-0.01411	-0.08153	-0.00211
609		2PZ	0.01116	-0.08217	0.02096	0.12445	0.00327
610		3S	-0.01198	-0.00133	-0.00123	-0.00160	-0.00059
611		3PX	0.02940	0.00292	-0.00017	-0.00371	0.00000
612		3PY	0.06195	0.04598	-0.01202	-0.07496	-0.00380
613		3PZ	0.05762	-0.06685	0.01733	0.11576	0.00556
614		4D 0	0.00119	-0.00263	0.00063	-0.00207	-0.00001
615		4D+1	0.00083	0.00261	-0.00056	0.00704	-0.00003
616		4D-1	0.00327	-0.00137	0.00032	-0.00131	-0.00001
617		4D+2	-0.00316	-0.00172	0.00044	-0.00150	-0.00001
618		4D-2	0.00297	-0.00149	0.00037	-0.00453	0.00002
619	60 C	1S	-0.00765	-0.00030	-0.00022	-0.00011	0.00000
620		2S	0.00748	0.00038	0.00046	0.00025	-0.00004
621		2PX	-0.02089	0.00137	-0.00119	-0.00373	-0.00005
622		2PY	-0.09356	0.04946	-0.01364	-0.09116	-0.00113
623		2PZ	-0.03958	-0.08167	0.02027	0.13793	0.00187
624		3S	0.14224	0.00436	0.00025	0.00129	0.00051
625		3PX	0.01937	0.00112	-0.00145	-0.00414	-0.00033
626		3PY	-0.16395	0.03658	-0.00912	-0.10637	-0.00185
627		3PZ	-0.09042	-0.06627	0.01745	0.16011	0.00269
628		4D 0	-0.00051	0.00326	-0.00078	0.00297	0.00003

629		4D+1	-0.00065	0.00173	-0.00041	0.00229	0.00022
630		4D-1	0.00147	0.00164	-0.00038	0.00141	0.00001
631		4D+2	-0.00242	0.00174	-0.00046	0.00161	0.00001
632		4D-2	-0.00006	-0.00125	0.00027	-0.00158	-0.00013
633	61 C	1S	-0.00076	-0.00007	-0.00007	-0.00009	0.00000
634		2S	0.00011	0.00008	0.00016	0.00014	0.00000
635		2PX	0.00355	-0.00089	-0.00010	-0.00162	0.00000
636		2PY	0.00954	-0.01969	0.00460	-0.03369	0.00030
637		2PZ	-0.00635	0.03038	-0.00693	0.05157	-0.00047
638		3S	-0.02893	-0.00044	0.00058	0.00128	0.00010
639		3PX	0.00846	-0.00040	-0.00002	-0.00256	-0.00002
640		3PY	-0.01274	-0.01483	0.00350	-0.04601	0.00069
641		3PZ	-0.01766	0.02212	-0.00493	0.06954	-0.00093
642		4D 0	-0.00100	0.00362	-0.00091	-0.00698	-0.00016
643		4D+1	-0.00076	0.00510	-0.00130	-0.00926	-0.00020
644		4D-1	-0.00036	0.00164	-0.00041	-0.00318	-0.00007
645		4D+2	0.00017	0.00185	-0.00048	-0.00355	-0.00008
646		4D-2	0.00079	-0.00341	0.00090	0.00628	0.00014
647	62 H	1S	0.00650	0.00017	-0.00002	-0.00017	-0.00002
648		2S	0.09333	0.00269	0.00010	0.00073	0.00008
649	63 C	1S	0.00494	0.00015	0.00008	0.00004	0.00000
650		2S	-0.01074	-0.00040	-0.00023	-0.00009	0.00002
651		2PX	0.02475	-0.00004	0.00058	-0.00008	-0.00007
652		2PY	0.02200	-0.01876	0.00469	-0.00462	-0.00148
653		2PZ	0.00609	0.02987	-0.00697	0.00717	0.00226
654		3S	-0.06426	-0.00116	0.00040	-0.00031	0.00004
655		3PX	0.02762	-0.00016	0.00024	0.00000	-0.00011
656		3PY	0.03992	-0.01233	0.00235	-0.00673	-0.00154
657		3PZ	0.02087	0.02082	-0.00532	0.01066	0.00256
658		4D 0	0.00087	-0.00222	0.00056	0.00431	0.00012
659		4D+1	0.00159	0.00586	-0.00146	-0.01112	-0.00017
660		4D-1	0.00135	-0.00132	0.00035	0.00262	0.00006
661		4D+2	-0.00111	-0.00161	0.00039	0.00304	0.00008
662		4D-2	0.00492	-0.00355	0.00096	0.00716	0.00010
663	64 H	1S	-0.01703	-0.00052	0.00015	-0.00008	-0.00001
664		2S	0.08317	0.00202	-0.00199	0.00061	-0.00020
665	65 C	1S	0.00474	0.00015	-0.00001	0.00004	0.00000
666		2S	-0.01298	-0.00040	0.00007	-0.00008	0.00001
667		2PX	0.01299	-0.00217	0.00060	0.00400	0.00007
668		2PY	0.00111	-0.06732	0.01679	0.10163	0.00212
669		2PZ	-0.02874	0.10222	-0.02572	-0.15576	-0.00321
670		3S	0.01864	0.00016	-0.00080	0.00003	0.00005
671		3PX	-0.01690	-0.00236	0.00089	0.00431	0.00009

672		3PY	0.00263	-0.05395	0.01365	0.11033	0.00228
673		3PZ	-0.02176	0.08239	-0.02094	-0.16940	-0.00336
674		4D 0	-0.00004	-0.00008	0.00001	-0.00197	0.00010
675		4D+1	0.00058	-0.00042	0.00010	-0.00250	-0.00008
676		4D-1	0.00062	-0.00001	0.00000	-0.00090	0.00005
677		4D+2	-0.00018	-0.00003	-0.00001	-0.00100	0.00006
678		4D-2	0.00054	0.00031	-0.00004	0.00171	0.00004
679	66 H	1S	-0.00151	-0.00013	-0.00011	-0.00012	0.00000
680		2S	-0.00652	-0.00027	-0.00020	-0.00038	0.00002
681	67 H	1S	0.02635	0.00080	0.00015	0.00017	-0.00002
682		2S	0.02997	0.00112	0.00060	0.00032	-0.00009
683	68 H	1S	0.00276	0.00011	-0.00004	0.00007	0.00000
684		2S	0.01429	0.00044	-0.00015	0.00018	-0.00002
685	69 H	1S	-0.00119	-0.01006	-0.01950	0.00036	0.00068
686		2S	0.06992	-0.02253	-0.03791	-0.00090	0.00154
687	70 F	1S	0.00036	-0.00008	-0.00019	-0.00011	-0.00059
688		2S	-0.00078	0.00011	0.00019	0.00019	0.00138
689		2PX	-0.01572	-0.02934	-0.02455	-0.00069	-0.01489
690		2PY	0.00138	-0.00683	-0.00896	-0.00088	-0.00780
691		2PZ	-0.00327	-0.00660	-0.00533	-0.00007	-0.00280
692		3S	-0.00295	0.00076	0.00292	0.00107	0.00406
693		3PX	-0.01222	-0.02327	-0.01751	-0.00090	-0.01385
694		3PY	0.00109	-0.00554	-0.00682	-0.00113	-0.00700
695		3PZ	-0.00268	-0.00520	-0.00336	0.00013	-0.00234
696		4D 0	0.00006	0.00025	0.00057	0.00006	0.00037
697		4D+1	0.00023	0.00073	0.00128	0.00019	0.00074
698		4D-1	0.00004	0.00012	0.00036	0.00001	0.00010
699		4D+2	-0.00004	-0.00003	-0.00035	-0.00004	0.00012
700		4D-2	-0.00017	-0.00031	0.00019	-0.00002	-0.00045
701	71 F	1S	-0.00004	-0.00001	0.00003	0.00004	0.00002
702		2S	0.00027	-0.00002	-0.00038	0.00011	0.00010
703		2PX	0.00737	0.01861	-0.02814	0.00259	0.02024
704		2PY	0.00180	0.00403	-0.00611	0.00079	0.00574
705		2PZ	0.00163	0.00371	-0.00594	0.00099	0.00524
706		3S	-0.00085	0.00016	0.00173	-0.00158	-0.00119
707		3PX	0.00602	0.01553	-0.02089	0.00213	0.01812
708		3PY	0.00158	0.00299	-0.00465	0.00056	0.00525
709		3PZ	0.00147	0.00278	-0.00472	0.00115	0.00510
710		4D 0	0.00005	0.00007	-0.00036	0.00006	0.00030
711		4D+1	-0.00003	0.00004	-0.00079	0.00008	0.00076
712		4D-1	0.00007	0.00019	0.00010	0.00007	0.00031
713		4D+2	-0.00008	-0.00026	-0.00042	-0.00006	-0.00023
714		4D-2	0.00017	0.00047	0.00124	0.00000	-0.00002

715	72	F	1S	-0.00132	-0.00027	-0.00162	0.00046	0.00073
716			2S	0.00283	0.00011	0.00326	-0.00127	-0.00153
717			2PX	0.01229	0.00157	0.00953	-0.00290	0.00581
718			2PY	0.01230	0.00234	0.02368	-0.00174	-0.02362
719			2PZ	-0.00179	0.00150	0.00314	0.00182	-0.01255
720			3S	0.01055	0.00455	0.01426	-0.00226	-0.00620
721			3PX	0.00849	0.00108	0.00748	-0.00220	0.00546
722			3PY	0.01021	0.00207	0.01814	-0.00147	-0.02211
723			3PZ	-0.00142	0.00010	0.00082	0.00153	-0.01143
724			4D 0	0.00008	0.00014	0.00088	-0.00015	-0.00133
725			4D+1	0.00004	0.00016	0.00030	-0.00007	0.00039
726			4D-1	-0.00007	0.00012	0.00047	-0.00006	-0.00066
727			4D+2	0.00010	-0.00002	-0.00018	0.00004	-0.00066
728			4D-2	-0.00047	-0.00001	0.00028	-0.00001	-0.00036
729	73	F	1S	-0.00104	-0.00171	-0.00086	-0.00008	0.00009
730			2S	0.00201	0.00391	0.00114	0.00020	-0.00025
731			2PX	0.02569	0.02052	0.00495	0.00081	-0.01251
732			2PY	-0.02057	0.00886	0.01544	0.00128	0.02892
733			2PZ	-0.01140	0.01093	0.01399	0.00108	0.01937
734			3S	0.00978	0.01236	0.01138	0.00062	-0.00030
735			3PX	0.01970	0.01567	0.00485	0.00091	-0.01096
736			3PY	-0.01637	0.00616	0.01143	0.00097	0.02568
737			3PZ	-0.00870	0.00921	0.01130	0.00107	0.01745
738			4D 0	0.00046	0.00013	-0.00056	0.00001	-0.00109
739			4D+1	-0.00034	-0.00008	0.00024	-0.00002	-0.00009
740			4D-1	0.00004	-0.00027	-0.00021	-0.00005	-0.00075
741			4D+2	-0.00009	-0.00045	-0.00088	0.00001	-0.00002
742			4D-2	0.00006	-0.00015	0.00011	-0.00009	-0.00093

B3

				171	172	173	174	175
				O	O	O	V	V
	Eigenvalues --			-0.21396	-0.20087	-0.19134	-0.08048	-0.05367
1	1	Ir	1S	0.00164	0.00792	0.01086	0.00008	-0.00819
2			2S	-0.00224	-0.01171	-0.01545	-0.00019	0.01166
3			3S	0.00473	0.04209	0.06889	-0.00708	-0.00702
4			4PX	-0.06376	0.06167	-0.06301	0.00087	-0.00702
5			4PY	0.01536	-0.01894	0.03473	0.00259	-0.01471

6		4PZ	0.00411	-0.00529	0.00381	-0.00767	-0.01012
7		5PX	0.03824	-0.03126	0.02471	0.01318	0.06333
8		5PY	0.00572	0.01789	-0.02608	-0.00620	0.09073
9		5PZ	-0.00728	-0.00574	0.00350	0.03620	0.06262
10		6PX	-0.01455	0.02066	-0.02008	-0.00597	-0.02246
11		6PY	-0.01138	0.00014	0.03550	-0.00109	-0.02848
12		6PZ	0.00235	-0.02333	-0.00191	0.01418	-0.01983
13		7D 0	0.05537	0.04667	0.02832	0.03240	-0.04911
14		7D+1	-0.14623	0.47038	0.26684	-0.04467	0.00426
15		7D-1	0.16900	-0.11592	-0.02844	0.06375	-0.14176
16		7D+2	0.03625	-0.09430	0.33317	0.01736	0.04751
17		7D-2	0.00629	-0.16370	0.35768	0.00816	0.03672
18		8D 0	0.01786	0.01072	-0.00139	0.01643	-0.02550
19		8D+1	-0.05724	0.16667	0.08981	-0.02143	0.00582
20		8D-1	0.06820	-0.03968	-0.00520	0.03628	-0.05167
21		8D+2	0.02630	-0.03882	0.12277	0.00768	0.01617
22		8D-2	0.00140	-0.06446	0.13235	0.00676	0.02697
23	2 C	1S	0.00128	0.00035	0.00139	-0.00043	-0.00374
24		2S	-0.00534	-0.00298	-0.00340	0.00066	0.01053
25		2PX	-0.00420	0.05835	-0.04616	-0.00398	-0.01379
26		2PY	-0.00519	-0.02211	0.01622	-0.00788	0.00576
27		2PZ	-0.00816	-0.00019	-0.00458	-0.00291	0.01117
28		3S	0.00602	0.00124	-0.01059	0.00852	0.01824
29		3PX	-0.00168	0.05155	-0.03067	0.00488	-0.00720
30		3PY	-0.00429	-0.02583	0.01068	-0.01300	0.00143
31		3PZ	-0.00395	0.00039	-0.00085	-0.00887	-0.00425
32		4D 0	-0.00003	-0.00072	-0.00010	0.00042	-0.00104
33		4D+1	-0.00522	0.00296	0.00508	0.00122	0.00535
34		4D-1	0.00147	-0.00081	-0.00198	-0.00028	-0.00080
35		4D+2	-0.00086	0.00080	0.00071	-0.00006	0.00014
36		4D-2	-0.00139	0.00135	0.00088	-0.00027	0.00101
37	3 C	1S	-0.00094	-0.00110	-0.00112	-0.00061	0.00282
38		2S	0.00288	0.00269	0.00265	0.00580	-0.00853
39		2PX	-0.06597	0.07667	-0.00384	-0.00902	-0.05377
40		2PY	0.01405	-0.03649	-0.00570	0.00215	0.03047
41		2PZ	-0.00263	0.00225	0.00117	0.00151	-0.00288
42		3S	0.00641	-0.00365	-0.00276	-0.01064	-0.01344
43		3PX	-0.04608	0.06131	-0.00497	-0.01068	-0.06189
44		3PY	0.01484	-0.02609	-0.01239	0.01687	0.01710
45		3PZ	-0.00362	-0.00446	-0.00786	-0.00661	-0.00009
46		4D 0	0.00032	-0.00026	-0.00053	0.00035	-0.00008
47		4D+1	0.00557	-0.00181	-0.00799	-0.00055	-0.00115
48		4D-1	-0.00223	0.00125	0.00298	-0.00039	-0.00003

49		4D+2	0.00306	-0.00155	-0.00289	-0.00007	-0.00229
50		4D-2	0.00375	-0.00228	-0.00409	-0.00023	-0.00262
51	4 C	1S	-0.00052	0.00049	-0.00039	-0.00034	0.00203
52		2S	0.00138	-0.00046	0.00058	0.00104	-0.00453
53		2PX	0.07003	-0.03675	-0.06871	-0.01133	-0.04333
54		2PY	-0.02432	0.01479	0.02396	0.00392	0.01868
55		2PZ	0.00380	-0.00245	0.00037	0.00071	-0.00657
56		3S	-0.00167	-0.00248	0.00439	-0.00305	-0.01722
57		3PX	0.05438	-0.02927	-0.06210	-0.01614	-0.05448
58		3PY	-0.02003	0.01291	0.02105	0.00545	0.02705
59		3PZ	0.00023	-0.00233	0.00074	-0.00050	-0.00495
60		4D 0	-0.00032	0.00003	-0.00005	-0.00039	0.00024
61		4D+1	-0.00060	0.00262	-0.00167	-0.00032	-0.00090
62		4D-1	-0.00013	-0.00096	0.00054	-0.00032	0.00047
63		4D+2	0.00078	-0.00260	0.00149	0.00010	0.00195
64		4D-2	0.00104	-0.00327	0.00176	0.00044	0.00236
65	5 H	1S	-0.00102	0.00003	-0.00099	-0.00208	0.00422
66		2S	-0.00738	-0.00886	0.00141	-0.00732	-0.00278
67	6 C	1S	-0.00003	0.00091	0.00072	-0.00066	-0.00099
68		2S	-0.00017	-0.00139	-0.00115	0.00149	0.00188
69		2PX	-0.04428	0.00296	0.07306	0.00824	0.00924
70		2PY	0.01749	0.00218	-0.02364	-0.00364	-0.00510
71		2PZ	0.00038	-0.00349	-0.00131	0.00206	0.00234
72		3S	-0.00191	-0.00770	-0.00527	0.00021	0.01018
73		3PX	-0.03786	0.00661	0.05803	0.00859	0.00832
74		3PY	0.01438	0.00133	-0.01546	-0.00629	-0.00171
75		3PZ	-0.00208	-0.00321	0.00030	-0.00213	0.00725
76		4D 0	-0.00044	-0.00025	-0.00021	0.00002	0.00023
77		4D+1	-0.00334	0.00542	-0.00136	-0.00066	-0.00460
78		4D-1	0.00094	-0.00216	0.00030	0.00023	0.00206
79		4D+2	0.00048	-0.00025	-0.00084	-0.00002	0.00016
80		4D-2	0.00083	0.00010	-0.00099	0.00005	-0.00028
81	7 C	1S	0.00004	0.00027	0.00034	-0.00070	-0.00036
82		2S	-0.00045	-0.00037	-0.00045	0.00140	0.00092
83		2PX	0.03778	-0.07975	0.02593	0.00645	0.04914
84		2PY	-0.01573	0.02693	-0.00929	-0.00441	-0.01761
85		2PZ	-0.00119	-0.00147	-0.00020	0.00004	0.00133
86		3S	0.00104	-0.00194	-0.00022	0.00274	0.00264
87		3PX	0.02834	-0.06523	0.02792	0.00721	0.06077
88		3PY	-0.01286	0.02283	-0.00885	-0.00573	-0.02042
89		3PZ	0.00103	-0.00022	-0.00003	-0.00085	0.00060
90		4D 0	-0.00009	-0.00012	-0.00003	-0.00006	0.00013
91		4D+1	-0.00178	0.00052	0.00254	0.00030	0.00024

92		4D-1	0.00044	-0.00010	-0.00089	0.00001	0.00026
93		4D+2	-0.00248	0.00082	0.00296	0.00047	0.00185
94		4D-2	-0.00297	0.00109	0.00373	0.00067	0.00209
95	8 H	1S	-0.00235	0.00020	-0.00050	-0.00222	0.00164
96		2S	-0.00416	-0.00042	-0.00121	-0.00431	0.00818
97	9 H	1S	0.00182	0.00255	0.00159	-0.00022	-0.00187
98		2S	0.00305	0.00249	0.00027	0.00044	-0.00568
99	10 H	1S	0.00045	-0.00069	0.00004	-0.00039	-0.00067
100		2S	0.00147	-0.00085	-0.00034	-0.00170	-0.00248
101	11 C	1S	0.01557	-0.01504	0.01843	-0.00091	-0.00255
102		2S	-0.02606	0.02580	-0.03450	0.00122	0.00729
103		2PX	-0.09364	0.08935	-0.07762	0.00412	0.04767
104		2PY	0.01992	-0.03173	0.08371	0.00460	0.13165
105		2PZ	0.00573	0.00816	0.04531	-0.00118	0.04858
106		3S	-0.05356	0.06058	-0.03431	0.00095	0.00692
107		3PX	-0.10409	0.08213	-0.12113	0.01555	0.05667
108		3PY	0.03225	-0.02832	0.09492	-0.00184	0.12628
109		3PZ	-0.00768	-0.00954	0.00318	-0.00419	0.03781
110		4D 0	0.00053	0.00186	0.00243	-0.00050	-0.00246
111		4D+1	0.00377	-0.00920	-0.00543	0.00179	-0.00277
112		4D-1	-0.00152	0.00309	0.00276	-0.00037	-0.00331
113		4D+2	0.00125	-0.00012	-0.00630	-0.00025	-0.00250
114		4D-2	-0.00052	0.00437	-0.01006	-0.00061	-0.00330
115	12 C	1S	-0.00209	-0.00335	-0.00594	0.00125	-0.00016
116		2S	0.00520	0.00592	0.01477	-0.00340	0.00068
117		2PX	0.01032	-0.00140	0.05070	-0.00219	-0.02199
118		2PY	-0.00734	0.00455	0.10629	-0.00378	-0.06809
119		2PZ	-0.01038	-0.02152	0.00780	0.00770	-0.02674
120		3S	-0.01122	0.04467	-0.00226	-0.00180	0.00729
121		3PX	0.04345	-0.03109	0.08146	-0.00908	-0.02174
122		3PY	-0.02091	0.01662	0.06038	0.00082	-0.06761
123		3PZ	0.00714	-0.01957	0.04342	-0.00420	-0.03704
124		4D 0	0.00193	-0.00184	0.00065	-0.00027	-0.00858
125		4D+1	0.00278	-0.00271	0.00338	-0.00081	-0.00828
126		4D-1	-0.00188	0.00162	-0.00377	-0.00005	-0.01078
127		4D+2	-0.00227	0.00153	-0.00256	-0.00023	-0.01106
128		4D-2	-0.00069	0.00035	0.00074	-0.00005	-0.00705
129	13 C	1S	-0.00715	0.01293	-0.00280	-0.00179	-0.00011
130		2S	0.01972	-0.03074	0.01186	0.00397	0.00242
131		2PX	0.02785	-0.04819	0.04697	0.00398	0.01048
132		2PY	-0.03352	0.02743	0.08165	-0.00276	0.02905
133		2PZ	0.01451	-0.03580	0.03979	0.00202	0.01057
134		3S	-0.03504	-0.00738	-0.07451	0.01124	0.00072

135		3PX	0.01526	-0.03610	0.02520	0.00358	0.00394
136		3PY	-0.01363	0.01376	0.09317	-0.00119	0.04596
137		3PZ	-0.02096	-0.00519	-0.02001	0.00693	0.01890
138		4D 0	0.00355	-0.00405	0.00514	0.00030	0.00208
139		4D+1	-0.00097	0.00036	-0.00028	0.00033	0.00533
140		4D-1	-0.00131	0.00148	0.00061	-0.00008	0.00100
141		4D+2	-0.00265	0.00302	-0.00109	0.00001	0.00850
142		4D-2	0.00196	-0.00220	0.00318	0.00041	0.00966
143	14 C	1S	0.00453	-0.00235	0.00633	-0.00074	-0.00024
144		2S	-0.01324	0.00785	-0.01788	0.00240	0.00202
145		2PX	-0.01344	0.01036	-0.02707	0.00251	0.04864
146		2PY	0.01618	-0.00370	-0.01604	0.00395	0.15267
147		2PZ	0.00273	-0.00037	-0.01147	0.00323	0.05746
148		3S	0.02546	-0.02894	0.02768	-0.00508	-0.00530
149		3PX	0.01465	-0.01270	0.01021	-0.00055	0.04035
150		3PY	0.00828	-0.00243	-0.00294	0.00326	0.11941
151		3PZ	-0.01533	0.01503	-0.03175	0.00817	0.05061
152		4D 0	0.00070	-0.00043	0.00358	-0.00035	-0.00256
153		4D+1	-0.00144	-0.00047	0.00139	0.00053	-0.00252
154		4D-1	-0.00100	0.00053	0.00134	-0.00008	-0.00285
155		4D+2	-0.00033	-0.00034	0.00623	-0.00021	-0.00373
156		4D-2	-0.00026	0.00014	0.00675	-0.00018	-0.00295
157	15 C	1S	0.00697	-0.00895	0.00592	0.00042	-0.00003
158		2S	-0.01906	0.02330	-0.01649	-0.00091	0.00029
159		2PX	-0.02538	0.03122	-0.02826	-0.00364	-0.05637
160		2PY	0.00264	-0.00285	-0.02282	-0.00535	-0.17544
161		2PZ	0.00987	-0.01334	-0.00228	-0.00092	-0.06631
162		3S	0.00946	0.00085	0.01566	-0.00483	-0.00670
163		3PX	0.00589	-0.00638	-0.00051	-0.00148	-0.05436
164		3PY	-0.01000	0.00848	-0.02433	-0.00448	-0.15231
165		3PZ	0.01900	-0.01500	0.02729	-0.00446	-0.05602
166		4D 0	0.00088	-0.00022	-0.00325	-0.00009	-0.00101
167		4D+1	0.00168	-0.00253	0.00166	0.00001	-0.00055
168		4D-1	-0.00061	0.00169	-0.00650	-0.00002	-0.00125
169		4D+2	-0.00008	-0.00035	0.00208	-0.00001	-0.00060
170		4D-2	-0.00201	0.00139	0.00521	-0.00015	0.00045
171	16 H	1S	0.01123	-0.00929	0.01419	0.00003	0.00076
172		2S	0.01392	-0.01761	0.00077	0.00225	0.00213
173	17 C	1S	-0.00102	0.00130	-0.00055	-0.00023	-0.00005
174		2S	0.00367	-0.00424	0.00306	0.00034	0.00031
175		2PX	0.00754	-0.00283	-0.03656	0.00078	0.00441
176		2PY	0.01442	0.00361	-0.11764	0.00038	0.01289
177		2PZ	0.00436	0.00200	-0.04624	0.00020	0.00488

178		3S	-0.01691	0.01078	-0.03554	0.00749	0.00310
179		3PX	-0.01463	0.01803	-0.05837	0.00259	0.01083
180		3PY	0.01609	-0.00157	-0.09758	0.00030	0.02560
181		3PZ	0.01029	-0.00238	-0.02998	-0.00069	0.01305
182		4D 0	0.00059	-0.00047	0.00029	0.00034	0.00814
183		4D+1	0.00050	-0.00036	0.00004	0.00017	0.00444
184		4D-1	0.00004	0.00017	0.00018	0.00025	0.01046
185		4D+2	-0.00013	0.00046	-0.00083	0.00006	0.00532
186		4D-2	0.00028	-0.00013	-0.00064	0.00001	-0.00050
187	18 H	1S	-0.00271	0.00333	-0.00192	-0.00067	-0.00034
188		2S	-0.01246	0.01372	-0.01262	-0.00136	-0.00037
189	19 C	1S	0.00336	-0.00310	-0.00018	-0.00017	0.00049
190		2S	-0.00810	0.00819	-0.00104	-0.00020	0.00142
191		2PX	-0.01320	0.00766	-0.03251	0.01053	0.00895
192		2PY	-0.01871	0.00139	0.00104	0.03690	0.00205
193		2PZ	0.04991	0.01994	0.00466	-0.15091	-0.01797
194		3S	0.00208	-0.01051	0.02512	0.00710	-0.00982
195		3PX	0.00336	-0.01262	-0.02335	0.00874	0.00414
196		3PY	-0.00724	-0.00593	0.02664	0.04419	0.00684
197		3PZ	0.02797	0.00869	0.01312	-0.15578	-0.01771
198		4D 0	-0.00344	-0.00291	-0.00094	-0.00232	0.00066
199		4D+1	-0.00902	-0.01053	-0.00183	-0.01263	-0.00104
200		4D-1	-0.00368	-0.00443	0.00001	-0.00110	0.00143
201		4D+2	0.00031	-0.00073	-0.00104	0.00032	-0.00234
202		4D-2	0.00219	0.00358	-0.00016	0.00346	-0.00089
203	20 C	1S	-0.00183	0.00073	0.00343	-0.00035	-0.00104
204		2S	0.00425	-0.00138	-0.01041	0.00085	0.00252
205		2PX	0.00585	0.00723	-0.02991	0.00204	-0.02076
206		2PY	0.01636	0.00631	-0.00613	0.00444	0.00981
207		2PZ	-0.03461	-0.04187	-0.00203	-0.01374	-0.00888
208		3S	0.00802	-0.00853	-0.01072	0.00252	0.02123
209		3PX	-0.00146	0.00877	-0.03934	0.00046	-0.04111
210		3PY	0.00351	0.01312	-0.00779	0.00117	0.00969
211		3PZ	-0.02567	-0.02537	-0.00307	-0.00403	0.00110
212		4D 0	0.00252	0.00269	0.00024	0.00524	0.00102
213		4D+1	0.00412	0.00505	0.00083	0.00909	0.00128
214		4D-1	0.00397	0.00441	0.00077	0.00901	0.00153
215		4D+2	0.00197	0.00039	-0.00124	0.00181	-0.00052
216		4D-2	-0.00248	-0.00111	-0.00056	-0.00297	0.00176
217	21 C	1S	-0.00087	0.00049	-0.00054	-0.00025	-0.00218
218		2S	0.00217	-0.00084	0.00066	0.00068	0.00535
219		2PX	-0.00269	-0.00799	0.00360	-0.00568	0.00135
220		2PY	-0.02305	-0.02290	0.00067	-0.01814	0.00850

221		2PZ	0.08757	0.09130	0.01125	0.07886	0.00061
222		3S	0.00555	-0.00242	0.01157	0.00392	0.01428
223		3PX	-0.00780	-0.00354	0.00472	-0.00693	0.00806
224		3PY	-0.02253	-0.02030	0.00700	-0.01795	0.00850
225		3PZ	0.06872	0.07682	0.01083	0.08033	-0.00003
226		4D 0	0.00080	0.00015	0.00004	-0.00455	-0.00042
227		4D+1	-0.00058	-0.00110	-0.00029	-0.00617	-0.00072
228		4D-1	0.00209	0.00065	0.00033	-0.00816	-0.00134
229		4D+2	0.00060	0.00017	-0.00032	-0.00169	-0.00002
230		4D-2	-0.00072	0.00064	-0.00138	0.00218	0.00131
231	22 C	1S	0.00138	-0.00067	-0.00168	0.00002	-0.00129
232		2S	-0.00303	0.00089	0.00369	-0.00039	0.00344
233		2PX	0.00609	0.00653	0.00483	0.00997	0.00063
234		2PY	0.01583	0.02615	0.01008	0.03448	0.00757
235		2PZ	-0.09756	-0.09362	-0.01030	-0.14097	-0.01169
236		3S	-0.01172	0.01231	0.00259	0.00073	0.00430
237		3PX	0.00780	0.00626	0.00722	0.01288	-0.00026
238		3PY	0.01296	0.02606	0.00067	0.04034	0.00677
239		3PZ	-0.08166	-0.08087	-0.01061	-0.16489	-0.01918
240		4D 0	-0.00054	-0.00077	0.00020	-0.00113	-0.00019
241		4D+1	-0.00001	0.00059	-0.00038	0.00406	0.00013
242		4D-1	-0.00112	-0.00177	0.00019	-0.00371	-0.00121
243		4D+2	-0.00025	-0.00045	-0.00055	-0.00123	-0.00096
244		4D-2	0.00017	0.00025	-0.00110	-0.00070	-0.00155
245	23 H	1S	0.00510	-0.00363	0.00145	-0.00004	-0.00559
246		2S	0.00129	0.00084	-0.02934	-0.00120	-0.05824
247	24 C	1S	0.00049	0.00016	0.00029	0.00017	-0.00200
248		2S	-0.00101	0.00025	-0.00148	-0.00002	0.00455
249		2PX	-0.00283	0.00159	-0.00771	-0.00740	-0.00373
250		2PY	0.00174	-0.00317	0.00044	-0.02473	-0.00217
251		2PZ	-0.00695	0.01074	-0.00535	0.10034	0.01983
252		3S	-0.00792	-0.00060	-0.00100	-0.00331	0.01640
253		3PX	-0.00400	-0.00003	0.00048	-0.00932	-0.00301
254		3PY	0.00148	-0.00652	0.00182	-0.03071	-0.00637
255		3PZ	-0.00081	0.01314	-0.00273	0.12004	0.02386
256		4D 0	0.00045	0.00055	-0.00004	-0.00020	0.00004
257		4D+1	0.00647	0.00668	0.00081	0.00924	0.00044
258		4D-1	-0.00096	-0.00091	0.00004	-0.00315	-0.00067
259		4D+2	-0.00044	-0.00079	-0.00043	-0.00149	0.00010
260		4D-2	-0.00151	-0.00161	-0.00026	-0.00199	0.00004
261	25 H	1S	0.00280	-0.00054	0.00434	0.00024	-0.00407
262		2S	-0.00057	-0.00283	0.01033	0.00096	-0.01477
263	26 H	1S	0.00135	0.00036	-0.00625	-0.00004	-0.00608

264		2S	0.00349	0.00032	-0.00932	0.00056	-0.01907
265	27 H	1S	-0.00077	0.00027	0.00183	0.00033	-0.00117
266		2S	0.00008	-0.00088	0.00449	0.00047	-0.00927
267	28 C	1S	-0.01476	0.01510	-0.01869	0.00007	0.00362
268		2S	0.02738	-0.02721	0.02927	0.00018	-0.00576
269		2PX	-0.07960	0.09072	-0.10525	-0.00699	0.01198
270		2PY	0.06484	-0.00348	0.04009	-0.03239	-0.01436
271		2PZ	-0.01832	-0.16161	-0.01899	0.10709	0.00598
272		3S	0.03111	-0.02528	0.09686	-0.00063	-0.02205
273		3PX	-0.09640	0.12073	-0.08063	-0.01078	0.00789
274		3PY	0.02764	-0.00468	0.04733	-0.03571	-0.02315
275		3PZ	-0.01695	-0.10874	-0.00693	0.10539	-0.00268
276		4D 0	0.00521	0.00223	0.00259	0.00509	-0.00051
277		4D+1	0.00718	-0.01083	-0.00456	0.00866	-0.00182
278		4D-1	0.00502	0.01024	0.00286	0.00644	0.00012
279		4D+2	0.00236	0.00404	-0.00809	0.00127	-0.00225
280		4D-2	-0.00329	0.00352	-0.00462	-0.00290	-0.00153
281	29 C	1S	0.00225	-0.00488	0.01146	0.00059	0.00208
282		2S	-0.00839	0.01583	-0.02802	-0.00298	-0.00432
283		2PX	0.02504	-0.02714	0.06957	-0.00925	0.00640
284		2PY	-0.05482	0.02538	0.03022	-0.04079	0.00468
285		2PZ	0.16400	-0.09094	-0.00561	0.14093	-0.01482
286		3S	0.05433	-0.05725	0.00328	0.00560	-0.00940
287		3PX	-0.01526	0.00775	0.05706	-0.01087	-0.00289
288		3PY	-0.04909	0.05873	0.00614	-0.04341	-0.00414
289		3PZ	0.11950	-0.05864	-0.00978	0.13259	-0.01570
290		4D 0	-0.00142	0.00248	-0.00095	-0.00149	-0.00037
291		4D+1	0.00651	0.00844	0.00022	-0.01058	-0.00035
292		4D-1	-0.00493	0.00212	-0.00039	-0.00070	0.00031
293		4D+2	0.00439	-0.00410	0.00380	0.00055	-0.00038
294		4D-2	-0.00479	0.00050	-0.00434	0.00314	0.00008
295	30 C	1S	0.00390	-0.00387	-0.00293	0.00022	-0.00129
296		2S	-0.00767	0.01026	0.00488	0.00006	0.00278
297		2PX	0.02372	0.00313	0.01138	0.00841	0.00570
298		2PY	0.00334	0.08140	0.01959	0.04280	0.01507
299		2PZ	-0.15789	-0.18915	-0.02408	-0.14948	0.00657
300		3S	-0.01288	-0.00965	0.03528	-0.00357	-0.00009
301		3PX	0.04223	-0.04229	0.03792	0.01366	0.00153
302		3PY	0.01222	0.04589	0.00869	0.03619	0.00117
303		3PZ	-0.10954	-0.15962	-0.02206	-0.14536	0.00472
304		4D 0	0.00010	-0.00261	-0.00025	0.00455	0.00055
305		4D+1	-0.00491	0.00188	-0.00143	0.00921	0.00078
306		4D-1	0.00090	-0.00519	-0.00115	0.00655	0.00082

307		4D+2	0.00104	-0.00149	-0.00083	0.00125	0.00042
308		4D-2	-0.00331	0.00435	-0.00472	-0.00297	0.00117
309	31 C	1S	-0.01233	0.00444	-0.00688	0.00017	-0.00020
310		2S	0.03023	-0.01333	0.01847	0.00020	0.00033
311		2PX	-0.00471	0.01745	-0.03502	0.00846	-0.00032
312		2PY	-0.00188	-0.04654	0.01319	0.03756	0.00025
313		2PZ	0.18731	0.10217	0.01491	-0.13194	-0.00195
314		3S	0.04172	0.01898	-0.01186	-0.00638	0.00322
315		3PX	-0.00286	-0.03008	0.01822	0.01248	0.00229
316		3PY	-0.03124	-0.04967	0.00889	0.04343	0.00340
317		3PZ	0.11854	0.05920	0.01257	-0.13498	-0.00061
318		4D 0	-0.00072	-0.00534	0.00044	-0.00645	0.00021
319		4D+1	-0.00967	0.00260	-0.00021	-0.01532	0.00143
320		4D-1	-0.00075	-0.00882	-0.00127	-0.00823	0.00019
321		4D+2	0.00353	-0.00206	-0.00314	-0.00206	-0.00004
322		4D-2	0.00076	0.00074	-0.00181	0.00533	-0.00034
323	32 H	1S	-0.01908	0.01243	-0.00461	-0.00076	0.00221
324		2S	-0.03513	0.00452	-0.02975	0.00349	0.01973
325	33 C	1S	-0.00543	0.00358	-0.00223	0.00023	0.00145
326		2S	0.01519	-0.01129	0.00716	-0.00076	-0.00361
327		2PX	-0.01076	0.01665	-0.01563	-0.00337	0.00386
328		2PY	0.05975	-0.02316	0.00545	-0.01893	-0.00384
329		2PZ	-0.11373	0.02752	0.00612	0.06360	0.00224
330		3S	-0.00699	0.03331	-0.03002	-0.00675	-0.00791
331		3PX	-0.00712	0.01041	-0.00649	-0.00382	0.00780
332		3PY	0.01968	0.02029	-0.02177	-0.02139	0.00424
333		3PZ	-0.09203	0.03330	-0.00161	0.06074	0.00360
334		4D 0	0.00059	0.00041	0.00068	0.00106	-0.00008
335		4D+1	0.00635	0.01324	0.00180	0.01101	-0.00014
336		4D-1	-0.00251	-0.00032	-0.00046	-0.00054	0.00033
337		4D+2	0.00252	-0.00258	-0.00025	-0.00082	-0.00091
338		4D-2	-0.00204	-0.00423	-0.00075	-0.00309	-0.00049
339	34 C	1S	0.00171	0.00046	-0.00044	-0.00039	0.00074
340		2S	-0.00368	0.00138	-0.00123	0.00020	-0.00164
341		2PX	0.00430	-0.01345	0.00212	-0.00727	0.00188
342		2PY	-0.04755	-0.05300	-0.00505	-0.02996	0.00098
343		2PZ	0.03684	0.19959	0.03004	0.10866	-0.00047
344		3S	0.00139	-0.04681	0.02749	0.00878	-0.00753
345		3PX	-0.00306	0.01874	-0.02491	-0.01261	0.00182
346		3PY	-0.04502	-0.05838	0.00561	-0.03361	0.00188
347		3PZ	0.02277	0.15331	0.02496	0.13061	0.00001
348		4D 0	0.00422	0.00192	-0.00018	-0.00360	-0.00014
349		4D+1	0.00294	-0.00046	-0.00036	-0.00350	-0.00008

350		4D-1	0.00715	0.00272	0.00029	-0.00575	-0.00010
351		4D+2	0.00342	0.00022	0.00033	-0.00163	-0.00021
352		4D-2	-0.00230	0.00114	-0.00117	0.00150	-0.00011
353	35 H	1S	-0.02042	0.01023	-0.00239	-0.00015	0.00382
354		2S	-0.03857	0.02770	-0.01045	-0.00082	0.01346
355	36 H	1S	0.01278	-0.00627	0.00474	-0.00040	0.00035
356		2S	-0.00297	-0.01861	0.01778	0.00166	0.00245
357	37 C	1S	-0.00148	0.00168	0.00287	0.00265	0.00001
358		2S	0.00495	-0.00757	-0.00535	-0.00341	-0.00062
359		2PX	-0.01323	0.03770	0.00843	-0.01838	-0.03098
360		2PY	-0.01200	-0.02489	0.02039	0.00542	-0.09655
361		2PZ	-0.01219	0.00863	0.01826	0.00402	-0.03335
362		3S	0.00257	0.00449	-0.02423	-0.03170	0.00301
363		3PX	-0.01811	0.03826	0.00779	-0.03151	-0.03247
364		3PY	-0.00306	-0.02057	0.01383	0.02501	-0.09469
365		3PZ	-0.00435	0.01948	0.00530	0.00972	-0.03090
366		4D 0	-0.00009	-0.00012	0.00260	-0.00067	-0.01127
367		4D+1	0.00066	-0.00120	0.00089	-0.00038	-0.00929
368		4D-1	-0.00006	-0.00022	0.00188	-0.00080	-0.01585
369		4D+2	0.00037	0.00056	0.00137	-0.00007	-0.01219
370		4D-2	0.00038	0.00067	0.00155	0.00041	-0.00591
371	38 C	1S	-0.00157	-0.00222	-0.00479	0.00099	-0.00089
372		2S	0.00390	0.00339	0.01120	-0.00376	0.00126
373		2PX	-0.02014	0.03293	0.00004	-0.00395	-0.08037
374		2PY	-0.00722	-0.01409	0.00062	-0.00743	-0.26095
375		2PZ	-0.01279	0.00123	-0.01388	-0.00068	-0.09306
376		3S	-0.01173	0.04479	0.00285	0.00438	0.01082
377		3PX	-0.00401	0.03515	0.02420	-0.00607	-0.08861
378		3PY	-0.01173	-0.01029	-0.01224	-0.00693	-0.26175
379		3PZ	0.00720	-0.01896	0.00546	-0.00695	-0.09102
380		4D 0	-0.00016	0.00083	-0.00247	-0.00025	-0.00192
381		4D+1	0.00059	-0.00132	-0.00264	0.00087	0.00482
382		4D-1	0.00045	0.00026	-0.00219	0.00028	-0.00477
383		4D+2	-0.00036	0.00031	-0.00426	0.00035	0.00913
384		4D-2	-0.00037	0.00012	-0.00290	-0.00045	0.01453
385	39 C	1S	0.00061	-0.00125	-0.00196	0.00005	-0.00022
386		2S	-0.00073	0.00293	0.00381	0.00035	0.00072
387		2PX	0.00105	-0.00579	0.01473	-0.00280	-0.05811
388		2PY	0.00094	-0.00148	0.04524	-0.01038	-0.18362
389		2PZ	0.00367	-0.00705	0.00745	-0.00521	-0.06335
390		3S	-0.00543	-0.00655	0.01783	-0.00258	-0.00192
391		3PX	0.00498	-0.00566	0.01297	-0.00082	-0.07192
392		3PY	-0.00351	-0.00501	0.04047	-0.01819	-0.23227

393		3PZ	0.00372	-0.00039	0.00659	-0.00509	-0.07770
394		4D 0	0.00055	0.00002	-0.00056	0.00021	0.00580
395		4D+1	0.00045	-0.00181	-0.00019	0.00094	-0.00137
396		4D-1	0.00083	0.00122	-0.00101	-0.00020	0.00998
397		4D+2	-0.00021	0.00036	0.00017	-0.00028	-0.00490
398		4D-2	-0.00089	0.00025	0.00091	-0.00031	-0.01273
399	40 H	1S	-0.00053	0.00577	-0.00400	0.00118	-0.00055
400		2S	0.01437	-0.03252	-0.00214	0.04543	0.00144
401	41 C	1S	0.00047	-0.00038	0.00114	0.00084	0.00020
402		2S	-0.00052	0.00059	-0.00242	-0.00156	-0.00018
403		2PX	0.00404	-0.00225	-0.01594	0.00263	0.00103
404		2PY	0.00553	0.00948	-0.04448	0.00894	0.00293
405		2PZ	0.00562	-0.00020	-0.01040	0.00504	0.00271
406		3S	-0.01056	0.00624	-0.01095	-0.00499	-0.00450
407		3PX	-0.00511	-0.00507	-0.02274	0.00326	-0.00454
408		3PY	0.00621	0.00989	-0.03056	0.00933	-0.01623
409		3PZ	0.00225	-0.00180	-0.01265	0.00566	-0.00072
410		4D 0	0.00090	-0.00037	0.00003	0.00023	0.01219
411		4D+1	0.00102	-0.00114	-0.00033	0.00004	0.00822
412		4D-1	0.00060	0.00078	-0.00016	0.00043	0.01728
413		4D+2	0.00018	0.00074	-0.00080	0.00018	0.01063
414		4D-2	0.00012	0.00023	-0.00060	-0.00006	0.00262
415	42 C	1S	-0.00041	-0.00050	0.00007	0.00122	0.00020
416		2S	0.00103	-0.00001	-0.00009	-0.00249	-0.00011
417		2PX	0.00253	0.01292	-0.00493	-0.00255	0.07938
418		2PY	0.01977	0.00207	-0.01068	0.00396	0.25044
419		2PZ	0.00385	0.00370	-0.00404	0.00218	0.08695
420		3S	0.01044	0.00764	0.00678	-0.00531	-0.00207
421		3PX	0.00204	0.00741	-0.00987	-0.00035	0.09880
422		3PY	0.01733	0.00488	-0.01105	0.00540	0.30667
423		3PZ	0.00233	-0.00232	-0.00484	0.00051	0.10433
424		4D 0	-0.00024	-0.00004	0.00030	0.00017	0.00246
425		4D+1	0.00009	-0.00039	0.00103	-0.00054	-0.00195
426		4D-1	-0.00007	0.00001	0.00031	-0.00003	0.00458
427		4D+2	-0.00009	-0.00012	0.00214	-0.00056	-0.00438
428		4D-2	-0.00021	-0.00033	0.00258	-0.00057	-0.00881
429	43 H	1S	0.00234	-0.00926	-0.00178	0.00333	-0.00014
430		2S	0.00120	-0.01398	-0.00356	0.00586	-0.00083
431	44 H	1S	-0.00241	0.00585	0.00074	0.00040	0.00054
432		2S	-0.00578	0.00745	-0.00178	0.00138	0.00046
433	45 H	1S	-0.00132	0.00030	0.00004	0.00137	0.00034
434		2S	-0.00263	0.00222	-0.00082	0.00511	0.00165
435	46 C	1S	-0.00265	0.00136	0.00208	0.00054	0.00549

436		2S	0.00559	-0.00168	-0.00474	-0.00012	-0.01080
437		2PX	0.02494	-0.00859	-0.10745	0.00709	0.04306
438		2PY	-0.02218	0.00511	0.04862	0.00041	-0.00209
439		2PZ	-0.01041	-0.00332	-0.00301	-0.00369	0.00085
440		3S	0.00644	-0.00946	0.00779	-0.00883	-0.06569
441		3PX	0.01684	-0.00409	-0.06783	0.00399	0.03758
442		3PY	-0.02011	0.01250	0.05404	0.00488	0.02619
443		3PZ	-0.00446	0.01836	0.01634	-0.00075	-0.02726
444		4D 0	-0.00112	-0.00045	-0.00042	-0.00063	0.00127
445		4D+1	-0.00729	0.00460	-0.00299	-0.00053	0.00111
446		4D-1	-0.00024	-0.00341	-0.00082	-0.00187	0.00024
447		4D+2	-0.00026	0.00147	-0.01190	-0.00027	0.00175
448		4D-2	0.00117	0.00153	-0.01450	0.00037	-0.00219
449	47 C	1S	0.00268	0.00157	0.00132	0.00196	-0.00116
450		2S	-0.00653	-0.00231	-0.00034	-0.00635	-0.00102
451		2PX	-0.08744	0.06902	-0.14306	0.00085	0.00227
452		2PY	0.04020	-0.02095	0.05327	0.00450	-0.00069
453		2PZ	0.01212	0.00612	0.00193	0.00430	-0.00569
454		3S	-0.00133	-0.02504	-0.03303	-0.00149	0.02111
455		3PX	-0.06437	0.05269	-0.11735	0.00836	-0.00438
456		3PY	0.03137	-0.01785	0.04073	0.00059	-0.04247
457		3PZ	0.00325	0.00998	0.02117	0.00397	-0.01911
458		4D 0	-0.00042	-0.00028	0.00002	-0.00029	-0.00076
459		4D+1	-0.00136	0.00057	0.00430	-0.00029	-0.00196
460		4D-1	0.00085	-0.00028	-0.00194	0.00026	0.00038
461		4D+2	-0.00362	0.00147	0.00114	-0.00065	-0.00261
462		4D-2	-0.00346	0.00177	0.00101	-0.00043	-0.00189
463	48 C	1S	-0.00186	-0.00150	-0.00141	-0.00166	0.00113
464		2S	0.00525	0.00240	0.00415	0.00654	-0.00643
465		2PX	0.09818	-0.02275	-0.16182	-0.00117	-0.01748
466		2PY	-0.04017	0.00314	0.05169	-0.00493	0.01007
467		2PZ	0.01031	0.00395	0.00438	0.00674	-0.00402
468		3S	0.01123	0.01274	-0.00340	0.00069	-0.00390
469		3PX	0.07612	-0.02538	-0.13238	-0.00947	-0.01422
470		3PY	-0.02652	-0.00699	0.02983	-0.01179	0.02674
471		3PZ	0.01022	-0.00059	-0.01674	0.00176	-0.01420
472		4D 0	-0.00029	-0.00014	0.00024	0.00055	-0.00039
473		4D+1	0.00290	-0.00296	-0.00304	0.00074	0.00423
474		4D-1	-0.00112	0.00107	0.00141	0.00009	-0.00135
475		4D+2	0.00204	-0.00136	0.00230	0.00039	0.00085
476		4D-2	0.00319	-0.00217	0.00197	0.00046	0.00110
477	49 C	1S	-0.00170	-0.00063	0.00004	-0.00055	-0.00019
478		2S	0.00445	0.00074	-0.00025	0.00142	-0.00072

479		2PX	-0.10551	0.04786	0.04240	-0.01231	-0.04479
480		2PY	0.03078	-0.01922	-0.01523	0.00184	0.01408
481		2PZ	-0.00020	0.00069	0.00063	0.00059	-0.00229
482		3S	-0.00073	0.01007	0.01148	0.00242	0.02171
483		3PX	-0.06035	0.02964	0.01769	-0.01021	-0.04722
484		3PY	0.02265	-0.01361	-0.00620	0.00762	-0.00610
485		3PZ	0.00349	-0.00233	-0.01028	-0.00164	0.00532
486		4D 0	-0.00037	-0.00010	-0.00012	-0.00003	0.00029
487		4D+1	0.00290	-0.00048	-0.00608	0.00012	0.00049
488		4D-1	-0.00157	-0.00003	0.00222	-0.00027	0.00050
489		4D+2	0.00289	-0.00280	0.00779	0.00017	0.00019
490		4D-2	0.00361	-0.00328	0.00958	0.00001	0.00037
491	50 H	1S	-0.00030	-0.00015	0.00091	-0.00093	-0.00081
492		2S	0.00036	0.00299	-0.00774	-0.00293	-0.01730
493	51 C	1S	0.00006	0.00063	0.00101	0.00077	-0.00013
494		2S	0.00021	-0.00163	-0.00268	-0.00218	0.00024
495		2PX	0.09275	-0.06045	0.04566	0.01155	0.03572
496		2PY	-0.03392	0.02366	-0.01311	-0.00300	-0.01333
497		2PZ	0.00095	0.00018	0.00172	0.00181	-0.00079
498		3S	-0.00462	0.00626	0.01216	0.00582	-0.00641
499		3PX	0.05474	-0.03504	0.01667	0.00793	0.03286
500		3PY	-0.01728	0.00939	-0.01359	-0.01028	0.00107
501		3PZ	-0.00101	0.00179	0.00833	0.00187	0.00374
502		4D 0	-0.00011	-0.00005	0.00011	-0.00004	0.00019
503		4D+1	0.00031	-0.00221	0.00915	0.00004	0.00148
504		4D-1	-0.00058	0.00052	-0.00363	-0.00051	-0.00041
505		4D+2	-0.00373	0.00064	0.00660	-0.00033	0.00074
506		4D-2	-0.00446	0.00087	0.00854	0.00006	0.00066
507	52 C	1S	0.00021	0.00013	0.00014	0.00018	0.00007
508		2S	-0.00083	0.00012	0.00075	-0.00027	-0.00089
509		2PX	-0.01248	-0.02680	0.19036	-0.00019	0.00821
510		2PY	0.00536	0.00969	-0.06770	0.00056	-0.00217
511		2PZ	0.00035	-0.00036	0.00173	-0.00010	-0.00116
512		3S	0.00249	-0.00472	-0.01490	-0.00435	0.00509
513		3PX	-0.01100	-0.02279	0.16733	0.00089	0.01043
514		3PY	0.00006	0.01244	-0.04898	0.00201	-0.00809
515		3PZ	-0.00027	0.00004	0.00085	-0.00330	0.00824
516		4D 0	-0.00019	0.00001	-0.00005	-0.00010	-0.00019
517		4D+1	-0.00606	0.00356	-0.00044	-0.00083	-0.00321
518		4D-1	0.00216	-0.00130	0.00012	0.00030	0.00105
519		4D+2	0.00061	-0.00009	-0.00098	0.00002	0.00019
520		4D-2	0.00089	-0.00012	-0.00144	0.00010	0.00059
521	53 H	1S	0.00077	-0.00003	-0.00034	0.00045	0.00090

522		2S	0.00307	-0.00131	-0.00355	0.00088	0.00343
523	54 N	1S	0.00155	0.00147	-0.00242	0.00028	-0.01214
524		2S	-0.00387	-0.00273	0.00534	-0.00006	0.02605
525		2PX	-0.00718	-0.00970	0.01778	-0.01186	0.00522
526		2PY	-0.03418	-0.02030	0.00810	-0.03607	0.04327
527		2PZ	0.07276	0.08778	0.01970	0.15010	0.02684
528		3S	-0.00109	-0.01553	0.01115	-0.00629	0.09288
529		3PX	-0.00491	-0.00827	-0.01895	-0.01382	0.00341
530		3PY	-0.02849	-0.01536	0.00597	-0.03403	0.04772
531		3PZ	0.06634	0.07696	0.01245	0.15558	0.01745
532		4D 0	-0.00231	-0.00111	0.00002	-0.00129	0.00044
533		4D+1	0.00184	0.00177	-0.00194	-0.00653	-0.00012
534		4D-1	-0.00425	-0.00332	-0.00192	-0.00038	0.00028
535		4D+2	-0.00150	-0.00084	-0.00220	0.00031	0.00305
536		4D-2	0.00179	-0.00067	-0.00648	0.00185	-0.00138
537	55 N	1S	-0.00020	0.00367	0.00211	-0.00431	0.00007
538		2S	0.00002	-0.00848	-0.00470	0.00804	-0.00025
539		2PX	-0.07550	0.05167	0.06695	0.00662	0.05666
540		2PY	0.03083	-0.00755	-0.01781	-0.00827	-0.02261
541		2PZ	0.00517	-0.01143	-0.00330	0.01287	-0.00436
542		3S	0.00364	-0.01961	-0.01352	0.04787	0.00073
543		3PX	-0.06287	0.04029	0.05687	-0.00162	0.05530
544		3PY	0.02522	-0.00659	-0.02481	-0.00066	-0.02555
545		3PZ	0.00477	-0.01339	-0.00126	0.01567	-0.00070
546		4D 0	-0.00209	-0.00171	-0.00140	-0.00044	0.00358
547		4D+1	0.00540	-0.01200	0.00012	0.00027	-0.00021
548		4D-1	-0.00353	0.00313	-0.00122	-0.00047	0.00234
549		4D+2	-0.00394	0.00398	0.00175	-0.00169	0.00023
550		4D-2	-0.00346	0.00462	0.00250	0.00038	-0.00253
551	56 N	1S	0.00111	-0.00271	0.00048	0.00402	0.00146
552		2S	-0.00290	0.00410	-0.00056	-0.00820	-0.00288
553		2PX	0.00337	-0.01704	-0.01617	-0.00221	0.08866
554		2PY	-0.01544	0.00757	-0.04238	-0.00416	0.28054
555		2PZ	0.00151	-0.02101	-0.02159	0.01602	0.10188
556		3S	-0.00578	0.01982	-0.01121	-0.03748	-0.01113
557		3PX	-0.00147	0.02056	0.00361	-0.00582	0.09119
558		3PY	-0.01267	-0.00722	-0.04040	-0.01317	0.29260
559		3PZ	-0.00919	-0.01782	-0.02159	0.00930	0.10718
560		4D 0	-0.00105	-0.00354	-0.00162	0.00051	0.00047
561		4D+1	0.00170	-0.00758	-0.00181	0.00071	0.00189
562		4D-1	-0.00312	0.00283	0.00038	-0.00079	0.00006
563		4D+2	-0.00160	0.00234	0.00218	-0.00095	0.00515
564		4D-2	0.00026	0.00168	0.00268	0.00105	0.00602

565	57	N	1S	0.01400	-0.00226	0.00414	-0.00033	0.00003
566			2S	-0.02521	0.00353	-0.00890	0.00096	0.00013
567			2PX	0.02249	-0.00698	0.01891	0.01350	-0.00106
568			2PY	-0.06557	0.01026	0.01179	0.08120	-0.00641
569			2PZ	-0.13551	-0.04617	0.00030	-0.25991	0.02036
570			3S	-0.08113	0.03117	-0.03298	-0.00009	-0.00288
571			3PX	0.00189	-0.00629	0.01075	0.01369	-0.00089
572			3PY	-0.04466	0.00184	0.01435	0.07489	-0.00484
573			3PZ	-0.09794	-0.03667	0.00163	-0.23848	0.01972
574			4D 0	-0.00168	0.00014	-0.00039	0.00437	-0.00025
575			4D+1	-0.01119	-0.00607	-0.00105	0.01666	-0.00056
576			4D-1	0.00660	0.00124	-0.00042	0.00457	-0.00035
577			4D+2	0.00381	-0.00021	0.00159	0.00063	-0.00012
578			4D-2	0.00428	0.00272	-0.00149	-0.00540	0.00017
579	58	N	1S	0.00978	0.00135	-0.00301	0.00025	0.00000
580			2S	-0.01741	-0.00293	0.00680	-0.00060	-0.00010
581			2PX	-0.00958	0.01086	-0.01153	-0.01490	0.00078
582			2PY	0.14156	0.02380	-0.00061	-0.09014	0.00508
583			2PZ	-0.11190	-0.07708	-0.00971	0.28982	-0.01595
584			3S	-0.03496	-0.01259	0.02126	-0.00204	0.00136
585			3PX	0.01026	0.00556	-0.00386	-0.01402	0.00066
586			3PY	0.10990	0.01442	0.00154	-0.08217	0.00539
587			3PZ	-0.08240	-0.05343	-0.00554	0.26291	-0.01468
588			4D 0	-0.00570	-0.00191	0.00018	0.00452	-0.00026
589			4D+1	0.00985	0.00328	-0.00013	0.01345	-0.00120
590			4D-1	-0.00405	-0.00363	-0.00041	0.00520	-0.00016
591			4D+2	-0.00200	-0.00101	-0.00096	0.00121	0.00001
592			4D-2	-0.00103	-0.00024	-0.00093	-0.00456	0.00039
593	59	C	1S	-0.00716	-0.00077	0.00177	-0.00009	0.00000
594			2S	0.01633	0.00165	-0.00396	-0.00009	0.00012
595			2PX	-0.03398	-0.00688	0.00952	-0.00317	0.00031
596			2PY	-0.06819	-0.01711	0.00299	-0.02251	0.00263
597			2PZ	0.12189	0.04746	0.00576	0.06868	-0.00823
598			3S	0.04871	0.00534	-0.01241	0.00234	-0.00117
599			3PX	0.01715	-0.00493	0.00410	-0.00423	0.00100
600			3PY	0.00102	-0.01339	0.00580	-0.02770	0.00275
601			3PZ	0.09526	0.02579	0.00421	0.08449	-0.00941
602			4D 0	0.00256	0.00162	0.00023	-0.00763	0.00052
603			4D+1	0.00824	0.00461	0.00035	-0.01550	0.00086
604			4D-1	0.00270	0.00206	0.00015	-0.01009	0.00068
605			4D+2	0.00419	0.00045	0.00008	-0.00277	0.00019
606			4D-2	-0.00448	-0.00131	-0.00053	0.00547	-0.00035
607	60	C	1S	-0.00245	0.00038	-0.00056	-0.00019	0.00001

608		2S	0.00681	-0.00080	0.00100	0.00046	0.00000
609		2PX	-0.01207	0.00019	-0.00368	0.00516	-0.00033
610		2PY	-0.03339	-0.01549	-0.00023	0.04145	-0.00250
611		2PZ	0.10224	0.04568	0.00460	-0.12848	0.00783
612		3S	0.00241	-0.00163	0.00449	0.00117	-0.00037
613		3PX	-0.00474	0.00162	-0.00511	0.00628	-0.00052
614		3PY	-0.05008	-0.01254	0.00067	0.03827	-0.00251
615		3PZ	0.07482	0.03900	0.00425	-0.11901	0.00745
616		4D 0	0.00085	0.00035	0.00002	-0.00090	0.00005
617		4D+1	-0.00579	-0.00211	-0.00026	-0.00595	0.00064
618		4D-1	0.00143	0.00083	0.00017	-0.00063	-0.00002
619		4D+2	0.00213	0.00050	-0.00023	-0.00002	-0.00003
620		4D-2	0.00201	0.00079	-0.00018	0.00194	-0.00021
621	61 C	1S	0.00170	-0.00002	-0.00009	0.00015	-0.00002
622		2S	-0.00125	-0.00002	0.00019	-0.00035	0.00007
623		2PX	-0.01200	-0.00164	-0.00075	0.00621	-0.00054
624		2PY	-0.00879	-0.01470	-0.00287	0.04479	-0.00305
625		2PZ	0.11051	0.04585	0.00388	-0.13583	0.00958
626		3S	-0.03660	0.00106	-0.00002	-0.00091	0.00041
627		3PX	-0.02931	-0.00113	0.00119	0.00681	-0.00045
628		3PY	0.02002	-0.01391	-0.00033	0.05005	-0.00438
629		3PZ	0.09082	0.03551	0.00392	-0.15249	0.01152
630		4D 0	-0.00307	-0.00120	-0.00014	-0.00149	0.00020
631		4D+1	-0.00063	-0.00006	-0.00009	-0.00094	0.00007
632		4D-1	-0.00527	-0.00191	-0.00018	-0.00224	0.00032
633		4D+2	-0.00141	-0.00075	0.00000	-0.00077	0.00011
634		4D-2	0.00091	0.00028	-0.00030	0.00044	-0.00003
635	62 C	1S	0.00036	-0.00024	0.00042	0.00008	-0.00001
636		2S	-0.00042	0.00058	-0.00094	-0.00014	0.00002
637		2PX	0.00316	-0.00047	0.00230	0.00210	-0.00025
638		2PY	0.01645	0.00567	0.00134	0.01317	-0.00154
639		2PZ	-0.05393	-0.01914	-0.00116	-0.04042	0.00474
640		3S	0.00875	-0.00016	-0.00149	-0.00114	0.00022
641		3PX	-0.00291	0.00073	0.00097	0.00296	-0.00033
642		3PY	0.01654	0.00507	-0.00021	0.01863	-0.00219
643		3PZ	-0.03895	-0.01420	-0.00132	-0.05551	0.00624
644		4D 0	-0.00408	-0.00173	-0.00021	0.00568	-0.00041
645		4D+1	-0.00393	-0.00173	-0.00020	0.00571	-0.00036
646		4D-1	-0.00607	-0.00255	-0.00027	0.00827	-0.00061
647		4D+2	-0.00201	-0.00094	0.00006	0.00276	-0.00020
648		4D-2	0.00140	0.00078	-0.00005	-0.00233	0.00015
649	63 H	1S	-0.00144	-0.00022	0.00060	0.00014	-0.00003
650		2S	-0.02424	-0.00065	0.00240	-0.00062	0.00004

651	64	C	1S	-0.00103	-0.00009	0.00026	-0.00006	0.00000
652			2S	0.00240	0.00015	-0.00047	0.00015	0.00003
653			2PX	-0.00004	0.00007	0.00150	0.00002	-0.00004
654			2PY	0.00877	0.00509	0.00118	0.00114	-0.00034
655			2PZ	-0.05029	-0.01656	-0.00096	-0.00400	0.00105
656			3S	0.01548	0.00027	-0.00221	0.00026	-0.00007
657			3PX	0.00225	-0.00110	0.00253	0.00010	-0.00027
658			3PY	-0.00268	0.00404	0.00077	0.00249	-0.00001
659			3PZ	-0.03753	-0.01118	-0.00059	-0.00789	0.00138
660			4D 0	-0.00049	-0.00023	-0.00002	0.00084	-0.00005
661			4D+1	-0.00841	-0.00356	-0.00034	0.01160	-0.00087
662			4D-1	0.00005	0.00012	0.00005	-0.00031	0.00004
663			4D+2	0.00167	0.00023	-0.00010	-0.00054	0.00006
664			4D-2	0.00208	0.00117	0.00012	-0.00377	0.00028
665	65	H	1S	0.00554	-0.00067	0.00093	0.00005	0.00000
666			2S	-0.02419	0.00067	0.00146	-0.00017	0.00042
667	66	C	1S	-0.00127	-0.00005	0.00013	-0.00003	0.00000
668			2S	0.00357	0.00007	-0.00030	0.00004	0.00000
669			2PX	0.00146	0.00285	0.00015	-0.00696	0.00048
670			2PY	0.04862	0.01886	0.00184	-0.04904	0.00358
671			2PZ	-0.14287	-0.05882	-0.00533	0.15188	-0.01105
672			3S	-0.00606	0.00081	-0.00056	0.00006	0.00038
673			3PX	0.00893	0.00150	0.00050	-0.00747	0.00045
674			3PY	0.03939	0.01565	0.00047	-0.05167	0.00408
675			3PZ	-0.10992	-0.04670	-0.00465	0.16038	-0.01255
676			4D 0	0.00052	0.00012	0.00000	0.00137	-0.00014
677			4D+1	0.00078	0.00021	-0.00001	0.00137	-0.00012
678			4D-1	0.00043	0.00017	0.00002	0.00199	-0.00020
679			4D+2	0.00032	0.00007	-0.00003	0.00067	-0.00007
680			4D-2	-0.00040	-0.00003	-0.00007	-0.00057	0.00005
681	67	H	1S	0.00090	-0.00064	0.00104	0.00011	-0.00001
682			2S	0.00259	-0.00109	0.00168	0.00037	-0.00008
683	68	H	1S	-0.00658	-0.00018	0.00065	-0.00016	-0.00002
684			2S	-0.00702	-0.00049	0.00113	-0.00041	-0.00026
685	69	H	1S	-0.00113	0.00023	-0.00033	-0.00004	0.00000
686			2S	-0.00450	0.00035	-0.00026	-0.00008	-0.00001
687	70	F	1S	-0.00098	0.00034	-0.00163	0.00045	0.00012
688			2S	0.00192	-0.00027	0.00322	-0.00090	-0.00035
689			2PX	0.00916	-0.00294	0.02105	-0.00306	-0.01765
690			2PY	-0.00762	0.00079	0.01381	-0.00227	-0.05346
691			2PZ	-0.00800	0.00023	-0.00473	0.00107	-0.02011
692			3S	0.00873	-0.00501	0.01461	-0.00389	-0.00087
693			3PX	0.00646	-0.00192	0.01585	-0.00268	-0.01629

694		3PY	-0.00549	0.00026	0.01025	-0.00214	-0.04987
695		3PZ	-0.00693	0.00112	-0.00528	0.00106	-0.01889
696		4D 0	-0.00002	0.00003	0.00050	-0.00002	-0.00220
697		4D+1	0.00022	-0.00020	0.00074	-0.00007	-0.00106
698		4D-1	-0.00018	0.00004	0.00036	-0.00005	-0.00293
699		4D+2	-0.00023	0.00006	0.00034	0.00003	-0.00127
700		4D-2	-0.00004	0.00003	0.00045	0.00003	0.00038
701	71 F	1S	-0.00139	0.00195	-0.00104	-0.00010	0.00013
702		2S	0.00292	-0.00447	0.00154	0.00031	-0.00033
703		2PX	0.02031	-0.02637	0.01802	0.00186	0.02302
704		2PY	-0.00639	0.00858	0.01057	0.00214	0.07455
705		2PZ	0.00285	-0.00396	0.00859	0.00092	0.02759
706		3S	0.01172	-0.01393	0.01254	0.00020	-0.00079
707		3PX	0.01533	-0.01992	0.01457	0.00141	0.02083
708		3PY	-0.00506	0.00689	0.00720	0.00200	0.06600
709		3PZ	0.00296	-0.00410	0.00719	0.00103	0.02436
710		4D 0	0.00034	-0.00041	-0.00035	0.00003	-0.00159
711		4D+1	-0.00012	0.00007	-0.00024	-0.00003	-0.00142
712		4D-1	0.00002	0.00014	-0.00071	-0.00007	-0.00186
713		4D+2	-0.00028	0.00034	-0.00018	-0.00009	-0.00203
714		4D-2	0.00011	-0.00024	0.00074	-0.00001	-0.00135
715	72 F	1S	-0.00012	-0.00008	-0.00022	-0.00039	0.00009
716		2S	0.00036	0.00019	0.00024	0.00078	-0.00008
717		2PX	-0.05367	0.03233	-0.02911	-0.00564	-0.01279
718		2PY	0.01748	-0.01374	0.00706	-0.00075	0.00577
719		2PZ	0.00046	0.00105	0.00067	0.00100	-0.00070
720		3S	0.00034	0.00074	0.00318	0.00325	-0.00127
721		3PX	-0.04324	0.02599	-0.02113	-0.00503	-0.01189
722		3PY	0.01415	-0.01090	0.00483	-0.00034	0.00482
723		3PZ	0.00020	0.00093	0.00105	0.00134	-0.00160
724		4D 0	0.00003	0.00004	0.00007	0.00007	-0.00014
725		4D+1	0.00065	-0.00073	0.00136	0.00016	0.00083
726		4D-1	-0.00027	0.00027	-0.00045	-0.00001	-0.00026
727		4D+2	-0.00042	0.00018	0.00047	-0.00001	-0.00018
728		4D-2	-0.00050	0.00016	0.00047	-0.00011	-0.00007
729	73 F	1S	0.00038	0.00011	0.00004	0.00016	-0.00051
730		2S	-0.00088	-0.00029	-0.00042	-0.00041	0.00161
731		2PX	0.07004	-0.02974	-0.02552	0.00569	0.01797
732		2PY	-0.01918	0.01246	0.00971	-0.00055	-0.00908
733		2PZ	0.00308	0.00055	-0.00009	0.00064	-0.00131
734		3S	-0.00268	-0.00039	0.00178	-0.00087	0.00120
735		3PX	0.05538	-0.02388	-0.01892	0.00509	0.01681
736		3PY	-0.01551	0.01024	0.00695	-0.00113	-0.00635

737		3PZ	0.00263	0.00063	-0.00036	0.00071	-0.00116
738		4D 0	-0.00007	-0.00005	-0.00008	-0.00007	0.00012
739		4D+1	0.00047	-0.00019	-0.00108	0.00018	0.00068
740		4D-1	-0.00011	0.00001	0.00038	0.00004	-0.00035
741		4D+2	0.00029	-0.00032	0.00074	-0.00002	0.00028
742		4D-2	0.00047	-0.00040	0.00086	0.00007	0.00024

A4

			176	177	178	179	180
			O	O	V	V	V
Eigenvalues --			-0.19094	-0.17561	-0.07584	-0.04833	-0.04619
1	1	Ir 1S	-0.00915	0.00870	0.00131	0.00441	-0.00731
2		2S	0.01344	-0.01232	-0.00190	-0.00628	0.01043
3		3S	-0.04752	0.06462	0.00069	0.00142	-0.00812
4		4PX	-0.06386	-0.06002	-0.00463	0.00489	-0.00916
5		4PY	-0.03271	-0.04701	-0.00157	-0.00808	0.01180
6		4PZ	-0.00359	-0.00036	-0.00349	-0.01364	-0.00413
7		5PX	0.03804	0.02478	-0.00549	-0.06643	0.04600
8		5PY	0.01987	0.02656	0.00097	0.05022	-0.07105
9		5PZ	-0.00557	-0.00693	0.01320	0.08961	0.03126
10		6PX	-0.02198	-0.01558	0.00035	0.02314	-0.00639
11		6PY	-0.00177	-0.03814	-0.00206	-0.01083	0.01929
12		6PZ	-0.02248	0.00625	0.01361	-0.01411	-0.00484
13		7D 0	-0.05434	0.01610	-0.01253	-0.01332	-0.03184
14		7D+1	0.49065	-0.16470	-0.01348	-0.02381	0.02744
15		7D-1	0.18819	-0.00842	-0.03712	0.01204	-0.19098
16		7D+2	0.03627	0.45649	0.00336	-0.04631	0.06538
17		7D-2	-0.04101	-0.26168	0.00289	-0.00301	-0.01504
18		8D 0	-0.01356	-0.00646	-0.00168	0.00148	-0.01561
19		8D+1	0.17508	-0.05195	-0.00522	-0.01247	0.00423
20		8D-1	0.06774	0.00032	-0.02143	0.00100	-0.07553
21		8D+2	0.02129	0.16551	0.00323	-0.01781	0.02724
22		8D-2	-0.01960	-0.09618	0.00186	0.01001	-0.01545
23	2	C 1S	-0.00088	0.00126	0.00035	0.00294	-0.00259
24		2S	0.00356	-0.00280	-0.00023	-0.00913	0.00616
25		2PX	-0.05604	-0.04015	0.00023	0.01576	0.01183
26		2PY	-0.03482	-0.02290	-0.00516	-0.00251	-0.00932
27		2PZ	-0.00021	0.00502	-0.00046	0.00565	-0.01010

28		3S	0.00402	-0.01232	-0.00696	-0.01378	0.01559
29		3PX	-0.04801	-0.02713	-0.00428	0.00738	0.01441
30		3PY	-0.03595	-0.01541	-0.00844	-0.01457	-0.00939
31		3PZ	0.00147	0.00158	-0.00378	-0.02444	-0.02283
32		4D 0	0.00046	0.00016	-0.00014	0.00042	-0.00102
33		4D+1	0.00219	-0.00450	0.00045	0.00589	-0.00017
34		4D-1	0.00132	-0.00276	0.00013	0.00253	-0.00001
35		4D+2	-0.00172	0.00163	0.00012	-0.00129	-0.00040
36		4D-2	0.00124	-0.00108	-0.00004	0.00129	-0.00049
37	3 C	1S	0.00125	-0.00092	0.00038	-0.00131	0.00263
38		2S	-0.00313	0.00212	-0.00306	0.00141	-0.01065
39		2PX	-0.07185	-0.02084	0.00178	0.06137	0.00282
40		2PY	-0.05262	-0.00568	0.00017	0.04231	-0.00915
41		2PZ	0.00557	-0.00090	0.00086	-0.00393	0.00375
42		3S	0.00323	-0.00212	0.00588	0.01076	-0.00993
43		3PX	-0.05597	-0.02027	0.00259	0.07129	-0.00237
44		3PY	-0.04025	0.00527	0.00587	0.03525	-0.00131
45		3PZ	-0.00071	0.00459	-0.00577	-0.00514	0.00219
46		4D 0	0.00046	-0.00091	-0.00021	-0.00019	-0.00028
47		4D+1	-0.00148	0.00639	-0.00031	-0.00117	0.00040
48		4D-1	-0.00128	0.00358	-0.00001	0.00043	0.00047
49		4D+2	0.00253	-0.00522	-0.00012	0.00347	0.00003
50		4D-2	-0.00177	0.00349	0.00000	-0.00200	-0.00010
51	4 C	1S	-0.00022	-0.00033	0.00011	-0.00128	0.00146
52		2S	0.00002	0.00032	-0.00042	0.00193	-0.00428
53		2PX	0.03214	-0.05993	0.00448	0.05054	-0.00329
54		2PY	0.01970	-0.03453	0.00268	0.03112	-0.00371
55		2PZ	-0.00222	0.00160	-0.00009	-0.00638	0.00512
56		3S	0.00041	0.00508	0.00287	0.02377	0.00112
57		3PX	0.02516	-0.05589	0.00663	0.06337	-0.00444
58		3PY	0.01699	-0.03222	0.00357	0.04351	-0.00486
59		3PZ	-0.00203	0.00017	-0.00129	-0.01201	-0.00187
60		4D 0	-0.00020	-0.00011	0.00013	0.00037	0.00068
61		4D+1	0.00304	0.00177	-0.00007	-0.00147	-0.00069
62		4D-1	0.00197	0.00108	0.00024	-0.00036	0.00053
63		4D+2	0.00336	0.00200	0.00006	-0.00278	-0.00016
64		4D-2	-0.00183	-0.00103	0.00005	0.00168	0.00025
65	5 H	1S	0.00031	-0.00068	0.00094	-0.00144	0.00462
66		2S	0.00721	0.00230	0.00306	0.01060	0.00711
67	6 C	1S	-0.00100	0.00076	0.00027	0.00116	-0.00036
68		2S	0.00169	-0.00138	-0.00056	-0.00278	0.00032
69		2PX	-0.00487	0.06224	-0.00454	-0.01341	0.00589
70		2PY	-0.00045	0.03474	-0.00295	-0.00930	0.00322

71		2PZ	-0.00327	-0.00034	0.00102	0.00391	-0.00012
72		3S	0.00663	-0.00358	0.00045	-0.00701	0.00494
73		3PX	-0.00632	0.05273	-0.00521	-0.01641	0.00831
74		3PY	-0.00202	0.02658	-0.00456	-0.00552	0.00164
75		3PZ	-0.00291	-0.00122	-0.00086	0.00720	-0.00096
76		4D 0	-0.00012	-0.00025	-0.00002	0.00022	0.00013
77		4D+1	0.00509	0.00198	-0.00005	-0.00495	-0.00021
78		4D-1	0.00334	0.00093	-0.00004	-0.00329	0.00030
79		4D+2	-0.00042	-0.00103	-0.00002	0.00051	0.00012
80		4D-2	0.00067	0.00067	0.00006	-0.00075	0.00004
81	7 C	1S	-0.00032	0.00031	0.00036	0.00111	0.00061
82		2S	0.00043	-0.00028	-0.00070	-0.00248	-0.00134
83		2PX	0.07484	0.02907	0.00056	-0.05041	-0.00165
84		2PY	0.04207	0.01681	-0.00082	-0.03229	-0.00407
85		2PZ	-0.00386	-0.00095	0.00014	0.00311	0.00001
86		3S	0.00326	-0.00141	-0.00194	-0.00914	-0.00362
87		3PX	0.06149	0.03022	0.00095	-0.06269	-0.00251
88		3PY	0.03574	0.01646	-0.00144	-0.03733	-0.00299
89		3PZ	-0.00315	-0.00004	0.00007	0.00406	0.00108
90		4D 0	0.00008	0.00005	0.00003	0.00010	0.00015
91		4D+1	0.00040	-0.00157	0.00015	0.00006	-0.00028
92		4D-1	0.00022	-0.00078	0.00003	-0.00056	-0.00002
93		4D+2	-0.00120	0.00424	-0.00033	-0.00316	0.00041
94		4D-2	0.00072	-0.00248	0.00024	0.00177	-0.00020
95	8 H	1S	0.00021	-0.00028	0.00099	0.00154	0.00397
96		2S	0.00090	-0.00057	0.00188	0.00122	0.01272
97	9 H	1S	-0.00250	0.00131	0.00000	0.00162	-0.00111
98		2S	-0.00346	0.00030	-0.00054	0.00658	-0.00441
99	10 H	1S	0.00037	0.00004	0.00019	0.00114	0.00014
100		2S	0.00063	-0.00051	0.00071	0.00491	0.00148
101	11 C	1S	0.01621	0.01926	0.00133	0.00337	0.00062
102		2S	-0.02664	-0.03516	-0.00208	-0.00790	0.00076
103		2PX	-0.10193	-0.06508	-0.00698	-0.05396	0.03997
104		2PY	-0.03530	-0.11000	0.00061	0.08411	-0.09254
105		2PZ	0.01485	-0.03663	-0.00199	0.01349	-0.02111
106		3S	-0.06923	-0.03793	-0.00205	-0.00849	-0.00785
107		3PX	-0.08598	-0.10789	-0.01198	-0.06318	0.04185
108		3PY	-0.03653	-0.11824	-0.00491	0.06941	-0.08750
109		3PZ	0.00262	0.00198	-0.00199	-0.00184	-0.02035
110		4D 0	-0.00148	0.00212	0.00021	0.00148	-0.00080
111		4D+1	-0.00926	0.00233	0.00076	-0.00073	0.00396
112		4D-1	-0.00551	0.00285	0.00039	0.00361	-0.00278
113		4D+2	0.00118	-0.00998	0.00021	0.00242	-0.00264

114		4D-2	0.00195	0.00786	0.00006	-0.00218	0.00223
115	12 C	1S	0.00337	-0.00572	-0.00075	-0.00097	-0.00130
116		2S	-0.00618	0.01397	0.00213	0.00201	0.00269
117		2PX	-0.00280	0.06991	0.00212	0.02746	-0.02497
118		2PY	0.01876	-0.09434	-0.00173	-0.05193	0.05202
119		2PZ	-0.01655	0.01240	0.00481	-0.00280	0.01984
120		3S	-0.03861	-0.00103	0.00054	-0.00358	0.00809
121		3PX	0.03090	0.09142	0.00480	0.03194	-0.02579
122		3PY	0.03498	-0.05297	0.00013	-0.05031	0.05761
123		3PZ	-0.01280	-0.03576	-0.00283	-0.02518	0.01914
124		4D 0	0.00267	0.00165	0.00022	0.00314	-0.00290
125		4D+1	-0.00349	-0.00265	-0.00052	-0.00664	0.00577
126		4D-1	-0.00156	-0.00444	-0.00002	0.00798	-0.00904
127		4D+2	-0.00146	-0.00050	0.00013	0.00768	-0.00863
128		4D-2	-0.00015	-0.00248	-0.00010	-0.00365	0.00387
129	13 C	1S	-0.01325	-0.00339	0.00061	0.00126	0.00085
130		2S	0.03110	0.01357	-0.00096	-0.00473	-0.00056
131		2PX	0.04767	0.06785	-0.00090	-0.01990	0.01818
132		2PY	0.04641	-0.07608	-0.00062	0.03068	-0.03928
133		2PZ	-0.03888	-0.02714	0.00008	0.00743	-0.00628
134		3S	0.01447	-0.07047	-0.00758	-0.00711	-0.00436
135		3PX	0.02603	0.04080	-0.00257	-0.01734	0.02302
136		3PY	0.02708	-0.08517	-0.00010	0.05197	-0.05420
137		3PZ	-0.00347	0.03279	0.00489	0.01427	-0.01276
138		4D 0	0.00400	0.00506	0.00012	-0.00093	0.00121
139		4D+1	-0.00013	-0.00032	0.00024	0.00284	-0.00247
140		4D-1	-0.00151	0.00151	0.00000	-0.00141	0.00152
141		4D+2	-0.00274	0.00015	-0.00027	-0.00731	0.00788
142		4D-2	-0.00242	-0.00389	0.00006	0.00483	-0.00490
143	14 C	1S	0.00106	0.00446	0.00043	0.00059	0.00088
144		2S	-0.00539	-0.01348	-0.00136	-0.00304	-0.00140
145		2PX	-0.01425	-0.03964	-0.00296	-0.05016	0.04894
146		2PY	-0.01338	0.01915	0.00218	0.09502	-0.10423
147		2PZ	0.00130	-0.00126	-0.00003	0.01789	-0.02078
148		3S	0.04232	0.02947	0.00151	0.00613	-0.00648
149		3PX	0.00915	-0.00951	-0.00165	-0.05036	0.05010
150		3PY	-0.00563	0.01620	0.00253	0.09269	-0.10201
151		3PZ	0.02456	0.04141	0.00550	0.03181	-0.01839
152		4D 0	0.00016	0.00205	0.00015	0.00048	-0.00006
153		4D+1	-0.00010	-0.00028	0.00030	-0.00042	0.00146
154		4D-1	-0.00062	0.00189	0.00010	0.00060	-0.00029
155		4D+2	-0.00055	0.00694	0.00014	0.00327	-0.00320
156		4D-2	0.00107	-0.00450	-0.00009	-0.00233	0.00228

157	15	C	1S	0.00724	0.00457	0.00007	-0.00025	-0.00016
158			2S	-0.01928	-0.01330	-0.00027	0.00022	0.00019
159			2PX	-0.03600	-0.03872	0.00131	0.05531	-0.05818
160			2PY	-0.02485	0.01427	-0.00335	-0.10915	0.11644
161			2PZ	-0.00163	0.00000	-0.00092	-0.02230	0.02355
162			3S	0.00256	0.01863	0.00165	0.00987	0.00003
163			3PX	-0.00619	-0.01162	0.00192	0.06606	-0.06632
164			3PY	-0.00307	0.02603	-0.00318	-0.12009	0.12908
165			3PZ	-0.02751	-0.03848	-0.00430	-0.02655	0.02650
166			4D 0	0.00014	-0.00135	0.00001	-0.00026	0.00034
167			4D+1	-0.00277	0.00010	-0.00002	0.00076	-0.00083
168			4D-1	-0.00089	-0.00559	-0.00008	-0.00069	0.00054
169			4D+2	-0.00025	0.00462	0.00001	-0.00191	0.00227
170			4D-2	0.00182	-0.00351	0.00000	0.00135	-0.00161
171	16	H	1S	0.00723	0.01471	0.00084	0.00003	0.00180
172			2S	0.01277	0.00219	-0.00109	0.00096	0.00624
173	17	C	1S	0.00068	0.00135	0.00025	0.00051	0.00024
174			2S	0.00145	0.00000	-0.00035	-0.00106	-0.00042
175			2PX	0.01334	-0.05371	-0.00067	-0.00610	0.00426
176			2PY	-0.01152	0.11153	0.00032	0.00969	-0.00913
177			2PZ	-0.00997	0.02558	0.00061	0.00312	-0.00149
178			3S	-0.04054	-0.06074	-0.00669	-0.01298	-0.00185
179			3PX	-0.01560	-0.07402	-0.00250	-0.01519	0.01069
180			3PY	-0.02101	0.08019	-0.00026	0.01799	-0.02014
181			3PZ	-0.01243	0.00995	-0.00034	0.00692	-0.00460
182			4D 0	0.00076	0.00069	-0.00007	-0.00288	0.00315
183			4D+1	-0.00116	-0.00035	0.00015	0.00446	-0.00457
184			4D-1	-0.00069	-0.00041	-0.00020	-0.00774	0.00839
185			4D+2	-0.00076	-0.00099	-0.00007	-0.00255	0.00282
186			4D-2	-0.00074	-0.00068	-0.00004	-0.00021	0.00015
187	18	H	1S	0.00061	0.01263	0.00138	0.00222	0.00191
188			2S	0.00730	0.03706	0.00569	0.01014	0.00751
189	19	H	1S	0.02020	0.00975	0.00017	0.00037	-0.00047
190			2S	0.04312	0.03004	0.00145	0.00159	-0.00069
191	20	H	1S	-0.00824	-0.00667	0.00002	0.00028	0.00005
192			2S	-0.01883	-0.01686	0.00010	0.00082	0.00113
193	21	C	1S	0.00392	0.00007	0.00009	-0.00006	0.00057
194			2S	-0.01005	-0.00197	-0.00019	-0.00161	0.00067
195			2PX	-0.00841	-0.03144	-0.00493	-0.01816	-0.00783
196			2PY	0.00542	-0.00717	0.00532	0.01094	0.01468
197			2PZ	0.01734	-0.00259	-0.08046	-0.20302	-0.18594
198			3S	0.01019	0.02736	-0.00138	0.00248	-0.01054
199			3PX	0.01887	-0.01770	-0.00574	-0.01223	-0.00840

200		3PY	-0.00251	-0.03456	0.00826	0.01879	0.01320
201		3PZ	0.00838	-0.00762	-0.08364	-0.20616	-0.18539
202		4D 0	0.00093	-0.00077	0.00084	0.00012	0.00022
203		4D+1	-0.01136	0.00096	-0.00723	-0.00951	-0.00874
204		4D-1	0.00279	0.00010	0.00011	-0.00752	-0.00807
205		4D+2	-0.00024	-0.00113	-0.00048	0.00092	-0.00312
206		4D-2	0.00157	0.00023	0.00051	0.00028	0.00019
207	22 C	1S	-0.00121	0.00303	0.00000	0.00122	-0.00064
208		2S	0.00280	-0.00933	-0.00005	-0.00261	0.00093
209		2PX	-0.00162	-0.03092	-0.00038	0.00834	-0.02089
210		2PY	-0.00245	-0.00087	0.00056	0.01221	-0.00394
211		2PZ	-0.03749	-0.00145	-0.00422	-0.05261	-0.06046
212		3S	0.00779	-0.01061	0.00139	-0.01982	0.01654
213		3PX	-0.00553	-0.04310	0.00010	0.02379	-0.03184
214		3PY	0.00726	0.00185	0.00086	0.01394	-0.00831
215		3PZ	-0.02384	0.00032	0.00162	-0.03940	-0.06771
216		4D 0	-0.00106	-0.00006	-0.00113	-0.00285	-0.00236
217		4D+1	0.00580	-0.00056	0.00587	0.01428	0.01380
218		4D-1	-0.00377	0.00009	-0.00448	-0.01024	-0.00841
219		4D+2	0.00060	-0.00130	0.00004	0.00023	0.00023
220		4D-2	0.00022	-0.00002	-0.00063	-0.00017	-0.00318
221	23 C	1S	-0.00068	-0.00056	-0.00023	0.00157	-0.00157
222		2S	0.00126	0.00073	0.00059	-0.00395	0.00374
223		2PX	0.00746	0.00411	0.00395	-0.00091	0.00162
224		2PY	-0.00582	-0.00234	-0.00168	0.00492	-0.00504
225		2PZ	0.08814	-0.00450	0.04687	0.01317	-0.00860
226		3S	0.00577	0.01186	-0.00181	-0.01121	0.00911
227		3PX	0.00064	0.00764	0.00612	-0.00558	0.00703
228		3PY	-0.00740	-0.00864	-0.00021	0.00537	-0.00255
229		3PZ	0.07439	-0.00414	0.04877	0.00710	-0.02001
230		4D 0	-0.00002	-0.00004	0.00095	0.00253	0.00277
231		4D+1	-0.00102	-0.00002	-0.00399	-0.01219	-0.01200
232		4D-1	-0.00078	0.00018	0.00407	0.01188	0.01097
233		4D+2	-0.00017	-0.00083	-0.00014	-0.00044	0.00029
234		4D-2	0.00045	0.00117	0.00058	0.00215	0.00091
235	24 C	1S	0.00105	-0.00149	-0.00001	0.00079	-0.00101
236		2S	-0.00186	0.00334	0.00029	-0.00189	0.00305
237		2PX	-0.00719	0.00497	-0.00483	-0.00997	-0.00824
238		2PY	0.01061	-0.00590	0.00548	0.01231	0.00499
239		2PZ	-0.09125	0.00469	-0.07791	-0.15162	-0.13300
240		3S	-0.01300	0.00064	-0.00169	-0.00250	0.00241
241		3PX	-0.00614	0.00596	-0.00705	-0.01231	-0.01444
242		3PY	0.01151	0.00401	0.00712	0.01267	0.00821

243		3PZ	-0.08021	0.00442	-0.09057	-0.19559	-0.16763
244		4D 0	0.00017	0.00016	0.00005	0.00037	0.00080
245		4D+1	0.00019	0.00014	0.00172	0.00479	0.00500
246		4D-1	0.00178	0.00025	0.00214	0.00998	0.01021
247		4D+2	0.00012	-0.00095	0.00022	0.00167	0.00008
248		4D-2	0.00018	0.00093	0.00001	-0.00049	0.00130
249	25 H	1S	0.00410	0.00200	0.00013	0.00352	-0.00419
250		2S	0.00341	-0.03008	0.00025	0.04176	-0.04111
251	26 C	1S	0.00000	0.00016	0.00002	0.00120	-0.00166
252		2S	-0.00047	-0.00125	-0.00045	-0.00311	0.00316
253		2PX	-0.00144	-0.00771	0.00275	0.01292	0.00997
254		2PY	-0.00128	-0.00134	-0.00319	-0.00963	-0.01374
255		2PZ	0.00966	0.00468	0.05022	0.18121	0.17936
256		3S	-0.00279	0.00023	0.00289	-0.00852	0.01731
257		3PX	-0.00064	0.00124	0.00536	0.01525	0.01358
258		3PY	-0.00326	-0.00165	-0.00543	-0.01542	-0.01600
259		3PZ	0.01313	0.00298	0.05999	0.22402	0.22238
260		4D 0	-0.00054	-0.00011	-0.00030	-0.00004	0.00038
261		4D+1	0.00627	-0.00036	0.00484	0.00574	0.00408
262		4D-1	0.00193	-0.00004	0.00258	0.00663	0.00604
263		4D+2	0.00068	-0.00032	0.00056	0.00059	0.00089
264		4D-2	-0.00029	-0.00007	-0.00009	0.00008	0.00015
265	27 H	1S	0.00058	0.00412	0.00007	0.00259	-0.00297
266		2S	0.00300	0.01026	-0.00235	0.00847	-0.01209
267	28 H	1S	0.00064	-0.00609	-0.00003	0.00403	-0.00457
268		2S	0.00172	-0.00943	-0.00067	0.01207	-0.01582
269	29 H	1S	-0.00038	0.00157	-0.00028	0.00054	-0.00114
270		2S	0.00062	0.00415	0.00011	0.00583	-0.00706
271	30 C	1S	-0.01590	-0.01986	0.00124	-0.00372	0.00052
272		2S	0.02882	0.03095	-0.00268	0.00674	0.00034
273		2PX	-0.08566	-0.10248	-0.00738	-0.00229	0.00814
274		2PY	-0.05598	-0.05857	-0.00716	-0.02380	-0.00483
275		2PZ	-0.14406	0.01295	0.04737	0.09996	0.08844
276		3S	0.01665	0.10201	-0.01861	0.01941	-0.00376
277		3PX	-0.13082	-0.07737	-0.02191	0.00175	0.00435
278		3PY	-0.04335	-0.06540	-0.00430	-0.03633	-0.00535
279		3PZ	-0.09519	0.00571	0.04652	0.08897	0.08882
280		4D 0	0.00061	0.00216	-0.00119	-0.00079	-0.00127
281		4D+1	-0.00896	0.00254	0.00569	0.00352	0.00491
282		4D-1	-0.01246	0.00196	-0.00370	-0.00136	-0.00083
283		4D+2	-0.00151	-0.00998	0.00005	0.00197	-0.00182
284		4D-2	0.00090	0.00158	0.00002	-0.00098	0.00038
285	31 C	1S	0.00257	0.01125	-0.00488	-0.00062	0.00232

286		2S	-0.01166	-0.02798	0.01125	0.00209	-0.00397
287		2PX	0.03292	0.07387	0.02294	-0.00453	0.00452
288		2PY	0.01401	-0.01852	0.00429	-0.00315	-0.00280
289		2PZ	-0.08825	0.01098	0.08355	0.02611	0.03601
290		3S	0.07934	0.01037	0.04051	0.00082	-0.00944
291		3PX	-0.02936	0.05815	-0.00316	0.01088	0.00922
292		3PY	0.04596	0.00717	0.00930	-0.00653	0.00596
293		3PZ	-0.06531	0.01103	0.08661	0.03938	0.04605
294		4D 0	-0.00126	-0.00106	0.00030	0.00048	-0.00010
295		4D+1	0.00763	-0.00026	-0.00478	-0.00920	-0.00840
296		4D-1	-0.00029	0.00007	-0.00053	-0.00249	-0.00226
297		4D+2	0.00349	0.00220	-0.00063	-0.00008	-0.00054
298		4D-2	0.00382	0.00548	0.00091	0.00089	0.00086
299	32 C	1S	0.00472	-0.00266	0.00022	0.00064	-0.00101
300		2S	-0.01182	0.00379	-0.00143	-0.00205	0.00179
301		2PX	-0.00711	0.01176	-0.00441	-0.00794	0.00414
302		2PY	0.05396	-0.00945	0.01131	0.01657	-0.00441
303		2PZ	-0.19095	0.01304	-0.08810	-0.05518	-0.05073
304		3S	0.00210	0.03764	0.00737	0.00483	0.00576
305		3PX	0.05182	0.03981	-0.00088	-0.00497	-0.00164
306		3PY	0.03229	0.00300	0.01511	0.00006	-0.00041
307		3PZ	-0.15773	0.01269	-0.08603	-0.06121	-0.05678
308		4D 0	0.00084	0.00020	-0.00100	-0.00209	-0.00183
309		4D+1	-0.00012	0.00072	0.00598	0.01264	0.01182
310		4D-1	0.00511	-0.00073	-0.00235	-0.00510	-0.00421
311		4D+2	-0.00130	-0.00253	0.00041	-0.00035	0.00061
312		4D-2	0.00489	0.00465	-0.00018	-0.00039	-0.00180
313	33 C	1S	-0.00469	-0.00663	-0.00001	-0.00011	-0.00042
314		2S	0.01204	0.01738	0.00140	-0.00002	0.00088
315		2PX	-0.01693	-0.03477	-0.00844	-0.00752	-0.00875
316		2PY	-0.03576	-0.02084	-0.00362	0.01255	0.01163
317		2PZ	0.09763	-0.00261	-0.06719	-0.12943	-0.12287
318		3S	-0.00009	-0.00676	-0.01034	0.00121	0.00146
319		3PX	0.04507	0.02897	-0.00350	-0.01048	-0.00285
320		3PY	-0.04620	-0.00810	0.00675	0.02192	0.01939
321		3PZ	0.05701	-0.00240	-0.06838	-0.12771	-0.11947
322		4D 0	0.00232	0.00082	0.00117	0.00018	0.00012
323		4D+1	0.00035	-0.00012	-0.00965	-0.00108	-0.00163
324		4D-1	0.01014	-0.00091	0.00148	-0.00042	-0.00107
325		4D+2	0.00081	-0.00319	0.00331	-0.00076	-0.00075
326		4D-2	0.00210	0.00041	0.00603	-0.00053	-0.00052
327	34 H	1S	-0.01379	-0.00474	0.00120	-0.00199	0.00081
328		2S	-0.00961	-0.03196	0.00003	-0.01289	0.01261

329	35	C	1S	-0.00463	-0.00228	-0.00266	-0.00091	0.00083
330			2S	0.01408	0.00741	0.00487	0.00270	-0.00180
331			2PX	-0.01473	-0.01572	0.00902	-0.00014	0.00427
332			2PY	-0.02364	-0.00940	-0.00826	-0.01236	-0.00747
333			2PZ	0.02081	-0.00574	0.04351	0.10570	0.10413
334			3S	-0.03574	-0.03286	0.03013	0.00502	-0.00436
335			3PX	-0.01618	-0.01221	0.02585	-0.00499	0.00894
336			3PY	0.02829	0.02245	-0.00559	-0.00978	-0.01372
337			3PZ	0.02020	-0.00233	0.04705	0.10601	0.10250
338			4D 0	0.00026	0.00068	-0.00046	-0.00008	-0.00026
339			4D+1	0.01298	-0.00096	0.00640	0.00374	0.00320
340			4D-1	0.00291	-0.00040	0.00127	0.00117	0.00116
341			4D+2	0.00329	-0.00006	0.00116	0.00111	-0.00040
342			4D-2	-0.00075	0.00017	-0.00015	-0.00037	-0.00015
343	36	C	1S	0.00014	-0.00108	0.00562	-0.00162	-0.00033
344			2S	-0.00372	0.00015	-0.01227	0.00382	0.00101
345			2PX	0.00906	0.00372	-0.00643	0.00313	0.00492
346			2PY	-0.00807	-0.00324	0.01214	-0.00087	-0.00081
347			2PZ	0.19831	-0.01765	0.06638	0.00873	0.00205
348			3S	0.05489	0.03238	-0.04521	0.00894	-0.00509
349			3PX	-0.01774	-0.02380	0.02034	0.00192	0.00435
350			3PY	-0.03399	-0.01766	-0.00774	0.00903	0.00513
351			3PZ	0.16018	-0.01450	0.06374	0.01988	0.01114
352			4D 0	-0.00112	-0.00034	0.00069	0.00203	0.00188
353			4D+1	0.00085	0.00019	-0.00389	-0.00630	-0.00627
354			4D-1	-0.00262	-0.00004	0.00344	0.00717	0.00689
355			4D+2	0.00037	-0.00043	0.00061	0.00026	-0.00007
356			4D-2	0.00101	0.00140	0.00012	0.00134	0.00146
357	37	H	1S	-0.01393	-0.00262	-0.00411	-0.00252	0.00263
358			2S	-0.03656	-0.01189	-0.01060	-0.00890	0.00863
359	38	H	1S	0.00553	0.00520	-0.00228	0.00089	0.00141
360			2S	0.01905	0.01939	0.00774	-0.01015	-0.00396
361	39	C	1S	-0.00205	0.00275	-0.00115	-0.00199	-0.00177
362			2S	0.00826	-0.00465	0.00077	0.00434	0.00371
363			2PX	-0.03365	0.00930	0.00744	0.03953	-0.02037
364			2PY	-0.02576	-0.01906	0.00487	-0.04484	0.07008
365			2PZ	0.01266	-0.01274	0.00117	-0.00608	0.01418
366			3S	-0.00028	-0.02739	0.01571	0.01945	0.02081
367			3PX	-0.03594	0.00815	0.01205	0.04631	-0.01313
368			3PY	-0.02275	-0.01079	0.01716	-0.02720	0.08087
369			3PZ	0.02380	0.00035	0.00650	-0.00760	0.00852
370			4D 0	-0.00005	0.00184	0.00037	0.00430	-0.00410
371			4D+1	-0.00098	-0.00125	-0.00034	-0.00846	0.00818

372		4D-1	-0.00057	0.00257	0.00054	0.01273	-0.01353
373		4D+2	-0.00106	0.00157	-0.00014	0.00745	-0.00886
374		4D-2	0.00029	-0.00124	0.00016	-0.00250	0.00305
375	40 C	1S	0.00128	-0.00470	-0.00069	0.00023	-0.00093
376		2S	-0.00107	0.01108	0.00226	0.00168	0.00330
377		2PX	-0.03092	0.00284	0.00310	0.08911	-0.09547
378		2PY	-0.02374	-0.00735	-0.00448	-0.17880	0.18669
379		2PZ	0.00496	0.01163	0.00050	-0.03185	0.03587
380		3S	-0.04138	0.00177	-0.00139	-0.01230	0.00272
381		3PX	-0.03416	0.02665	0.00434	0.09916	-0.09832
382		3PY	-0.02197	0.00881	-0.00501	-0.17640	0.18337
383		3PZ	-0.02336	-0.00796	-0.00261	-0.03555	0.03225
384		4D 0	-0.00037	-0.00149	0.00017	0.00088	-0.00027
385		4D+1	-0.00154	0.00251	0.00051	0.00189	-0.00006
386		4D-1	-0.00007	-0.00291	-0.00014	0.00274	-0.00324
387		4D+2	0.00048	-0.00476	-0.00011	-0.00950	0.01042
388		4D-2	-0.00067	0.00189	-0.00020	0.00668	-0.00838
389	41 C	1S	0.00114	-0.00180	-0.00021	0.00011	-0.00012
390		2S	-0.00264	0.00316	0.00005	-0.00045	0.00064
391		2PX	0.00143	0.02230	0.00343	0.06693	-0.06744
392		2PY	0.00630	-0.04095	-0.00668	-0.13014	0.13177
393		2PZ	-0.00485	-0.00022	-0.00144	-0.02420	0.02274
394		3S	0.00608	0.02011	0.00473	-0.00038	-0.00325
395		3PX	0.00370	0.01966	0.00349	0.08320	-0.08638
396		3PY	0.00362	-0.03897	-0.01148	-0.16720	0.16566
397		3PZ	0.00238	0.00263	0.00022	-0.02891	0.02739
398		4D 0	0.00028	-0.00019	-0.00008	-0.00196	0.00182
399		4D+1	-0.00157	0.00038	0.00042	0.00242	-0.00118
400		4D-1	-0.00135	-0.00102	0.00016	-0.00582	0.00773
401		4D+2	-0.00015	0.00066	0.00013	0.00698	-0.00761
402		4D-2	-0.00003	-0.00066	-0.00002	-0.00616	0.00700
403	42 H	1S	-0.00606	-0.00394	-0.00102	-0.00122	-0.00170
404		2S	0.03116	-0.00013	-0.02288	-0.03408	-0.03238
405	43 C	1S	0.00015	0.00137	-0.00035	-0.00102	-0.00061
406		2S	-0.00006	-0.00308	0.00053	0.00205	0.00157
407		2PX	0.00385	-0.02103	-0.00276	-0.00511	-0.00168
408		2PY	0.00102	0.04022	0.00599	0.01076	0.00529
409		2PZ	-0.00332	0.00288	0.00193	0.00517	0.00265
410		3S	-0.00746	-0.00737	0.00314	0.00862	0.00184
411		3PX	0.00409	-0.02502	-0.00274	-0.00535	-0.00608
412		3PY	0.00274	0.03005	0.00685	0.00380	0.01693
413		3PZ	-0.00903	0.00438	0.00200	0.00563	0.00363
414		4D 0	0.00051	-0.00001	-0.00005	-0.00434	0.00482

415		4D+1	-0.00110	0.00027	0.00007	0.00751	-0.00875
416		4D-1	-0.00111	-0.00073	-0.00032	-0.01377	0.01457
417		4D+2	-0.00051	-0.00091	-0.00003	-0.00563	0.00623
418		4D-2	-0.00023	0.00025	-0.00004	0.00068	-0.00111
419	44 C	1S	0.00037	0.00012	-0.00058	-0.00124	-0.00095
420		2S	0.00033	0.00036	0.00121	0.00270	0.00243
421		2PX	-0.01276	-0.00825	0.00048	-0.07983	0.09459
422		2PY	0.00027	0.01125	0.00230	0.16099	-0.17844
423		2PZ	0.00328	0.00253	0.00079	0.02942	-0.03114
424		3S	-0.00657	0.00127	0.00181	0.00827	0.00381
425		3PX	-0.00606	-0.01095	-0.00033	-0.09973	0.11570
426		3PY	0.00332	0.01215	0.00301	0.19660	-0.21950
427		3PZ	-0.00252	0.00003	-0.00068	0.03276	-0.04031
428		4D 0	-0.00008	0.00015	-0.00007	-0.00101	0.00078
429		4D+1	-0.00015	-0.00059	-0.00021	-0.00010	-0.00073
430		4D-1	-0.00010	0.00050	0.00001	-0.00309	0.00357
431		4D+2	-0.00027	0.00274	0.00049	0.00612	-0.00566
432		4D-2	0.00005	-0.00190	-0.00029	-0.00498	0.00477
433	45 H	1S	0.00866	-0.00105	-0.00155	-0.00289	-0.00283
434		2S	0.01309	-0.00175	-0.00261	-0.00684	-0.00766
435	46 H	1S	-0.00578	0.00036	-0.00021	-0.00148	-0.00066
436		2S	-0.01224	-0.00276	-0.00037	-0.00661	-0.00089
437	47 H	1S	-0.00061	0.00020	-0.00056	-0.00135	-0.00084
438		2S	-0.00251	-0.00117	-0.00234	-0.00677	-0.00472
439	48 C	1S	-0.00184	0.00198	-0.00057	-0.00418	0.00324
440		2S	0.00299	-0.00428	0.00072	0.00761	-0.00652
441		2PX	0.01304	-0.10406	-0.00235	-0.04273	0.00873
442		2PY	0.01258	-0.07027	0.00144	-0.01197	-0.00246
443		2PZ	-0.00678	0.00827	-0.00238	-0.00208	-0.00368
444		3S	0.00710	0.00616	0.00487	0.04620	-0.04115
445		3PX	0.00496	-0.05917	-0.00374	-0.04144	0.00811
446		3PY	0.02047	-0.07103	0.00743	0.01134	-0.01838
447		3PZ	0.01340	-0.00605	-0.00159	-0.01528	0.02625
448		4D 0	-0.00026	0.00011	-0.00002	-0.00071	0.00076
449		4D+1	0.00257	0.00063	-0.00038	0.00070	-0.00208
450		4D-1	0.00394	-0.00199	0.00093	0.00224	0.00322
451		4D+2	-0.00155	-0.01627	-0.00021	-0.00106	-0.00003
452		4D-2	0.00037	0.00964	0.00016	-0.00121	0.00214
453	49 C	1S	-0.00189	0.00104	-0.00094	-0.00145	-0.00324
454		2S	0.00308	0.00062	0.00308	0.00630	0.00505
455		2PX	-0.04394	-0.13508	-0.00275	-0.01375	-0.00538
456		2PY	-0.01981	-0.08050	0.00140	-0.00216	0.00454
457		2PZ	0.00884	0.00503	0.00149	0.00076	0.01039

458		3S	0.02692	-0.03187	0.00323	-0.00190	0.03101
459		3PX	-0.03082	-0.11328	-0.00529	-0.01340	-0.01897
460		3PY	-0.01445	-0.06779	-0.00277	-0.03051	0.03085
461		3PZ	0.01302	-0.01456	0.00356	0.00009	0.00919
462		4D 0	0.00003	0.00047	0.00011	0.00080	-0.00023
463		4D+1	0.00056	-0.00382	-0.00008	-0.00160	0.00022
464		4D-1	0.00061	-0.00247	0.00004	-0.00038	-0.00006
465		4D+2	-0.00182	0.00282	0.00025	0.00353	-0.00061
466		4D-2	0.00086	-0.00145	-0.00010	-0.00126	0.00003
467	50 C	1S	0.00190	-0.00102	0.00092	0.00100	0.00310
468		2S	-0.00338	0.00349	-0.00327	-0.00119	-0.01027
469		2PX	0.02109	-0.14832	0.00020	0.02191	-0.00133
470		2PY	0.00572	-0.08236	-0.00258	0.01047	-0.00917
471		2PZ	0.00700	0.00163	0.00383	0.00458	0.01307
472		3S	-0.01236	-0.00622	-0.00116	-0.00267	-0.01934
473		3PX	0.02367	-0.12611	0.00551	0.02553	0.00331
474		3PY	-0.00353	-0.05655	-0.00533	0.01425	-0.01622
475		3PZ	0.00094	0.01962	-0.00144	-0.01018	0.01973
476		4D 0	0.00024	-0.00014	-0.00020	-0.00045	-0.00067
477		4D+1	-0.00246	0.00277	0.00015	0.00413	-0.00022
478		4D-1	-0.00134	0.00218	-0.00018	0.00181	-0.00040
479		4D+2	0.00197	0.00391	-0.00028	-0.00249	-0.00008
480		4D-2	-0.00168	-0.00165	0.00017	0.00139	-0.00007
481	51 C	1S	0.00052	0.00005	0.00021	0.00098	0.00038
482		2S	-0.00036	-0.00031	-0.00049	-0.00152	-0.00202
483		2PX	-0.03950	0.03780	0.00434	0.04641	-0.00254
484		2PY	-0.02495	0.02162	0.00163	0.02374	-0.00375
485		2PZ	0.00086	-0.00148	-0.00039	-0.00181	-0.00075
486		3S	-0.00961	0.01000	-0.00263	-0.01857	0.01480
487		3PX	-0.03130	0.02510	0.00502	0.05592	-0.00945
488		3PY	-0.02286	0.01730	0.00290	0.02354	0.00562
489		3PZ	-0.00297	0.00863	-0.00193	-0.00046	-0.00238
490		4D 0	-0.00005	-0.00046	-0.00004	0.00003	-0.00015
491		4D+1	0.00062	0.00531	0.00001	-0.00046	-0.00016
492		4D-1	0.00083	0.00362	0.00008	-0.00040	0.00069
493		4D+2	0.00182	0.00924	0.00007	0.00057	0.00012
494		4D-2	-0.00092	-0.00500	-0.00009	-0.00034	-0.00033
495	52 H	1S	-0.00093	0.00118	0.00023	0.00109	-0.00065
496		2S	-0.00322	-0.00737	0.00262	0.00990	-0.02025
497	53 C	1S	-0.00089	0.00068	-0.00033	-0.00062	-0.00123
498		2S	0.00216	-0.00174	0.00102	0.00179	0.00249
499		2PX	0.04647	0.05419	-0.00485	-0.04062	-0.00023
500		2PY	0.03106	0.02849	-0.00141	-0.02108	0.00342

501		2PZ	-0.00388	-0.00187	-0.00015	0.00153	-0.00041
502		3S	-0.00489	0.00946	-0.00356	0.00184	0.00366
503		3PX	0.03592	0.03727	-0.00404	-0.04230	0.00355
504		3PY	0.01984	0.02601	-0.00469	-0.02090	-0.00256
505		3PZ	0.00202	-0.01143	0.00367	0.00715	0.00051
506		4D 0	-0.00004	0.00049	-0.00003	-0.00010	0.00001
507		4D+1	-0.00081	-0.00485	-0.00020	0.00028	-0.00052
508		4D-1	0.00001	-0.00276	0.00018	0.00056	0.00056
509		4D+2	-0.00017	0.00984	0.00013	-0.00134	0.00045
510		4D-2	0.00007	-0.00594	0.00003	0.00083	-0.00011
511	54 C	1S	-0.00016	0.00025	-0.00013	-0.00046	0.00001
512		2S	-0.00021	0.00038	0.00015	0.00122	-0.00032
513		2PX	0.01504	0.16837	0.00138	-0.00602	0.00475
514		2PY	0.00882	0.09841	0.00108	-0.00245	0.00259
515		2PZ	0.00084	-0.00951	0.00035	-0.00027	0.00270
516		3S	0.00740	-0.01501	0.00400	0.00476	0.00138
517		3PX	0.01126	0.14281	0.00076	-0.00990	0.00541
518		3PY	0.01222	0.07419	0.00238	-0.00442	0.00249
519		3PZ	-0.00032	-0.00601	-0.00063	0.00188	-0.00317
520		4D 0	-0.00025	-0.00008	0.00004	0.00036	-0.00003
521		4D+1	0.00290	0.00064	-0.00034	-0.00353	0.00012
522		4D-1	0.00185	0.00028	-0.00010	-0.00186	0.00026
523		4D+2	-0.00029	-0.00048	0.00003	0.00011	0.00007
524		4D-2	0.00023	0.00050	-0.00004	-0.00014	-0.00008
525	55 H	1S	0.00160	-0.00002	0.00033	-0.00015	0.00244
526		2S	0.00124	0.00201	0.00056	0.00119	0.00576
527	56 H	1S	-0.00240	0.00200	-0.00103	-0.00141	-0.00291
528		2S	-0.00506	0.00642	-0.00433	-0.00566	-0.00928
529	57 H	1S	0.00026	-0.00053	-0.00007	-0.00058	0.00011
530		2S	0.00182	-0.00293	-0.00009	-0.00224	0.00010
531	58 N	1S	-0.00090	-0.00258	0.00002	0.00762	-0.00916
532		2S	0.00146	0.00566	-0.00048	-0.01702	0.01903
533		2PX	0.00564	0.01949	0.00516	0.00341	0.02462
534		2PY	-0.00021	-0.00825	-0.00417	0.01784	-0.04644
535		2PZ	0.08742	-0.01071	0.08034	0.20060	0.19711
536		3S	0.01315	0.01274	0.00267	-0.05376	0.07234
537		3PX	0.00646	-0.02010	0.00670	0.00597	0.02475
538		3PY	0.00299	-0.01227	-0.00368	0.02251	-0.04699
539		3PZ	0.07616	-0.00537	0.08193	0.20363	0.21684
540		4D 0	0.00006	0.00070	0.00045	0.00064	0.00103
541		4D+1	0.00083	0.00113	-0.00380	-0.00616	-0.00566
542		4D-1	0.00401	-0.00140	-0.00016	-0.00225	-0.00079
543		4D+2	0.00075	-0.00391	-0.00018	-0.00216	0.00113

544		4D-2	-0.00129	0.00548	0.00024	-0.00098	0.00239
545	59 N	1S	-0.00316	0.00193	0.00184	0.00451	0.00485
546		2S	0.00747	-0.00415	-0.00337	-0.00801	-0.00886
547		2PX	-0.04817	0.06289	-0.00028	-0.05865	-0.00094
548		2PY	-0.01892	0.03159	-0.00157	-0.04146	-0.00322
549		2PZ	-0.00872	0.00215	0.00550	0.01277	0.01732
550		3S	0.01619	-0.01353	-0.02135	-0.05232	-0.05404
551		3PX	-0.03595	0.05198	0.00346	-0.04586	0.00785
552		3PY	-0.01744	0.03711	0.00294	-0.04830	-0.01050
553		3PZ	-0.01086	-0.00025	0.00752	0.01729	0.01470
554		4D 0	0.00209	-0.00078	0.00010	-0.00146	0.00248
555		4D+1	-0.01251	-0.00004	-0.00014	0.00024	-0.00093
556		4D-1	-0.00526	-0.00144	0.00038	-0.00156	0.00320
557		4D+2	-0.00421	0.00182	0.00063	0.00262	0.00088
558		4D-2	0.00182	-0.00106	0.00044	-0.00123	0.00207
559	60 N	1S	0.00248	0.00079	-0.00191	-0.00550	-0.00407
560		2S	-0.00398	-0.00094	0.00417	0.01119	0.00863
561		2PX	0.02133	-0.02359	0.00086	-0.08877	0.10855
562		2PY	-0.00075	0.04292	-0.00079	0.17959	-0.20436
563		2PZ	-0.02019	0.01228	0.00840	0.05110	-0.02140
564		3S	-0.01617	-0.01458	0.01539	0.04985	0.03918
565		3PX	-0.01673	-0.00465	0.00292	-0.08392	0.11696
566		3PY	-0.02086	0.04449	-0.00563	0.17894	-0.21855
567		3PZ	-0.01378	0.01354	0.00429	0.05445	-0.02301
568		4D 0	0.00372	-0.00124	-0.00045	-0.00054	0.00028
569		4D+1	-0.00774	0.00196	0.00028	0.00078	-0.00121
570		4D-1	-0.00308	0.00050	0.00051	-0.00015	0.00140
571		4D+2	-0.00197	0.00224	0.00010	-0.00487	0.00614
572		4D-2	0.00033	-0.00120	0.00074	0.00443	-0.00201
573	61 C	1S	0.00280	0.00454	-0.00020	0.00008	0.00005
574		2S	-0.00011	-0.00999	-0.00106	-0.00091	-0.00159
575		2PX	0.01789	0.02540	0.02546	-0.00097	0.00007
576		2PY	0.02987	-0.00203	0.11886	-0.01205	-0.00804
577		2PZ	-0.05121	-0.00265	-0.14307	0.02140	0.01629
578		3S	-0.07851	-0.03151	0.01158	0.00760	0.01085
579		3PX	0.02116	0.02655	0.01990	-0.00254	0.00271
580		3PY	0.01388	-0.01763	0.10105	-0.01071	-0.01281
581		3PZ	-0.03111	-0.01052	-0.14604	0.01399	0.00503
582		4D 0	0.00110	0.00003	-0.00238	-0.00058	-0.00065
583		4D+1	-0.00535	0.00012	0.00511	0.00751	0.00717
584		4D-1	0.00195	-0.00003	-0.00193	-0.00227	-0.00217
585		4D+2	0.00115	0.00068	-0.00138	0.00060	0.00038
586		4D-2	0.00210	0.00168	-0.00104	-0.00098	-0.00087

587	62	C	1S	0.00293	-0.00230	-0.00188	-0.00395	-0.00392
588			2S	-0.00536	0.00475	0.00396	0.00901	0.00879
589			2PX	0.01564	-0.00991	-0.00983	-0.01947	-0.01884
590			2PY	0.02785	0.00048	-0.01945	-0.03576	-0.03372
591			2PZ	-0.04765	-0.00949	0.01455	0.03443	0.03273
592			3S	-0.02513	0.01528	0.02213	0.03085	0.03297
593			3PX	-0.01774	-0.00504	0.00101	0.00315	0.00362
594			3PY	0.01379	0.00255	-0.02352	-0.03939	-0.03583
595			3PZ	-0.05100	-0.00744	0.01168	0.03921	0.03832
596			4D 0	0.00143	0.00048	0.00434	-0.00035	-0.00023
597			4D+1	0.00178	0.00027	0.01006	-0.00174	-0.00134
598			4D-1	-0.00012	0.00039	-0.00109	0.00038	0.00030
599			4D+2	0.00071	-0.00068	-0.00095	-0.00043	-0.00039
600			4D-2	-0.00157	0.00010	-0.00857	0.00167	0.00130
601	63	C	1S	-0.00166	0.00010	0.00154	0.00370	0.00336
602			2S	0.00371	0.00013	-0.00311	-0.00851	-0.00765
603			2PX	0.00461	-0.00053	-0.00881	0.00189	0.00092
604			2PY	0.04399	0.00419	-0.05181	-0.03153	-0.03168
605			2PZ	-0.03854	-0.00674	0.04858	0.01912	0.01926
606			3S	0.01107	-0.01364	-0.02009	-0.02841	-0.02923
607			3PX	0.00057	-0.00791	-0.01856	-0.01438	-0.01537
608			3PY	0.04413	-0.00340	-0.06454	-0.02286	-0.03015
609			3PZ	-0.03045	-0.01257	0.05359	0.01973	0.01603
610			4D 0	-0.00200	0.00008	-0.00710	0.00094	0.00069
611			4D+1	0.00146	0.00059	0.00794	-0.00123	-0.00103
612			4D-1	-0.00042	0.00010	-0.00339	0.00049	0.00030
613			4D+2	-0.00202	-0.00027	-0.00647	0.00131	0.00114
614			4D-2	-0.00035	0.00080	-0.00453	0.00018	0.00019
615	64	C	1S	-0.00115	0.00142	0.00100	0.00164	0.00164
616			2S	0.00169	-0.00290	-0.00117	-0.00299	-0.00274
617			2PX	-0.00823	0.00678	-0.01776	0.01177	0.01075
618			2PY	-0.01290	-0.00300	-0.09454	0.02526	0.02098
619			2PZ	0.02054	0.00264	0.11771	-0.03350	-0.02827
620			3S	0.02062	-0.00638	-0.01557	-0.02018	-0.02140
621			3PX	-0.01503	0.00425	-0.01348	0.02070	0.02002
622			3PY	0.00173	-0.00350	-0.11051	0.02295	0.01806
623			3PZ	0.02187	0.00121	0.13557	-0.04169	-0.03558
624			4D 0	-0.00279	-0.00031	0.00330	0.00149	0.00153
625			4D+1	0.00248	0.00061	-0.00234	-0.00179	-0.00173
626			4D-1	-0.00120	-0.00014	0.00119	0.00070	0.00068
627			4D+2	-0.00187	-0.00007	0.00263	0.00168	0.00162
628			4D-2	-0.00139	0.00022	0.00172	0.00169	0.00164
629	65	H	1S	-0.00548	0.00174	0.00048	0.00229	0.00232

630		2S	0.02237	0.00060	0.00181	-0.00369	-0.00619
631	66 C	1S	0.00068	0.00041	-0.00081	-0.00147	-0.00139
632		2S	-0.00161	-0.00155	0.00121	0.00258	0.00239
633		2PX	-0.00003	0.00324	-0.01897	-0.00069	-0.00072
634		2PY	-0.02090	-0.00117	-0.08823	0.02317	0.02052
635		2PZ	0.02185	0.00065	0.11039	-0.02570	-0.02289
636		3S	0.00352	0.00724	0.00992	0.01669	0.01690
637		3PX	-0.00411	0.00051	-0.02192	-0.00964	-0.00693
638		3PY	-0.01840	0.00490	-0.07842	0.02059	0.02020
639		3PZ	0.01789	0.00476	0.10504	-0.02273	-0.01858
640		4D 0	0.00169	0.00010	-0.00206	-0.00101	-0.00102
641		4D+1	0.00310	0.00041	-0.00648	-0.00113	-0.00122
642		4D-1	-0.00011	0.00008	0.00085	-0.00011	-0.00007
643		4D+2	-0.00028	0.00003	0.00144	0.00027	0.00030
644		4D-2	-0.00321	-0.00046	0.00577	0.00150	0.00159
645	67 H	1S	0.00005	0.00272	0.00027	-0.00134	-0.00105
646		2S	0.00348	-0.00272	-0.00847	-0.00104	-0.00650
647	68 C	1S	0.00059	0.00000	-0.00026	-0.00006	-0.00012
648		2S	-0.00109	0.00034	0.00034	0.00013	0.00038
649		2PX	-0.00693	-0.00082	0.01316	0.00337	0.00342
650		2PY	-0.05205	-0.00643	0.06565	0.01706	0.01769
651		2PZ	0.06067	0.00620	-0.08451	-0.02250	-0.02330
652		3S	0.00667	-0.00592	0.00031	-0.00128	-0.00381
653		3PX	-0.00157	0.00233	0.01377	0.00001	0.00055
654		3PY	-0.03431	-0.00418	0.07439	0.00900	0.01163
655		3PZ	0.04614	0.00558	-0.09480	-0.02117	-0.02139
656		4D 0	-0.00040	0.00013	0.00554	-0.00184	-0.00153
657		4D+1	-0.00121	0.00007	-0.01537	0.00489	0.00433
658		4D-1	0.00019	0.00005	0.00431	-0.00144	-0.00126
659		4D+2	0.00046	-0.00010	0.00815	-0.00250	-0.00223
660		4D-2	0.00074	0.00020	0.01103	-0.00312	-0.00277
661	69 H	1S	0.00016	0.00318	0.00216	0.00262	0.00250
662		2S	-0.00359	0.00519	0.00261	0.00643	0.00611
663	70 H	1S	0.00241	0.00064	-0.00168	-0.00267	-0.00253
664		2S	0.00216	0.00339	-0.00250	-0.00592	-0.00533
665	71 N	1S	0.00056	0.00030	0.00019	-0.00016	-0.00012
666		2S	-0.00026	-0.00066	-0.00050	0.00015	-0.00001
667		2PX	0.00013	0.00105	0.03947	-0.01343	-0.01184
668		2PY	0.01634	0.00091	0.19286	-0.06811	-0.06113
669		2PZ	-0.01040	0.00005	-0.23395	0.08193	0.07335
670		3S	-0.00844	-0.00216	-0.00043	0.00206	0.00279
671		3PX	0.00067	-0.00001	0.03553	-0.01315	-0.01211
672		3PY	0.00950	0.00030	0.17821	-0.06457	-0.05792

673		3PZ	-0.00847	-0.00022	-0.21605	0.07948	0.07147
674		4D 0	-0.00231	-0.00025	0.00040	0.00056	0.00054
675		4D+1	-0.00363	-0.00038	0.01386	-0.00191	-0.00151
676		4D-1	0.00035	0.00006	-0.00278	0.00050	0.00042
677		4D+2	-0.00001	0.00013	-0.00432	0.00098	0.00087
678		4D-2	0.00324	0.00037	-0.01095	0.00125	0.00097
679	72 N	1S	0.00044	0.00030	-0.00010	0.00029	0.00026
680		2S	-0.00078	-0.00067	0.00011	-0.00081	-0.00073
681		2PX	0.00843	0.00094	-0.04071	0.00984	0.00850
682		2PY	0.03533	0.00262	-0.19980	0.04657	0.04039
683		2PZ	-0.04986	-0.00668	0.24176	-0.05753	-0.04998
684		3S	-0.00137	-0.00038	0.00215	-0.00109	-0.00080
685		3PX	0.00477	0.00143	-0.03601	0.01062	0.00988
686		3PY	0.02739	0.00189	-0.18485	0.04619	0.04018
687		3PZ	-0.03840	-0.00521	0.22286	-0.05677	-0.04950
688		4D 0	0.00261	0.00025	-0.00033	-0.00134	-0.00128
689		4D+1	0.00071	-0.00004	0.01293	-0.00462	-0.00418
690		4D-1	0.00049	0.00016	-0.00262	0.00072	0.00063
691		4D+2	0.00148	0.00011	-0.00455	0.00078	0.00065
692		4D-2	-0.00106	-0.00012	-0.01025	0.00379	0.00341
693	73 C	1S	-0.00044	-0.00012	0.00007	-0.00008	-0.00006
694		2S	0.00100	0.00030	0.00008	0.00013	0.00010
695		2PX	-0.00591	-0.00078	-0.01106	0.00540	0.00504
696		2PY	-0.01809	-0.00105	-0.05532	0.02838	0.02618
697		2PZ	0.02307	0.00192	0.06574	-0.03355	-0.03095
698		3S	0.00441	-0.00004	-0.00265	0.00014	-0.00033
699		3PX	-0.00239	0.00029	-0.01206	0.00675	0.00650
700		3PY	-0.01157	-0.00161	-0.06609	0.02984	0.02707
701		3PZ	0.01351	0.00029	0.07731	-0.03712	-0.03450
702		4D 0	-0.00053	-0.00006	0.00574	-0.00202	-0.00182
703		4D+1	0.00299	0.00038	-0.01547	0.00392	0.00344
704		4D-1	-0.00071	-0.00011	0.00425	-0.00120	-0.00107
705		4D+2	-0.00113	-0.00010	0.00826	-0.00241	-0.00215
706		4D-2	-0.00221	-0.00018	0.01120	-0.00264	-0.00228
707	74 C	1S	0.00006	0.00009	-0.00008	0.00006	0.00006
708		2S	-0.00003	-0.00016	0.00019	-0.00014	-0.00012
709		2PX	-0.00436	-0.00025	0.01974	-0.00618	-0.00553
710		2PY	-0.02166	-0.00248	0.09814	-0.03120	-0.02803
711		2PZ	0.02395	0.00214	-0.11621	0.03657	0.03284
712		3S	-0.00067	-0.00129	0.00003	-0.00103	-0.00136
713		3PX	-0.00317	-0.00065	0.02195	-0.00875	-0.00810
714		3PY	-0.01869	-0.00236	0.11161	-0.03899	-0.03533
715		3PZ	0.01830	0.00150	-0.13276	0.04492	0.04049

716		4D 0	0.00111	0.00009	0.00246	-0.00156	-0.00145
717		4D+1	-0.00041	-0.00003	-0.00156	0.00067	0.00061
718		4D-1	0.00027	0.00001	0.00077	-0.00043	-0.00040
719		4D+2	0.00077	0.00007	0.00187	-0.00107	-0.00100
720		4D-2	0.00007	-0.00001	0.00077	-0.00025	-0.00023
721	75 C	1S	-0.00008	-0.00008	0.00011	-0.00005	-0.00005
722		2S	0.00025	0.00017	-0.00023	0.00014	0.00013
723		2PX	-0.00454	-0.00069	0.01868	-0.00497	-0.00439
724		2PY	-0.02145	-0.00223	0.09037	-0.02373	-0.02086
725		2PZ	0.02577	0.00248	-0.10783	0.02818	0.02474
726		3S	-0.00029	0.00068	-0.00080	0.00034	0.00055
727		3PX	-0.00358	-0.00084	0.01586	-0.00477	-0.00439
728		3PY	-0.01700	-0.00181	0.08345	-0.02219	-0.01953
729		3PZ	0.02223	0.00215	-0.10002	0.02625	0.02301
730		4D 0	-0.00093	-0.00008	-0.00155	0.00110	0.00103
731		4D+1	-0.00070	-0.00003	-0.00541	0.00250	0.00230
732		4D-1	-0.00007	-0.00002	0.00081	-0.00031	-0.00029
733		4D+2	-0.00022	-0.00001	0.00104	-0.00024	-0.00020
734		4D-2	0.00075	0.00006	0.00465	-0.00221	-0.00203
735	76 C	1S	-0.00004	-0.00005	0.00003	-0.00004	-0.00004
736		2S	0.00015	0.00010	-0.00007	0.00006	0.00005
737		2PX	0.00125	-0.00007	0.00075	-0.00075	-0.00070
738		2PY	0.00726	0.00067	0.00336	-0.00305	-0.00286
739		2PZ	-0.00826	-0.00059	-0.00408	0.00369	0.00346
740		3S	-0.00013	0.00057	0.00041	0.00104	0.00116
741		3PX	0.00138	-0.00014	0.00121	-0.00111	-0.00110
742		3PY	0.00516	0.00054	0.00613	-0.00335	-0.00304
743		3PZ	-0.00538	-0.00033	-0.00702	0.00457	0.00428
744		4D 0	-0.00078	-0.00008	0.00409	-0.00148	-0.00134
745		4D+1	-0.00176	-0.00017	0.00933	-0.00312	-0.00281
746		4D-1	0.00020	0.00001	-0.00113	0.00036	0.00032
747		4D+2	0.00021	0.00004	-0.00096	0.00028	0.00025
748		4D-2	0.00164	0.00017	-0.00834	0.00281	0.00254
749	77 H	1S	0.00026	0.00001	-0.00006	-0.00004	-0.00004
750		2S	-0.00125	-0.00031	-0.00029	-0.00107	-0.00103
751	78 C	1S	0.00000	0.00002	-0.00005	0.00001	0.00001
752		2S	0.00000	-0.00002	0.00009	-0.00001	0.00000
753		2PX	0.00130	0.00015	0.00638	-0.00341	-0.00316
754		2PY	0.00674	0.00046	0.03249	-0.01696	-0.01577
755		2PZ	-0.00797	-0.00053	-0.03868	0.02022	0.01878
756		3S	0.00032	0.00000	0.00103	0.00003	0.00005
757		3PX	0.00066	0.00009	0.00844	-0.00452	-0.00418
758		3PY	0.00465	0.00042	0.04463	-0.02242	-0.02077

759		3PZ	-0.00594	-0.00025	-0.05235	0.02691	0.02503
760		4D 0	0.00134	0.00013	-0.00694	0.00238	0.00215
761		4D+1	-0.00148	-0.00015	0.00728	-0.00212	-0.00188
762		4D-1	0.00055	0.00005	-0.00276	0.00087	0.00078
763		4D+2	0.00123	0.00012	-0.00625	0.00201	0.00181
764		4D-2	0.00093	0.00010	-0.00450	0.00124	0.00110
765	79 H	1S	-0.00005	-0.00004	-0.00012	-0.00003	-0.00003
766		2S	-0.00119	-0.00025	0.00053	0.00003	0.00003
767	80 C	1S	-0.00007	-0.00001	0.00003	-0.00001	-0.00001
768		2S	0.00017	0.00004	-0.00004	0.00004	0.00004
769		2PX	0.00505	0.00045	-0.02207	0.00716	0.00645
770		2PY	0.02586	0.00242	-0.10933	0.03554	0.03199
771		2PZ	-0.03103	-0.00295	0.13037	-0.04241	-0.03818
772		3S	-0.00022	0.00008	-0.00011	-0.00001	-0.00002
773		3PX	0.00439	0.00048	-0.02340	0.00846	0.00770
774		3PY	0.02122	0.00209	-0.11670	0.04095	0.03709
775		3PZ	-0.02522	-0.00245	0.13938	-0.04884	-0.04423
776		4D 0	0.00000	0.00000	-0.00184	0.00091	0.00085
777		4D+1	0.00009	0.00000	0.00183	-0.00075	-0.00069
778		4D-1	-0.00002	0.00000	-0.00071	0.00032	0.00029
779		4D+2	-0.00003	0.00001	-0.00162	0.00075	0.00069
780		4D-2	-0.00007	0.00000	-0.00113	0.00043	0.00038
781	81 H	1S	-0.00029	-0.00013	0.00010	-0.00009	-0.00008
782		2S	-0.00037	-0.00021	0.00026	-0.00016	-0.00012
783	82 H	1S	-0.00002	0.00003	-0.00006	0.00002	0.00002
784		2S	0.00008	0.00000	-0.00025	-0.00002	-0.00004
785	83 H	1S	-0.00005	0.00000	0.00004	-0.00002	-0.00001
786		2S	-0.00017	-0.00005	0.00005	-0.00013	-0.00013

B4

			191	192	193	194	195
			O	O	O	V	V
	Eigenvalues --		-0.20944	-0.19979	-0.19135	-0.07923	-0.05496
1	1 Ir	1S	-0.00501	-0.00661	0.01072	0.00124	0.00487
2		2S	0.00735	0.00984	-0.01521	-0.00180	-0.00692
3		3S	-0.02103	-0.03725	0.06919	0.00039	0.00266
4		4PX	-0.04118	-0.05192	-0.06081	-0.00440	0.00596
5		4PY	-0.01920	-0.02531	-0.04572	-0.00105	-0.00886
6		4PZ	-0.00525	-0.00286	-0.00032	-0.00433	-0.01395

7		5PX	0.02616	0.02762	0.02375	-0.00646	-0.06844
8		5PY	0.00859	0.01772	0.02950	0.00074	0.05706
9		5PZ	0.00751	-0.00919	-0.00666	0.01815	0.09036
10		6PX	-0.01191	-0.01991	-0.01446	0.00168	0.03151
11		6PY	-0.00157	-0.00354	-0.03710	-0.00241	-0.01718
12		6PZ	-0.01587	-0.02164	0.00715	0.01435	-0.02128
13		7D 0	-0.00268	-0.05088	0.01589	-0.01438	-0.01137
14		7D+1	0.27382	0.42447	-0.19101	-0.01543	-0.02212
15		7D-1	0.22173	0.14930	-0.01043	-0.04155	0.02445
16		7D+2	0.05231	0.05918	0.44243	0.00279	-0.05064
17		7D-2	-0.03546	-0.04902	-0.27554	0.00387	0.00108
18		8D 0	-0.00212	-0.01276	-0.00728	-0.00221	0.00211
19		8D+1	0.09688	0.15061	-0.06154	-0.00654	-0.01158
20		8D-1	0.08865	0.05179	-0.00058	-0.02369	0.00672
21		8D+2	0.02430	0.02826	0.16319	0.00289	-0.01969
22		8D-2	-0.01220	-0.02113	-0.10101	0.00230	0.01175
23	2 C	1S	0.00073	-0.00050	0.00137	0.00041	0.00302
24		2S	-0.00259	0.00314	-0.00330	-0.00040	-0.00939
25		2PX	-0.03244	-0.04677	-0.04455	0.00032	0.02068
26		2PY	-0.01111	-0.02775	-0.02321	-0.00584	0.00091
27		2PZ	0.00624	0.00028	0.00553	-0.00046	0.00608
28		3S	0.00593	-0.00117	-0.01097	-0.00750	-0.01313
29		3PX	-0.02395	-0.04138	-0.02992	-0.00498	0.01417
30		3PY	-0.01248	-0.02996	-0.01590	-0.00945	-0.01040
31		3PZ	0.00317	0.00176	0.00181	-0.00490	-0.02397
32		4D 0	0.00038	0.00050	0.00014	-0.00014	0.00056
33		4D+1	0.00320	0.00216	-0.00443	0.00052	0.00586
34		4D-1	0.00146	0.00116	-0.00255	0.00011	0.00222
35		4D+2	-0.00156	-0.00135	0.00153	0.00014	-0.00135
36		4D-2	0.00149	0.00117	-0.00111	-0.00007	0.00146
37	3 C	1S	-0.00048	0.00114	-0.00102	0.00049	-0.00142
38		2S	0.00261	-0.00322	0.00237	-0.00344	0.00210
39		2PX	-0.06016	-0.06130	-0.00711	0.00190	0.06073
40		2PY	-0.02945	-0.04238	0.00308	0.00032	0.04000
41		2PZ	0.00289	0.00499	-0.00191	0.00121	-0.00368
42		3S	0.00068	0.00479	-0.00285	0.00506	0.00901
43		3PX	-0.04430	-0.05010	-0.00899	0.00281	0.06953
44		3PY	-0.02865	-0.02986	0.01148	0.00657	0.03329
45		3PZ	0.00586	-0.00359	0.00543	-0.00665	-0.00282
46		4D 0	0.00061	0.00039	-0.00088	-0.00021	-0.00022
47		4D+1	-0.00234	-0.00120	0.00667	-0.00035	-0.00091
48		4D-1	-0.00154	-0.00107	0.00346	0.00002	0.00056
49		4D+2	0.00353	0.00207	-0.00487	-0.00011	0.00353

50		4D-2	-0.00224	-0.00168	0.00378	0.00001	-0.00236
51	4 C	1S	-0.00066	-0.00035	-0.00037	0.00013	-0.00143
52		2S	0.00146	0.00010	0.00053	-0.00052	0.00227
53		2PX	0.04293	0.03018	-0.06282	0.00505	0.04835
54		2PY	0.02296	0.01758	-0.03338	0.00286	0.02785
55		2PZ	-0.00507	-0.00266	0.00121	-0.00009	-0.00634
56		3S	-0.00053	0.00259	0.00435	0.00358	0.02421
57		3PX	0.03224	0.02435	-0.05697	0.00760	0.06025
58		3PY	0.02003	0.01476	-0.02990	0.00377	0.03962
59		3PZ	-0.00209	-0.00304	0.00062	-0.00171	-0.01151
60		4D 0	-0.00029	-0.00011	-0.00012	0.00015	0.00035
61		4D+1	0.00195	0.00254	0.00191	-0.00009	-0.00178
62		4D-1	0.00074	0.00153	0.00103	0.00029	-0.00051
63		4D+2	0.00201	0.00270	0.00181	0.00006	-0.00286
64		4D-2	-0.00128	-0.00176	-0.00108	0.00005	0.00198
65	5 H	1S	-0.00140	0.00026	-0.00092	0.00109	-0.00165
66		2S	-0.00045	0.00819	0.00153	0.00340	0.01070
67	6 C	1S	-0.00044	-0.00082	0.00072	0.00033	0.00119
68		2S	0.00072	0.00121	-0.00119	-0.00077	-0.00280
69		2PX	-0.01484	-0.00397	0.06784	-0.00520	-0.01032
70		2PY	-0.00790	0.00054	0.03427	-0.00289	-0.00695
71		2PZ	-0.00189	-0.00330	-0.00002	0.00102	0.00371
72		3S	0.00001	0.00775	-0.00516	0.00138	-0.00721
73		3PX	-0.01488	-0.00660	0.05424	-0.00596	-0.01049
74		3PY	-0.00615	-0.00093	0.02370	-0.00394	-0.00167
75		3PZ	0.00149	-0.00401	-0.00113	-0.00088	0.00746
76		4D 0	-0.00030	0.00000	-0.00021	-0.00002	0.00017
77		4D+1	0.00377	0.00432	0.00131	-0.00007	-0.00506
78		4D-1	0.00188	0.00267	0.00043	-0.00003	-0.00309
79		4D+2	-0.00017	-0.00041	-0.00123	-0.00001	0.00066
80		4D-2	0.00024	0.00065	0.00086	0.00005	-0.00090
81	7 C	1S	-0.00016	-0.00023	0.00033	0.00043	0.00107
82		2S	0.00003	0.00030	-0.00042	-0.00077	-0.00234
83		2PX	0.05181	0.06528	0.02634	0.00037	-0.05445
84		2PY	0.02906	0.03321	0.01418	-0.00113	-0.03191
85		2PZ	-0.00132	-0.00285	-0.00057	0.00017	0.00300
86		3S	0.00194	0.00195	-0.00021	-0.00306	-0.00873
87		3PX	0.04039	0.05351	0.02817	0.00049	-0.06785
88		3PY	0.02442	0.02777	0.01373	-0.00168	-0.03648
89		3PZ	-0.00199	-0.00148	-0.00054	0.00057	0.00408
90		4D 0	0.00001	0.00011	0.00004	0.00005	0.00011
91		4D+1	0.00059	0.00030	-0.00173	0.00017	-0.00007
92		4D-1	0.00008	0.00012	-0.00080	0.00001	-0.00062

93		4D+2	-0.00188	-0.00105	0.00415	-0.00034	-0.00275
94		4D-2	0.00124	0.00077	-0.00286	0.00031	0.00180
95	8 H	1S	-0.00207	0.00018	-0.00042	0.00118	0.00132
96		2S	-0.00337	0.00109	-0.00109	0.00234	0.00031
97	9 H	1S	0.00009	-0.00246	0.00149	0.00004	0.00171
98		2S	0.00124	-0.00246	0.00025	-0.00030	0.00650
99	10 H	1S	0.00062	0.00056	0.00001	0.00029	0.00120
100		2S	0.00134	0.00063	-0.00042	0.00089	0.00476
101	11 C	1S	0.01100	0.01324	0.01929	0.00137	0.00343
102		2S	-0.01867	-0.02248	-0.03580	-0.00218	-0.00811
103		2PX	-0.06065	-0.07568	-0.06745	-0.00682	-0.05588
104		2PY	-0.03469	-0.03432	-0.10180	0.00116	0.09384
105		2PZ	0.00600	0.00941	-0.03451	-0.00158	0.01683
106		3S	-0.04580	-0.05439	-0.03779	-0.00269	-0.01314
107		3PX	-0.05764	-0.06889	-0.11232	-0.01203	-0.06458
108		3PY	-0.03279	-0.03388	-0.11379	-0.00455	0.08356
109		3PZ	-0.00088	-0.00709	0.00834	-0.00131	0.00371
110		4D 0	-0.00063	-0.00136	0.00195	0.00018	0.00125
111		4D+1	-0.00637	-0.00801	0.00295	0.00090	-0.00059
112		4D-1	-0.00276	-0.00428	0.00298	0.00041	0.00315
113		4D+2	0.00018	0.00048	-0.00954	0.00026	0.00219
114		4D-2	0.00190	0.00247	0.00840	0.00006	-0.00232
115	12 C	1S	0.00179	0.00298	-0.00610	-0.00080	-0.00088
116		2S	-0.00333	-0.00504	0.01516	0.00231	0.00153
117		2PX	0.00386	-0.00048	0.06608	0.00178	0.02518
118		2PY	-0.00066	0.00535	-0.09714	-0.00179	-0.05049
119		2PZ	-0.01433	-0.01803	0.01087	0.00512	-0.00393
120		3S	-0.02563	-0.04052	-0.00269	0.00055	-0.00234
121		3PX	0.02521	0.02501	0.09391	0.00528	0.02800
122		3PY	0.01073	0.01978	-0.05177	0.00023	-0.04788
123		3PZ	-0.01339	-0.01772	-0.03152	-0.00158	-0.01977
124		4D 0	0.00149	0.00187	0.00164	0.00024	0.00372
125		4D+1	-0.00172	-0.00241	-0.00296	-0.00065	-0.00725
126		4D-1	-0.00163	-0.00136	-0.00440	-0.00006	0.00907
127		4D+2	-0.00114	-0.00102	-0.00153	0.00014	0.00818
128		4D-2	-0.00024	-0.00028	-0.00166	-0.00008	-0.00395
129	13 C	1S	-0.00871	-0.01141	-0.00322	0.00074	0.00113
130		2S	0.02100	0.02720	0.01308	-0.00138	-0.00455
131		2PX	0.03014	0.03844	0.06170	-0.00105	-0.01242
132		2PY	0.02442	0.02855	-0.07844	-0.00134	0.01741
133		2PZ	-0.02663	-0.03253	-0.02636	0.00017	0.00518
134		3S	-0.00181	0.00710	-0.07646	-0.00720	-0.00461
135		3PX	0.02183	0.02869	0.03755	-0.00338	-0.00719

136		3PY	0.01592	0.01874	-0.08436	-0.00094	0.03415
137		3PZ	-0.00232	-0.00493	0.03584	0.00487	0.00814
138		4D 0	0.00306	0.00385	0.00509	0.00006	-0.00102
139		4D+1	0.00033	0.00051	0.00030	0.00027	0.00309
140		4D-1	-0.00045	-0.00080	0.00171	0.00001	-0.00142
141		4D+2	-0.00132	-0.00197	-0.00046	-0.00026	-0.00791
142		4D-2	-0.00208	-0.00245	-0.00349	0.00014	0.00573
143	14 C	1S	0.00197	0.00206	0.00659	0.00066	0.00102
144		2S	-0.00626	-0.00692	-0.01872	-0.00197	-0.00391
145		2PX	-0.00618	-0.00788	-0.03059	-0.00254	-0.05375
146		2PY	-0.00816	-0.00566	0.01314	0.00252	0.10836
147		2PZ	-0.00067	-0.00033	0.00812	0.00178	0.02434
148		3S	0.01978	0.02650	0.02940	0.00213	0.00418
149		3PX	0.01053	0.01125	0.00882	-0.00030	-0.04308
150		3PY	-0.00038	0.00103	0.00940	0.00293	0.08543
151		3PZ	0.00935	0.01432	0.03227	0.00495	0.02731
152		4D 0	0.00041	0.00041	0.00301	0.00026	0.00140
153		4D+1	-0.00016	-0.00026	-0.00067	0.00035	-0.00138
154		4D-1	-0.00041	-0.00047	0.00291	0.00019	0.00273
155		4D+2	0.00033	0.00004	0.00768	0.00017	0.00316
156		4D-2	0.00006	0.00038	-0.00494	-0.00005	-0.00177
157	15 C	1S	0.00625	0.00789	0.00629	0.00013	-0.00010
158		2S	-0.01652	-0.02053	-0.01752	-0.00039	-0.00008
159		2PX	-0.02294	-0.02551	-0.03215	0.00206	0.06217
160		2PY	-0.00286	-0.00971	0.01750	-0.00379	-0.12605
161		2PZ	-0.00870	-0.01238	-0.00287	-0.00063	-0.02596
162		3S	0.00191	-0.00091	0.01603	0.00099	0.00771
163		3PX	0.00374	0.00552	-0.00205	0.00101	0.05793
164		3PY	0.00748	0.00539	0.01947	-0.00348	-0.10906
165		3PZ	-0.01122	-0.01420	-0.03205	-0.00423	-0.02132
166		4D 0	0.00041	0.00054	-0.00145	0.00005	0.00050
167		4D+1	-0.00175	-0.00225	0.00026	-0.00009	-0.00065
168		4D-1	-0.00130	-0.00135	-0.00697	-0.00005	0.00093
169		4D+2	0.00003	0.00016	0.00457	0.00007	0.00031
170		4D-2	0.00099	0.00123	-0.00402	-0.00006	0.00018
171	16 H	1S	0.00617	0.00839	0.01490	0.00070	-0.00010
172		2S	0.01308	0.01561	0.00192	-0.00118	0.00219
173	17 C	1S	-0.00095	-0.00112	-0.00059	0.00014	0.00018
174		2S	0.00301	0.00374	0.00322	-0.00015	-0.00059
175		2PX	0.00209	0.00434	-0.05496	-0.00072	-0.00564
176		2PY	0.00232	-0.00147	0.11649	0.00056	0.01022
177		2PZ	0.00065	0.00034	0.02615	0.00016	0.00221
178		3S	-0.00661	-0.01013	-0.03651	-0.00564	-0.00595

179		3PX	-0.01187	-0.01364	-0.07393	-0.00219	-0.01216
180		3PY	-0.00373	-0.00857	0.09097	0.00028	0.01927
181		3PZ	-0.00309	-0.00315	0.01215	-0.00087	0.00709
182		4D 0	0.00045	0.00042	0.00026	-0.00017	-0.00349
183		4D+1	-0.00039	-0.00031	-0.00020	0.00014	0.00474
184		4D-1	0.00010	-0.00016	0.00008	-0.00022	-0.00877
185		4D+2	-0.00018	-0.00028	-0.00100	-0.00002	-0.00253
186		4D-2	-0.00020	-0.00030	0.00033	0.00003	-0.00028
187	18 H	1S	-0.00245	-0.00290	-0.00202	0.00045	0.00089
188		2S	-0.00986	-0.01215	-0.01319	0.00073	0.00208
189	19 C	1S	0.00213	0.00305	0.00011	0.00006	-0.00021
190		2S	-0.00583	-0.00792	-0.00175	-0.00011	-0.00144
191		2PX	-0.01023	-0.00699	-0.03253	-0.00574	-0.01779
192		2PY	0.00548	0.00355	-0.00646	0.00690	0.01097
193		2PZ	-0.03219	0.02255	-0.00369	-0.09554	-0.18823
194		3S	0.00963	0.00982	0.02494	-0.00137	0.00471
195		3PX	0.00753	0.01417	-0.01724	-0.00647	-0.01259
196		3PY	0.00038	-0.00379	-0.03191	0.01042	0.01770
197		3PZ	-0.01414	0.01010	-0.00854	-0.09878	-0.18985
198		4D 0	-0.00131	0.00136	-0.00080	0.00091	-0.00009
199		4D+1	0.00585	-0.01268	0.00135	-0.00788	-0.00890
200		4D-1	-0.00160	0.00361	-0.00001	-0.00001	-0.00761
201		4D+2	0.00048	-0.00044	-0.00110	-0.00054	0.00104
202		4D-2	-0.00019	0.00166	0.00020	0.00059	0.00018
203	20 C	1S	-0.00088	-0.00080	0.00327	0.00000	0.00107
204		2S	0.00135	0.00179	-0.00999	-0.00009	-0.00265
205		2PX	0.00025	-0.00503	-0.03073	-0.00059	0.00894
206		2PY	-0.00586	-0.00087	0.00102	0.00080	0.01284
207		2PZ	0.02103	-0.04559	-0.00035	-0.00657	-0.05919
208		3S	0.00769	0.00718	-0.01008	0.00167	-0.01818
209		3PX	-0.00220	-0.00850	-0.04067	0.00039	0.02604
210		3PY	0.00197	0.00733	0.00247	0.00076	0.01446
211		3PZ	0.01568	-0.02956	0.00092	-0.00021	-0.04918
212		4D 0	0.00061	-0.00129	-0.00003	-0.00139	-0.00288
213		4D+1	-0.00297	0.00638	-0.00078	0.00666	0.01327
214		4D-1	0.00253	-0.00454	0.00027	-0.00532	-0.00967
215		4D+2	0.00038	0.00036	-0.00134	0.00001	0.00021
216		4D-2	0.00101	-0.00019	0.00005	-0.00080	-0.00004
217	21 C	1S	-0.00030	-0.00065	-0.00053	-0.00024	0.00166
218		2S	0.00059	0.00121	0.00063	0.00061	-0.00414
219		2PX	-0.00284	0.00850	0.00429	0.00418	-0.00165
220		2PY	0.00275	-0.00756	-0.00219	-0.00219	0.00589
221		2PZ	-0.05410	0.10215	-0.00729	0.04962	0.00318

222		3S	0.00281	0.00457	0.01172	-0.00196	-0.01175
223		3PX	-0.00643	0.00323	0.00602	0.00647	-0.00626
224		3PY	0.00332	-0.00841	-0.00857	-0.00047	0.00651
225		3PZ	-0.04226	0.08560	-0.00649	0.05181	-0.00472
226		4D 0	0.00012	-0.00001	-0.00004	0.00119	0.00249
227		4D+1	0.00015	-0.00118	0.00000	-0.00465	-0.01140
228		4D-1	0.00148	-0.00100	0.00024	0.00500	0.01139
229		4D+2	0.00011	-0.00022	-0.00079	-0.00009	-0.00035
230		4D-2	0.00043	0.00040	0.00125	0.00072	0.00219
231	22 C	1S	0.00074	0.00069	-0.00156	-0.00003	0.00080
232		2S	-0.00149	-0.00099	0.00343	0.00036	-0.00197
233		2PX	0.00293	-0.00731	0.00547	-0.00557	-0.00922
234		2PY	-0.00098	0.01068	-0.00669	0.00663	0.01238
235		2PZ	0.05860	-0.10537	0.00800	-0.08838	-0.13629
236		3S	-0.00963	-0.01115	0.00135	-0.00164	-0.00227
237		3PX	0.00206	-0.00666	0.00644	-0.00825	-0.01196
238		3PY	-0.00003	0.01226	0.00293	0.00835	0.01233
239		3PZ	0.04959	-0.09187	0.00723	-0.10351	-0.17576
240		4D 0	-0.00007	0.00026	0.00016	0.00009	0.00045
241		4D+1	0.00014	0.00023	0.00016	0.00210	0.00469
242		4D-1	-0.00069	0.00216	0.00022	0.00266	0.00997
243		4D+2	-0.00009	0.00008	-0.00090	0.00029	0.00173
244		4D-2	0.00005	0.00029	0.00093	0.00001	-0.00060
245	23 H	1S	0.00301	0.00335	0.00194	0.00005	0.00377
246		2S	0.00077	-0.00038	-0.02876	0.00035	0.04466
247	24 C	1S	-0.00002	-0.00006	0.00026	0.00000	0.00129
248		2S	-0.00015	-0.00036	-0.00146	-0.00046	-0.00336
249		2PX	-0.00138	-0.00147	-0.00792	0.00354	0.01284
250		2PY	-0.00072	-0.00150	-0.00089	-0.00426	-0.01019
251		2PZ	0.00369	0.01155	0.00504	0.06142	0.17579
252		3S	-0.00200	-0.00119	-0.00092	0.00334	-0.00828
253		3PX	-0.00261	0.00025	0.00061	0.00613	0.01496
254		3PY	-0.00245	-0.00346	-0.00145	-0.00698	-0.01659
255		3PZ	-0.00035	0.01519	0.00309	0.07318	0.21634
256		4D 0	0.00028	-0.00063	-0.00009	-0.00031	0.00001
257		4D+1	-0.00387	0.00727	-0.00057	0.00542	0.00484
258		4D-1	-0.00109	0.00205	-0.00010	0.00287	0.00598
259		4D+2	-0.00029	0.00073	-0.00039	0.00064	0.00052
260		4D-2	0.00016	-0.00038	-0.00003	-0.00014	0.00008
261	25 H	1S	0.00068	0.00056	0.00435	0.00001	0.00280
262		2S	0.00090	0.00273	0.01087	-0.00272	0.00936
263	26 H	1S	0.00011	-0.00009	-0.00620	-0.00005	0.00430
264		2S	0.00068	0.00023	-0.00913	-0.00084	0.01258

265	27	H	1S	-0.00005	-0.00026	0.00178	-0.00030	0.00063
266			2S	0.00084	0.00070	0.00446	0.00011	0.00637
267	28	C	1S	-0.01245	-0.01203	-0.01917	0.00138	-0.00392
268			2S	0.02427	0.02144	0.03015	-0.00283	0.00724
269			2PX	-0.04519	-0.07613	-0.10492	-0.00613	-0.00299
270			2PY	-0.03973	-0.03747	-0.05523	-0.00755	-0.02390
271			2PZ	-0.04645	-0.14813	0.02132	0.05527	0.09276
272			3S	0.02341	0.01005	0.09456	-0.02000	0.02199
273			3PX	-0.06158	-0.11106	-0.08097	-0.02070	0.00223
274			3PY	-0.03721	-0.02723	-0.05844	-0.00501	-0.03562
275			3PZ	-0.03303	-0.09814	0.01183	0.05405	0.08294
276			4D 0	0.00263	-0.00014	0.00201	-0.00137	-0.00068
277			4D+1	-0.01277	-0.00698	0.00322	0.00590	0.00262
278			4D-1	0.00156	-0.01263	0.00237	-0.00400	-0.00107
279			4D+2	-0.00091	-0.00209	-0.00980	0.00010	0.00207
280			4D-2	0.00152	0.00095	0.00241	-0.00003	-0.00108
281	29	C	1S	0.00806	0.00097	0.01141	-0.00489	-0.00046
282			2S	-0.02182	-0.00696	-0.02845	0.01138	0.00178
283			2PX	-0.00820	0.03546	0.07607	0.02310	-0.00616
284			2PY	0.01963	0.00927	-0.01926	0.00340	-0.00270
285			2PZ	-0.21942	-0.05271	0.01751	0.08508	0.01629
286			3S	0.01659	0.07019	0.01254	0.04070	-0.00097
287			3PX	-0.01183	-0.02218	0.05548	-0.00189	0.01086
288			3PY	0.04444	0.03416	0.00626	0.00963	-0.00821
289			3PZ	-0.16422	-0.03715	0.01666	0.08968	0.02661
290			4D 0	-0.00088	-0.00120	-0.00103	0.00038	0.00059
291			4D+1	-0.00248	0.00869	-0.00062	-0.00563	-0.00843
292			4D-1	-0.00465	0.00042	0.00009	-0.00067	-0.00201
293			4D+2	0.00223	0.00296	0.00236	-0.00071	0.00000
294			4D-2	0.00234	0.00283	0.00544	0.00098	0.00083
295	30	C	1S	0.00265	0.00330	-0.00270	0.00021	0.00075
296			2S	-0.00568	-0.00873	0.00440	-0.00145	-0.00202
297			2PX	0.00824	-0.00740	0.01296	-0.00458	-0.00778
298			2PY	0.01223	0.04759	-0.01092	0.01209	0.01667
299			2PZ	0.08637	-0.21419	0.01948	-0.09228	-0.04640
300			3S	-0.00101	0.00582	0.03428	0.00772	0.00332
301			3PX	0.03368	0.04195	0.04076	-0.00129	-0.00501
302			3PY	-0.00574	0.03096	0.00294	0.01520	0.00084
303			3PZ	0.05480	-0.17268	0.01793	-0.09138	-0.05094
304			4D 0	0.00053	0.00092	0.00013	-0.00121	-0.00206
305			4D+1	0.00315	-0.00035	0.00073	0.00691	0.01139
306			4D-1	0.00497	0.00485	-0.00113	-0.00279	-0.00522
307			4D+2	-0.00076	-0.00069	-0.00228	0.00046	-0.00042

308		4D-2	0.00258	0.00417	0.00476	-0.00038	-0.00028
309	31 C	1S	-0.00329	-0.00387	-0.00664	0.00003	-0.00007
310		2S	0.00782	0.00991	0.01741	0.00131	-0.00006
311		2PX	-0.01740	-0.01287	-0.03756	-0.00941	-0.00681
312		2PY	0.01381	-0.03820	-0.02022	-0.00138	0.01233
313		2PZ	-0.12907	0.12670	-0.00552	-0.08007	-0.11577
314		3S	0.00510	0.00012	-0.00687	-0.01035	0.00122
315		3PX	0.02687	0.03527	0.02738	-0.00408	-0.01044
316		3PY	-0.00067	-0.04449	-0.00953	0.00986	0.02137
317		3PZ	-0.09426	0.07769	-0.00474	-0.08061	-0.11328
318		4D 0	0.00004	0.00246	0.00076	0.00128	0.00014
319		4D+1	0.01111	-0.00161	-0.00032	-0.00964	-0.00034
320		4D-1	0.00492	0.00980	-0.00139	0.00162	-0.00023
321		4D+2	-0.00259	0.00161	-0.00314	0.00357	-0.00090
322		4D-2	-0.00409	0.00313	0.00070	0.00590	-0.00078
323	32 H	1S	-0.01269	-0.00966	-0.00469	0.00130	-0.00217
324		2S	0.00462	-0.01132	-0.03043	0.00084	-0.01610
325	33 C	1S	-0.00060	-0.00414	-0.00221	-0.00264	-0.00087
326		2S	0.00429	0.01207	0.00721	0.00481	0.00265
327		2PX	-0.01383	-0.01049	-0.01681	0.00947	-0.00083
328		2PY	-0.02053	-0.01860	-0.00878	-0.00946	-0.01169
329		2PZ	0.13242	0.00423	-0.00856	0.05323	0.09481
330		3S	-0.03996	-0.02579	-0.03263	0.03047	0.00357
331		3PX	-0.02604	-0.00744	-0.01059	0.02639	-0.00654
332		3PY	0.00566	0.02439	0.02224	-0.00781	-0.00834
333		3PZ	0.10482	0.00678	-0.00452	0.05688	0.09345
334		4D 0	0.00050	-0.00007	0.00070	-0.00053	-0.00007
335		4D+1	-0.00210	0.01408	-0.00145	0.00668	0.00329
336		4D-1	-0.00118	0.00285	-0.00048	0.00121	0.00085
337		4D+2	0.00050	0.00297	-0.00013	0.00119	0.00107
338		4D-2	0.00010	-0.00099	0.00026	-0.00024	-0.00044
339	34 C	1S	-0.00564	0.00150	-0.00087	0.00560	-0.00184
340		2S	0.01010	-0.00604	-0.00030	-0.01221	0.00438
341		2PX	0.01522	0.00822	0.00355	-0.00538	0.00314
342		2PY	-0.01342	-0.00787	-0.00188	0.01200	-0.00175
343		2PZ	0.01284	0.20879	-0.02595	0.06665	0.00687
344		3S	0.06642	0.03576	0.03052	-0.04599	0.01057
345		3PX	-0.02291	-0.01001	-0.02365	0.02097	0.00083
346		3PY	-0.00137	-0.03310	-0.01674	-0.00764	0.00875
347		3PZ	0.01172	0.16690	-0.02097	0.06469	0.01790
348		4D 0	0.00153	-0.00140	-0.00035	0.00095	0.00195
349		4D+1	-0.00430	0.00130	0.00023	-0.00436	-0.00539
350		4D-1	0.00683	-0.00400	-0.00001	0.00424	0.00654

351		4D+2	0.00005	0.00037	-0.00041	0.00064	0.00030
352		4D-2	0.00226	0.00046	0.00154	0.00024	0.00127
353	35 H	1S	-0.00399	-0.01182	-0.00252	-0.00401	-0.00251
354		2S	-0.01183	-0.03026	-0.01114	-0.01028	-0.00907
355	36 H	1S	0.00712	0.00381	0.00582	-0.00223	0.00090
356		2S	-0.00189	0.01847	0.02048	0.00705	-0.00988
357	37 C	1S	-0.00232	-0.00117	0.00280	-0.00136	-0.00177
358		2S	0.00788	0.00590	-0.00518	0.00105	0.00409
359		2PX	-0.02401	-0.03067	0.01196	0.00845	0.04374
360		2PY	-0.00555	-0.02570	-0.02170	0.00556	-0.05999
361		2PZ	0.01394	0.00866	-0.01449	0.00165	-0.00910
362		3S	0.00258	-0.00467	-0.02349	0.01833	0.01672
363		3PX	-0.03019	-0.03101	0.01016	0.01334	0.05137
364		3PY	-0.01397	-0.01929	-0.01294	0.01882	-0.04546
365		3PZ	0.00755	0.02074	-0.00234	0.00702	-0.01118
366		4D 0	-0.00052	0.00013	0.00199	0.00042	0.00467
367		4D+1	-0.00111	-0.00109	-0.00110	-0.00038	-0.00856
368		4D-1	-0.00009	-0.00006	0.00249	0.00058	0.01332
369		4D+2	0.00043	-0.00083	0.00149	-0.00016	0.00809
370		4D-2	-0.00002	0.00029	-0.00134	0.00018	-0.00319
371	38 C	1S	0.00115	0.00198	-0.00493	-0.00080	0.00025
372		2S	-0.00235	-0.00263	0.01158	0.00258	0.00146
373		2PX	-0.02631	-0.02629	-0.00092	0.00278	0.08843
374		2PY	-0.00224	-0.01728	0.00042	-0.00479	-0.18904
375		2PZ	0.00484	0.00176	0.01417	0.00076	-0.03541
376		3S	-0.02192	-0.04258	0.00201	-0.00045	-0.01094
377		3PX	-0.01922	-0.02993	0.02235	0.00396	0.09716
378		3PY	-0.00162	-0.01753	0.01431	-0.00546	-0.18854
379		3PZ	-0.00931	-0.01777	-0.00761	-0.00280	-0.03742
380		4D 0	-0.00071	-0.00059	-0.00162	0.00019	0.00100
381		4D+1	-0.00086	-0.00113	0.00258	0.00059	0.00199
382		4D-1	-0.00041	-0.00051	-0.00291	-0.00018	0.00312
383		4D+2	-0.00052	0.00002	-0.00471	-0.00012	-0.01002
384		4D-2	0.00045	-0.00032	0.00205	-0.00024	0.00779
385	39 C	1S	0.00151	0.00092	-0.00197	-0.00023	0.00015
386		2S	-0.00270	-0.00231	0.00378	0.00010	-0.00052
387		2PX	0.00377	0.00514	0.02145	0.00351	0.06500
388		2PY	-0.00244	-0.00020	-0.04298	-0.00746	-0.13446
389		2PZ	-0.00782	-0.00466	-0.00014	-0.00173	-0.02572
390		3S	-0.00819	0.00849	0.01832	0.00452	-0.00053
391		3PX	0.00713	0.00474	0.01884	0.00378	0.07995
392		3PY	0.00213	-0.00356	-0.03883	-0.01246	-0.17175
393		3PZ	-0.00558	0.00213	0.00004	-0.00046	-0.03108

394		4D 0	0.00026	0.00019	-0.00028	-0.00008	-0.00237
395		4D+1	-0.00120	-0.00145	0.00050	0.00049	0.00249
396		4D-1	-0.00006	-0.00137	-0.00108	0.00020	-0.00697
397		4D+2	-0.00036	-0.00011	0.00056	0.00013	0.00716
398		4D-2	0.00039	-0.00004	-0.00072	-0.00003	-0.00719
399	40 H	1S	-0.00116	-0.00581	-0.00410	-0.00120	-0.00107
400		2S	0.03011	0.02643	-0.00303	-0.02522	-0.03156
401	41 C	1S	0.00036	0.00030	0.00114	-0.00047	-0.00095
402		2S	-0.00027	-0.00047	-0.00243	0.00081	0.00197
403		2PX	0.00307	0.00117	-0.02264	-0.00319	-0.00390
404		2PY	0.00221	0.00739	0.04265	0.00674	0.00853
405		2PZ	-0.00293	-0.00122	0.00297	0.00218	0.00485
406		3S	-0.00763	-0.00535	-0.01144	0.00302	0.00738
407		3PX	-0.00071	0.00464	-0.02763	-0.00365	-0.00030
408		3PY	0.00151	0.00878	0.02827	0.00721	-0.00389
409		3PZ	-0.00243	-0.00326	0.00713	0.00254	0.00532
410		4D 0	0.00057	0.00044	0.00011	-0.00004	-0.00480
411		4D+1	-0.00115	-0.00091	0.00024	0.00006	0.00770
412		4D-1	0.00009	-0.00087	-0.00026	-0.00031	-0.01443
413		4D+2	-0.00014	-0.00050	-0.00095	-0.00005	-0.00642
414		4D-2	-0.00012	-0.00011	0.00039	-0.00005	0.00124
415	42 C	1S	-0.00006	0.00052	0.00005	-0.00068	-0.00114
416		2S	0.00061	-0.00009	-0.00004	0.00132	0.00235
417		2PX	-0.00169	-0.01215	-0.00697	0.00082	-0.08310
418		2PY	-0.01187	0.00111	0.01064	0.00227	0.17708
419		2PZ	0.00085	0.00247	0.00240	0.00086	0.03361
420		3S	0.00445	-0.00870	0.00677	0.00325	0.00761
421		3PX	0.00132	-0.00728	-0.01205	-0.00033	-0.10440
422		3PY	-0.00884	0.00351	0.01033	0.00288	0.21570
423		3PZ	-0.00027	-0.00360	0.00289	-0.00020	0.03778
424		4D 0	-0.00012	0.00004	0.00012	-0.00010	-0.00111
425		4D+1	-0.00029	-0.00024	-0.00067	-0.00025	-0.00013
426		4D-1	-0.00011	-0.00004	0.00052	0.00002	-0.00328
427		4D+2	0.00013	0.00012	0.00279	0.00054	0.00580
428		4D-2	-0.00008	-0.00025	-0.00198	-0.00033	-0.00528
429	43 H	1S	0.00602	0.00806	-0.00171	-0.00182	-0.00263
430		2S	0.00688	0.01257	-0.00336	-0.00338	-0.00612
431	44 H	1S	-0.00396	-0.00514	0.00065	-0.00030	-0.00138
432		2S	-0.00665	-0.00629	-0.00194	-0.00087	-0.00447
433	45 H	1S	-0.00115	-0.00004	-0.00001	-0.00071	-0.00134
434		2S	-0.00254	-0.00172	-0.00093	-0.00269	-0.00636
435	46 C	1S	-0.00093	-0.00134	0.00190	-0.00068	-0.00463
436		2S	0.00224	0.00141	-0.00431	0.00088	0.00863

437		2PX	0.01274	0.01122	-0.09622	-0.00213	-0.04515
438		2PY	0.01029	0.00825	-0.06150	0.00179	-0.01160
439		2PZ	0.00473	-0.00474	0.00690	-0.00227	-0.00215
440		3S	0.00135	0.00994	0.00815	0.00656	0.05452
441		3PX	0.00676	0.00441	-0.05616	-0.00326	-0.04295
442		3PY	0.01018	0.01682	-0.06382	0.00813	0.00914
443		3PZ	0.00759	0.01528	-0.00975	0.00040	-0.01605
444		4D 0	-0.00046	-0.00013	0.00005	0.00004	-0.00065
445		4D+1	0.00557	0.00286	0.00083	-0.00046	0.00042
446		4D-1	0.00111	0.00362	-0.00201	0.00108	0.00188
447		4D+2	-0.00135	-0.00175	-0.01575	-0.00015	-0.00107
448		4D-2	0.00067	0.00085	0.01058	0.00018	-0.00140
449	47 C	1S	0.00123	-0.00169	0.00128	-0.00110	-0.00122
450		2S	-0.00407	0.00280	0.00006	0.00366	0.00607
451		2PX	-0.06565	-0.04897	-0.13420	-0.00209	-0.00637
452		2PY	-0.04043	-0.02137	-0.07533	0.00213	0.00155
453		2PZ	-0.00282	0.00728	0.00268	0.00169	0.00057
454		3S	0.00690	0.02437	-0.03321	0.00267	-0.00479
455		3PX	-0.04858	-0.03730	-0.11021	-0.00616	-0.00245
456		3PY	-0.02868	-0.01778	-0.06212	-0.00085	-0.02823
457		3PZ	0.00142	0.01102	-0.01739	0.00425	-0.00503
458		4D 0	-0.00003	0.00018	0.00031	0.00018	0.00084
459		4D+1	0.00042	0.00035	-0.00367	-0.00004	-0.00171
460		4D-1	0.00019	0.00029	-0.00228	0.00002	-0.00030
461		4D+2	-0.00290	-0.00173	0.00178	0.00030	0.00362
462		4D-2	0.00167	0.00105	-0.00098	-0.00009	-0.00142
463	48 C	1S	-0.00106	0.00162	-0.00124	0.00106	0.00097
464		2S	0.00413	-0.00318	0.00385	-0.00371	-0.00046
465		2PX	0.04901	0.02072	-0.15037	-0.00014	0.01925
466		2PY	0.02953	0.00610	-0.07653	-0.00276	0.00868
467		2PZ	-0.00884	0.00528	-0.00032	0.00431	0.00424
468		3S	0.00083	-0.01137	-0.00427	-0.00153	-0.00569
469		3PX	0.03895	0.02609	-0.12586	0.00643	0.02066
470		3PY	0.02083	-0.00462	-0.04777	-0.00793	0.01391
471		3PZ	-0.00597	0.00215	0.01757	0.00014	-0.00581
472		4D 0	0.00020	0.00019	-0.00003	-0.00029	-0.00040
473		4D+1	-0.00204	-0.00227	0.00290	0.00022	0.00446
474		4D-1	-0.00091	-0.00122	0.00210	-0.00027	0.00181
475		4D+2	0.00268	0.00173	0.00229	-0.00034	-0.00218
476		4D-2	-0.00205	-0.00159	-0.00087	0.00022	0.00146
477	49 C	1S	-0.00053	0.00061	0.00001	0.00023	0.00076
478		2S	0.00151	-0.00057	-0.00019	-0.00059	-0.00112
479		2PX	-0.06450	-0.03676	0.03729	0.00516	0.05031

480		2PY	-0.03273	-0.02196	0.02046	0.00155	0.02274
481		2PZ	0.00169	0.00209	-0.00173	0.00030	-0.00186
482		3S	-0.00203	-0.01050	0.01144	-0.00201	-0.01703
483		3PX	-0.03753	-0.02248	0.01470	0.00403	0.04974
484		3PY	-0.02239	-0.01566	0.00981	0.00457	0.01362
485		3PZ	0.00024	-0.00161	0.00951	-0.00257	0.00376
486		4D 0	-0.00003	0.00006	-0.00050	-0.00004	-0.00016
487		4D+1	-0.00077	-0.00017	0.00704	0.00009	0.00047
488		4D-1	-0.00058	0.00028	0.00417	0.00013	-0.00006
489		4D+2	0.00363	0.00269	0.00957	-0.00002	-0.00025
490		4D-2	-0.00234	-0.00169	-0.00602	-0.00008	0.00019
491	50 H	1S	0.00042	0.00002	0.00093	0.00044	0.00115
492		2S	-0.00217	-0.00253	-0.00769	0.00298	0.00872
493	51 C	1S	0.00025	-0.00071	0.00091	-0.00051	-0.00089
494		2S	-0.00071	0.00192	-0.00239	0.00153	0.00232
495		2PX	0.06627	0.04354	0.04335	-0.00570	-0.04157
496		2PY	0.03558	0.02617	0.02032	-0.00201	-0.02119
497		2PZ	-0.00297	-0.00121	-0.00239	0.00121	0.00286
498		3S	-0.00087	-0.00733	0.01195	-0.00483	0.00478
499		3PX	0.03847	0.02637	0.01487	-0.00304	-0.03565
500		3PY	0.02109	0.01029	0.01476	-0.00668	-0.01414
501		3PZ	-0.00192	0.00200	-0.00948	0.00234	0.00394
502		4D 0	0.00015	0.00004	0.00055	-0.00008	-0.00028
503		4D+1	-0.00137	-0.00168	-0.00708	-0.00013	0.00112
504		4D-1	-0.00123	-0.00058	-0.00384	0.00031	0.00109
505		4D+2	-0.00245	-0.00067	0.00990	0.00023	-0.00092
506		4D-2	0.00148	0.00044	-0.00697	0.00003	0.00074
507	52 C	1S	0.00008	-0.00015	0.00015	-0.00009	-0.00020
508		2S	-0.00041	-0.00011	0.00062	0.00006	0.00095
509		2PX	0.00780	0.01579	0.17680	0.00119	-0.00660
510		2PY	0.00369	0.00872	0.09552	0.00093	-0.00277
511		2PZ	-0.00066	-0.00067	-0.00685	-0.00018	-0.00079
512		3S	0.00038	0.00539	-0.01431	0.00361	-0.00161
513		3PX	0.00655	0.01255	0.15720	0.00060	-0.00923
514		3PY	0.00510	0.01203	0.07428	0.00212	-0.00701
515		3PZ	-0.00030	-0.00120	-0.00384	-0.00245	0.00357
516		4D 0	-0.00030	-0.00014	-0.00006	0.00008	0.00040
517		4D+1	0.00411	0.00266	0.00027	-0.00036	-0.00364
518		4D-1	0.00218	0.00147	0.00008	-0.00018	-0.00183
519		4D+2	-0.00010	-0.00023	-0.00137	0.00005	0.00006
520		4D-2	0.00020	0.00020	0.00109	0.00000	0.00010
521	53 H	1S	0.00032	0.00005	-0.00033	-0.00028	-0.00116
522		2S	0.00126	0.00153	-0.00343	-0.00041	-0.00386

523	54	N	1S	-0.00023	-0.00127	-0.00241	-0.00001	0.00840
524			2S	0.00037	0.00219	0.00529	-0.00047	-0.01860
525			2PX	-0.00233	0.00832	0.01977	0.00613	0.00308
526			2PY	0.00738	-0.00504	-0.00772	-0.00574	0.02008
527			2PZ	-0.04442	0.09715	-0.01432	0.09291	0.19263
528			3S	0.00458	0.01444	0.01179	0.00295	-0.06136
529			3PX	-0.00207	0.00713	-0.01716	0.00804	0.00541
530			3PY	0.00676	-0.00249	-0.00993	-0.00514	0.02392
531			3PZ	-0.04270	0.08583	-0.00850	0.09516	0.19569
532			4D 0	-0.00060	0.00025	0.00062	0.00053	0.00056
533			4D+1	0.00009	0.00116	0.00112	-0.00435	-0.00515
534			4D-1	-0.00304	0.00424	-0.00163	-0.00031	-0.00203
535			4D+2	-0.00031	0.00055	-0.00383	-0.00020	-0.00225
536			4D-2	-0.00081	-0.00061	0.00574	0.00032	-0.00099
537	55	N	1S	-0.00221	-0.00310	0.00205	0.00216	0.00425
538			2S	0.00450	0.00729	-0.00454	-0.00392	-0.00753
539			2PX	-0.05625	-0.04288	0.06173	-0.00026	-0.06192
540			2PY	-0.02905	-0.01435	0.02757	-0.00193	-0.04047
541			2PZ	-0.00980	-0.00920	0.00259	0.00643	0.01173
542			3S	0.01634	0.01511	-0.01316	-0.02543	-0.05004
543			3PX	-0.04501	-0.03318	0.05101	0.00449	-0.05141
544			3PY	-0.02786	-0.01096	0.03298	0.00234	-0.04813
545			3PZ	-0.01138	-0.01121	-0.00074	0.00892	0.01550
546			4D 0	-0.00025	0.00191	-0.00097	0.00011	-0.00164
547			4D+1	-0.00788	-0.01077	0.00023	-0.00012	0.00045
548			4D-1	-0.00553	-0.00411	-0.00136	0.00042	-0.00167
549			4D+2	-0.00364	-0.00336	0.00248	0.00074	0.00213
550			4D-2	0.00119	0.00169	-0.00165	0.00047	-0.00126
551	56	N	1S	0.00225	0.00219	0.00048	-0.00228	-0.00536
552			2S	-0.00456	-0.00319	-0.00058	0.00489	0.01093
553			2PX	0.00577	0.01624	-0.02271	0.00125	-0.09159
554			2PY	0.01732	0.00275	0.04187	-0.00124	0.19610
555			2PZ	-0.01535	-0.01804	0.01439	0.00975	0.05519
556			3S	-0.01370	-0.01561	-0.01068	0.01874	0.04867
557			3PX	-0.01293	-0.01677	-0.00336	0.00356	-0.08897
558			3PY	0.00876	-0.01565	0.04257	-0.00681	0.19844
559			3PZ	-0.00339	-0.01538	0.01562	0.00585	0.05871
560			4D 0	0.00166	0.00341	-0.00152	-0.00049	-0.00037
561			4D+1	-0.00427	-0.00668	0.00217	0.00030	0.00058
562			4D-1	-0.00425	-0.00262	0.00054	0.00053	0.00003
563			4D+2	-0.00148	-0.00161	0.00266	0.00018	-0.00439
564			4D-2	-0.00073	0.00023	-0.00159	0.00084	0.00444
565	57	C	1S	0.00192	0.00237	0.00453	-0.00020	0.00011

566		2S	0.00083	-0.00003	-0.01026	-0.00108	-0.00061
567		2PX	-0.01078	0.02134	0.02676	0.02746	-0.00250
568		2PY	-0.09724	0.05203	-0.00137	0.11831	-0.01759
569		2PZ	0.13681	-0.08212	-0.00380	-0.13953	0.02737
570		3S	-0.05700	-0.06623	-0.02942	0.01236	0.00492
571		3PX	0.00134	0.01970	0.02645	0.02181	-0.00481
572		3PY	-0.06733	0.03007	-0.01734	0.10084	-0.01513
573		3PZ	0.09719	-0.05279	-0.01198	-0.14401	0.02138
574		4D 0	-0.00165	0.00149	0.00004	-0.00256	-0.00051
575		4D+1	0.00788	-0.00701	0.00028	0.00581	0.00652
576		4D-1	-0.00237	0.00259	-0.00010	-0.00225	-0.00214
577		4D+2	-0.00037	0.00133	0.00071	-0.00143	0.00065
578		4D-2	-0.00157	0.00239	0.00167	-0.00118	-0.00091
579	58 C	1S	-0.00348	0.00377	-0.00252	-0.00224	-0.00352
580		2S	0.00869	-0.00743	0.00513	0.00479	0.00803
581		2PX	-0.02892	0.02321	-0.01119	-0.01239	-0.01793
582		2PY	-0.06618	0.04203	0.00061	-0.02313	-0.03095
583		2PZ	0.06092	-0.06162	-0.00917	0.01826	0.02948
584		3S	0.01171	-0.02789	0.01694	0.02466	0.02730
585		3PX	-0.01874	-0.01365	-0.00449	0.00029	0.00204
586		3PY	-0.05291	0.02516	0.00282	-0.02744	-0.03483
587		3PZ	0.04634	-0.06218	-0.00658	0.01573	0.03315
588		4D 0	-0.00351	0.00220	0.00052	0.00420	-0.00056
589		4D+1	-0.00540	0.00304	0.00040	0.00984	-0.00207
590		4D-1	0.00055	-0.00035	0.00038	-0.00134	0.00046
591		4D+2	-0.00010	0.00072	-0.00070	-0.00141	-0.00026
592		4D-2	0.00602	-0.00296	0.00009	-0.00848	0.00203
593	59 C	1S	0.00446	-0.00258	0.00012	0.00186	0.00349
594		2S	-0.00946	0.00563	0.00008	-0.00388	-0.00798
595		2PX	-0.00234	0.00654	-0.00082	-0.00992	0.00215
596		2PY	-0.07678	0.06119	0.00395	-0.05622	-0.02588
597		2PZ	0.07869	-0.05461	-0.00698	0.05113	0.01445
598		3S	-0.02409	0.01704	-0.01404	-0.02234	-0.02614
599		3PX	-0.02398	0.00641	-0.00818	-0.02159	-0.01200
600		3PY	-0.03558	0.05302	-0.00400	-0.06834	-0.01534
601		3PZ	0.07604	-0.04543	-0.01297	0.05599	0.01558
602		4D 0	0.00504	-0.00318	0.00005	-0.00714	0.00127
603		4D+1	-0.00376	0.00230	0.00069	0.00763	-0.00149
604		4D-1	0.00205	-0.00087	0.00006	-0.00335	0.00062
605		4D+2	0.00466	-0.00311	-0.00029	-0.00656	0.00156
606		4D-2	0.00130	-0.00059	0.00084	-0.00427	0.00030
607	60 C	1S	0.00157	-0.00148	0.00154	0.00109	0.00147
608		2S	-0.00362	0.00251	-0.00310	-0.00128	-0.00277

609			2PX	0.02190	-0.01356	0.00734	-0.01863	0.01214
610			2PY	0.06276	-0.02570	-0.00408	-0.09346	0.02754
611			2PZ	-0.06849	0.03661	0.00379	0.11384	-0.03557
612			3S	-0.00468	0.02059	-0.00763	-0.01658	-0.01771
613			3PX	0.01536	-0.01804	0.00490	-0.01426	0.02005
614			3PY	0.04835	-0.00696	-0.00456	-0.11032	0.02628
615			3PZ	-0.04952	0.03486	0.00202	0.13082	-0.04386
616			4D 0	0.00554	-0.00406	-0.00032	0.00355	0.00114
617			4D+1	-0.00345	0.00317	0.00060	-0.00249	-0.00142
618			4D-1	0.00200	-0.00166	-0.00015	0.00125	0.00055
619			4D+2	0.00501	-0.00301	-0.00007	0.00294	0.00141
620			4D-2	0.00226	-0.00183	0.00026	0.00178	0.00137
621	61	H	1S	-0.00204	-0.00576	0.00193	0.00074	0.00200
622			2S	0.00067	0.02255	-0.00041	0.00136	-0.00298
623	62	C	1S	-0.00216	0.00100	0.00042	-0.00087	-0.00137
624			2S	0.00409	-0.00219	-0.00157	0.00123	0.00244
625			2PX	0.00512	-0.00167	0.00349	-0.02107	0.00061
626			2PY	0.05607	-0.03415	-0.00180	-0.08611	0.02544
627			2PZ	-0.06153	0.03586	0.00134	0.10662	-0.02797
628			3S	0.02461	-0.00077	0.00713	0.01110	0.01516
629			3PX	-0.01024	-0.00281	0.00086	-0.02395	-0.00805
630			3PY	0.04071	-0.02861	0.00447	-0.07608	0.02271
631			3PZ	-0.05547	0.02990	0.00543	0.10196	-0.02556
632			4D 0	-0.00410	0.00254	0.00011	-0.00214	-0.00075
633			4D+1	-0.00638	0.00444	0.00042	-0.00665	-0.00066
634			4D-1	0.00030	-0.00029	0.00006	0.00102	-0.00011
635			4D+2	0.00071	-0.00054	0.00003	0.00179	0.00022
636			4D-2	0.00583	-0.00451	-0.00044	0.00599	0.00102
637	63	H	1S	-0.00311	0.00042	0.00309	-0.00002	-0.00135
638			2S	0.01433	0.00005	-0.00289	-0.00893	0.00118
639	64	C	1S	-0.00042	0.00041	-0.00010	-0.00021	-0.00002
640			2S	0.00099	-0.00070	0.00056	0.00037	-0.00001
641			2PX	0.03067	-0.01284	-0.00103	0.01506	0.00259
642			2PY	0.10453	-0.07633	-0.00685	0.06930	0.01160
643			2PZ	-0.13621	0.08955	0.00635	-0.08772	-0.01526
644			3S	0.01065	0.00663	-0.00584	-0.00110	-0.00052
645			3PX	0.01743	-0.00674	0.00192	0.01582	-0.00084
646			3PY	0.07059	-0.04908	-0.00423	0.07686	0.00357
647			3PZ	-0.09437	0.06685	0.00557	-0.09766	-0.01342
648			4D 0	-0.00089	-0.00024	0.00018	0.00563	-0.00199
649			4D+1	0.00523	-0.00233	0.00003	-0.01477	0.00501
650			4D-1	-0.00148	0.00050	0.00007	0.00441	-0.00156
651			4D+2	-0.00136	0.00093	-0.00005	0.00842	-0.00273

652		4D-2	-0.00315	0.00153	0.00030	0.01040	-0.00317
653	65 H	1S	0.00567	-0.00085	0.00350	0.00237	0.00234
654		2S	0.00387	-0.00556	0.00537	0.00347	0.00559
655	66 H	1S	-0.00312	0.00315	0.00059	-0.00206	-0.00233
656		2S	-0.00917	0.00323	0.00323	-0.00261	-0.00527
657	67 N	1S	0.00139	0.00077	0.00039	0.00008	-0.00015
658		2S	-0.00189	-0.00079	-0.00085	-0.00030	0.00019
659		2PX	-0.01416	0.00304	0.00147	0.04167	-0.01501
660		2PY	-0.04123	0.02974	0.00204	0.18649	-0.06908
661		2PZ	0.07303	-0.02400	-0.00073	-0.22611	0.08291
662		3S	-0.01181	-0.00835	-0.00233	0.00056	0.00164
663		3PX	-0.01106	0.00218	0.00011	0.03758	-0.01445
664		3PY	-0.03093	0.01953	0.00126	0.17235	-0.06522
665		3PZ	0.05220	-0.01840	-0.00081	-0.20847	0.07979
666		4D 0	0.00619	-0.00373	-0.00031	0.00035	0.00050
667		4D+1	0.00722	-0.00519	-0.00037	0.01372	-0.00237
668		4D-1	-0.00007	0.00056	0.00007	-0.00300	0.00061
669		4D+2	0.00103	-0.00001	0.00014	-0.00475	0.00114
670		4D-2	-0.00752	0.00479	0.00037	-0.01080	0.00160
671	68 N	1S	0.00203	0.00048	0.00037	0.00002	0.00026
672		2S	-0.00413	-0.00077	-0.00081	-0.00014	-0.00076
673		2PX	-0.01667	0.01303	0.00100	-0.04372	0.01166
674		2PY	-0.09824	0.05278	0.00222	-0.19668	0.05063
675		2PZ	0.09455	-0.07282	-0.00721	0.23782	-0.06220
676		3S	-0.00759	-0.00174	-0.00062	0.00129	-0.00090
677		3PX	-0.01216	0.00872	0.00166	-0.03855	0.01195
678		3PY	-0.07345	0.04030	0.00148	-0.18154	0.04958
679		3PZ	0.07033	-0.05529	-0.00550	0.21883	-0.06075
680		4D 0	-0.00753	0.00416	0.00029	-0.00064	-0.00111
681		4D+1	-0.00360	0.00155	0.00002	0.01242	-0.00463
682		4D-1	-0.00021	0.00061	0.00018	-0.00282	0.00086
683		4D+2	-0.00224	0.00200	0.00010	-0.00491	0.00106
684		4D-2	0.00400	-0.00213	-0.00020	-0.00969	0.00376
685	69 C	1S	-0.00128	-0.00052	-0.00015	0.00001	-0.00006
686		2S	0.00294	0.00117	0.00037	0.00007	0.00015
687		2PX	0.00850	-0.00977	-0.00108	-0.01132	0.00556
688		2PY	0.06967	-0.03240	-0.00158	-0.05127	0.02671
689		2PZ	-0.07855	0.04097	0.00282	0.06199	-0.03200
690		3S	0.00889	0.00491	0.00008	-0.00146	-0.00023
691		3PX	0.01182	-0.00429	0.00034	-0.01214	0.00664
692		3PY	0.03997	-0.02120	-0.00225	-0.06228	0.02850
693		3PZ	-0.05182	0.02463	0.00077	0.07307	-0.03545
694		4D 0	0.00092	-0.00078	-0.00007	0.00572	-0.00206

695		4D+1	-0.00648	0.00444	0.00041	-0.01506	0.00414
696		4D-1	0.00153	-0.00114	-0.00013	0.00446	-0.00134
697		4D+2	0.00339	-0.00184	-0.00009	0.00855	-0.00262
698		4D-2	0.00534	-0.00323	-0.00017	0.01069	-0.00276
699	70 C	1S	-0.00030	-0.00010	-0.00010	0.00000	-0.00002
700		2S	0.00091	0.00029	0.00022	0.00001	0.00006
701		2PX	0.01185	-0.00760	-0.00085	0.01941	-0.00555
702		2PY	0.05694	-0.03351	-0.00249	0.08803	-0.02497
703		2PZ	-0.06877	0.04071	0.00280	-0.10646	0.03007
704		3S	-0.00046	-0.00025	0.00074	-0.00009	0.00015
705		3PX	0.00989	-0.00603	-0.00097	0.01707	-0.00543
706		3PY	0.04904	-0.02653	-0.00189	0.08136	-0.02340
707		3PZ	-0.05366	0.03452	0.00245	-0.09826	0.02786
708		4D 0	0.00281	-0.00155	-0.00011	-0.00133	0.00097
709		4D+1	0.00290	-0.00135	-0.00006	-0.00515	0.00240
710		4D-1	-0.00022	-0.00005	-0.00002	0.00087	-0.00035
711		4D+2	0.00065	-0.00028	0.00000	0.00119	-0.00033
712		4D-2	-0.00285	0.00139	0.00010	0.00435	-0.00209
713	71 C	1S	0.00032	0.00005	0.00011	-0.00001	0.00005
714		2S	-0.00041	0.00004	-0.00018	0.00002	-0.00011
715		2PX	0.01239	-0.00749	-0.00034	0.02083	-0.00674
716		2PY	0.05308	-0.03371	-0.00287	0.09455	-0.03124
717		2PZ	-0.07054	0.03850	0.00239	-0.11422	0.03736
718		3S	-0.00466	-0.00111	-0.00157	-0.00072	-0.00076
719		3PX	0.00726	-0.00568	-0.00085	0.02270	-0.00918
720		3PY	0.03781	-0.02815	-0.00268	0.10677	-0.03826
721		3PZ	-0.05694	0.02908	0.00153	-0.12999	0.04548
722		4D 0	-0.00373	0.00193	0.00012	0.00228	-0.00145
723		4D+1	0.00145	-0.00073	-0.00005	-0.00144	0.00063
724		4D-1	-0.00114	0.00052	0.00002	0.00076	-0.00043
725		4D+2	-0.00248	0.00133	0.00009	0.00175	-0.00101
726		4D-2	-0.00049	0.00013	-0.00001	0.00065	-0.00021
727	72 C	1S	0.00000	-0.00001	0.00003	-0.00001	0.00000
728		2S	0.00003	0.00001	-0.00003	0.00001	0.00001
729		2PX	-0.00596	0.00264	0.00024	0.00665	-0.00349
730		2PY	-0.02588	0.01242	0.00074	0.03029	-0.01573
731		2PZ	0.03160	-0.01493	-0.00086	-0.03660	0.01901
732		3S	0.00140	0.00042	0.00004	0.00061	0.00012
733		3PX	-0.00503	0.00165	0.00015	0.00887	-0.00463
734		3PY	-0.01978	0.00886	0.00063	0.04159	-0.02076
735		3PZ	0.02291	-0.01120	-0.00054	-0.04979	0.02538
736		4D 0	-0.00387	0.00219	0.00015	-0.00681	0.00240
737		4D+1	0.00390	-0.00230	-0.00016	0.00703	-0.00217

738		4D-1	-0.00162	0.00094	0.00006	-0.00289	0.00095
739		4D+2	-0.00352	0.00201	0.00014	-0.00624	0.00208
740		4D-2	-0.00225	0.00135	0.00010	-0.00411	0.00120
741	73 H	1S	-0.00033	-0.00005	-0.00005	-0.00007	-0.00005
742		2S	-0.00354	-0.00149	-0.00038	0.00009	0.00017
743	74 C	1S	-0.00021	-0.00004	-0.00006	0.00000	-0.00004
744		2S	0.00050	0.00014	0.00012	-0.00002	0.00005
745		2PX	-0.00621	0.00256	-0.00005	0.00061	-0.00074
746		2PY	-0.02336	0.01256	0.00093	0.00277	-0.00273
747		2PZ	0.02987	-0.01470	-0.00084	-0.00333	0.00335
748		3S	0.00235	-0.00004	0.00070	0.00078	0.00089
749		3PX	-0.00419	0.00229	-0.00014	0.00102	-0.00110
750		3PY	-0.01527	0.00892	0.00077	0.00557	-0.00312
751		3PZ	0.02143	-0.00978	-0.00048	-0.00616	0.00419
752		4D 0	0.00224	-0.00125	-0.00009	0.00386	-0.00143
753		4D+1	0.00512	-0.00284	-0.00019	0.00914	-0.00315
754		4D-1	-0.00074	0.00036	0.00002	-0.00125	0.00041
755		4D+2	-0.00049	0.00042	0.00005	-0.00125	0.00040
756		4D-2	-0.00431	0.00258	0.00019	-0.00802	0.00279
757	75 H	1S	0.00058	0.00035	0.00003	-0.00004	-0.00005
758		2S	-0.00389	-0.00146	-0.00042	-0.00074	-0.00070
759	76 C	1S	-0.00019	-0.00009	-0.00002	0.00001	-0.00001
760		2S	0.00053	0.00022	0.00005	0.00002	0.00001
761		2PX	-0.01730	0.00901	0.00057	-0.02328	0.00782
762		2PY	-0.07617	0.04197	0.00285	-0.10562	0.03555
763		2PZ	0.09128	-0.05093	-0.00354	0.12754	-0.04295
764		3S	-0.00073	-0.00028	0.00005	-0.00021	0.00006
765		3PX	-0.01253	0.00759	0.00061	-0.02448	0.00903
766		3PY	-0.05992	0.03376	0.00236	-0.11219	0.04037
767		3PZ	0.07175	-0.04077	-0.00284	0.13559	-0.04875
768		4D 0	0.00017	-0.00003	0.00000	-0.00177	0.00086
769		4D+1	-0.00052	0.00022	0.00001	0.00172	-0.00072
770		4D-1	0.00012	-0.00006	-0.00001	-0.00073	0.00032
771		4D+2	0.00031	-0.00010	0.00000	-0.00158	0.00073
772		4D-2	0.00040	-0.00015	-0.00001	-0.00099	0.00038
773	77 H	1S	0.00000	-0.00003	0.00005	0.00000	0.00000
774		2S	0.00019	0.00008	0.00002	-0.00007	-0.00008
775	78 H	1S	-0.00106	-0.00035	-0.00017	0.00000	-0.00006
776		2S	-0.00127	-0.00040	-0.00026	0.00007	-0.00011
777	79 H	1S	-0.00007	-0.00007	-0.00001	0.00001	0.00000
778		2S	-0.00052	-0.00023	-0.00007	-0.00006	-0.00007
779	80 F	1S	-0.00017	0.00012	-0.00019	0.00026	0.00037
780		2S	0.00038	-0.00025	0.00018	-0.00052	-0.00094

781		2PX	-0.03811	-0.02256	-0.02753	0.00313	0.01607
782		2PY	-0.01886	-0.01479	-0.01190	-0.00008	0.00643
783		2PZ	0.00062	0.00215	-0.00028	0.00084	0.00063
784		3S	0.00112	-0.00108	0.00300	-0.00215	-0.00218
785		3PX	-0.03070	-0.01822	-0.01999	0.00271	0.01485
786		3PY	-0.01528	-0.01174	-0.00847	0.00020	0.00587
787		3PZ	0.00049	0.00186	-0.00080	0.00093	0.00026
788		4D 0	0.00005	-0.00002	0.00012	-0.00004	-0.00002
789		4D+1	-0.00061	-0.00055	-0.00120	0.00008	0.00094
790		4D-1	-0.00035	-0.00034	-0.00056	-0.00002	0.00045
791		4D+2	-0.00025	-0.00012	0.00074	0.00003	0.00008
792		4D-2	0.00015	0.00001	-0.00046	-0.00006	0.00000
793	81 F	1S	0.00018	-0.00013	0.00003	-0.00006	0.00022
794		2S	-0.00045	0.00034	-0.00040	0.00020	-0.00077
795		2PX	0.04184	0.02246	-0.02227	-0.00241	-0.02049
796		2PY	0.02012	0.01438	-0.01270	-0.00056	-0.01157
797		2PZ	-0.00217	-0.00030	0.00081	0.00015	0.00050
798		3S	-0.00110	0.00046	0.00176	0.00011	0.00006
799		3PX	0.03320	0.01802	-0.01650	-0.00214	-0.01891
800		3PY	0.01633	0.01178	-0.00911	-0.00091	-0.00957
801		3PZ	-0.00178	-0.00009	0.00086	0.00024	0.00051
802		4D 0	-0.00003	0.00004	-0.00013	0.00005	-0.00006
803		4D+1	-0.00022	-0.00013	0.00113	0.00008	0.00075
804		4D-1	-0.00008	0.00001	0.00062	0.00000	0.00037
805		4D+2	0.00042	0.00034	0.00084	0.00002	-0.00041
806		4D-2	-0.00033	-0.00023	-0.00048	0.00003	0.00031
807	82 F	1S	-0.00030	-0.00031	-0.00169	-0.00034	-0.00054
808		2S	0.00039	0.00023	0.00334	0.00070	0.00119
809		2PX	0.00183	0.00211	0.02306	0.00242	0.02110
810		2PY	0.00349	0.00180	-0.00958	-0.00106	-0.03800
811		2PZ	0.00103	0.00038	0.00780	0.00122	-0.00604
812		3S	0.00353	0.00461	0.01516	0.00285	0.00445
813		3PX	0.00095	0.00135	0.01722	0.00213	0.01960
814		3PY	0.00254	0.00113	-0.00684	-0.00098	-0.03546
815		3PZ	0.00139	0.00122	0.00759	0.00120	-0.00557
816		4D 0	-0.00001	-0.00004	0.00035	0.00001	0.00087
817		4D+1	-0.00016	-0.00015	-0.00076	-0.00006	-0.00124
818		4D-1	-0.00011	-0.00010	0.00040	0.00002	0.00240
819		4D+2	-0.00004	-0.00007	0.00044	-0.00002	0.00051
820		4D-2	-0.00002	0.00000	-0.00047	0.00000	0.00022
821	83 F	1S	-0.00137	-0.00171	-0.00112	-0.00003	-0.00012
822		2S	0.00314	0.00393	0.00171	-0.00003	0.00034
823		2PX	0.01944	0.02151	0.02048	-0.00078	-0.02552

824	2PY	0.00600	0.01110	-0.00814	0.00183	0.05387
825	2PZ	-0.00353	-0.00375	-0.00639	0.00000	0.01068
826	3S	0.00980	0.01227	0.01321	0.00082	0.00059
827	3PX	0.01458	0.01627	0.01635	-0.00048	-0.02296
828	3PY	0.00455	0.00861	-0.00530	0.00180	0.04765
829	3PZ	-0.00348	-0.00386	-0.00565	0.00006	0.00957
830	4D 0	0.00030	0.00040	-0.00011	-0.00002	0.00063
831	4D+1	0.00007	0.00007	0.00049	-0.00002	-0.00110
832	4D-1	-0.00006	-0.00003	-0.00076	0.00004	0.00164
833	4D+2	-0.00020	-0.00022	0.00012	0.00005	0.00156
834	4D-2	-0.00019	-0.00025	-0.00068	-0.00001	-0.00076

Cartesian coordinates (optimized at the B3LYP/6-31G*&LANL2DZ level) of all the compounds discussed in the main text.

$[Ir(ppy)_2(1)]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.150015	-0.308205	0.006219
2	6	0	1.611201	0.205309	2.469544
3	6	0	2.605612	-1.013418	0.721962
4	6	0	2.731542	0.074163	3.275389
5	1	0	0.740463	0.754185	2.803998
6	6	0	3.756899	-1.184052	1.505444
7	6	0	3.822219	-0.649100	2.784058
8	1	0	2.743009	0.525563	4.261261
9	1	0	4.598578	-1.734134	1.102047
10	1	0	4.714003	-0.784540	3.388548
11	6	0	-0.680610	-2.207354	0.473525
12	6	0	-1.855870	-2.671219	-0.167684
13	6	0	-0.049747	-3.074002	1.377642

14	6	0	-2.386270	-3.939498	0.122060
15	6	0	-0.577937	-4.337404	1.660075
16	1	0	0.864809	-2.771552	1.878552
17	6	0	-1.751972	-4.771063	1.038613
18	1	0	-3.291790	-4.286405	-0.367098
19	1	0	-0.068081	-4.987514	2.366504
20	1	0	-2.162817	-5.751231	1.260395
21	6	0	-2.281012	1.611317	1.564991
22	6	0	-1.696050	-0.304145	2.742209
23	6	0	-3.055366	2.043190	2.656408
24	6	0	-2.471323	0.050302	3.838477
25	1	0	-1.143839	-1.235397	2.736019
26	6	0	-3.157714	1.261713	3.800233
27	1	0	-3.553778	3.003603	2.606129
28	1	0	-2.518876	-0.608437	4.698930
29	1	0	-3.755022	1.595896	4.643165
30	6	0	-3.412557	3.149250	-0.015189
31	6	0	-3.439263	4.061146	-1.066852
32	6	0	-2.243283	2.451755	0.342551
33	6	0	-2.270547	4.323687	-1.781233
34	1	0	-4.366325	4.566338	-1.319318
35	6	0	-1.085880	2.687690	-0.426039
36	6	0	-1.102909	3.638831	-1.456348
37	6	0	-2.144559	0.269600	-2.287101
38	6	0	-2.428135	-1.770034	-1.166482
39	6	0	-3.212238	0.017424	-3.135589
40	1	0	-1.562968	1.175771	-2.379426
41	6	0	-3.528425	-2.062973	-1.985442
42	6	0	-3.929023	-1.169571	-2.968764
43	1	0	-3.469092	0.737438	-3.904468
44	1	0	-4.053400	-3.001937	-1.857326
45	1	0	-4.777285	-1.400511	-3.606049
46	6	0	1.191414	-1.137637	-1.257304
47	6	0	1.011624	-1.486199	-2.603637

48	6	0	2.433518	-1.470737	-0.653715
49	6	0	2.015195	-2.141071	-3.321846
50	1	0	0.077396	-1.257131	-3.106864
51	6	0	3.434116	-2.142986	-1.375362
52	6	0	3.226506	-2.479347	-2.708169
53	1	0	1.848363	-2.400120	-4.364374
54	1	0	4.378750	-2.401344	-0.905237
55	1	0	3.998272	-3.001261	-3.265803
56	7	0	-1.582177	0.452325	1.629231
57	7	0	1.532710	-0.333924	1.236388
58	7	0	-1.767622	-0.580327	-1.311080
59	7	0	0.148650	1.952734	-0.266801
60	7	0	1.110036	2.766073	-0.116502
61	6	0	2.444687	2.377905	-0.305010
62	6	0	2.861674	1.612513	-1.406928
63	6	0	3.396515	3.002796	0.524363
64	6	0	4.225144	1.449397	-1.648839
65	1	0	2.126301	1.196382	-2.084113
66	6	0	4.751072	2.791996	0.300156
67	1	0	3.051386	3.640619	1.332068
68	6	0	5.168522	2.019106	-0.791394
69	1	0	4.546768	0.873735	-2.511182
70	1	0	5.485230	3.254696	0.952926
71	1	0	6.228702	1.886450	-0.986691
72	1	0	-2.265884	5.047543	-2.590398
73	1	0	-4.325555	2.959147	0.539310
74	1	0	-0.187930	3.814045	-2.011670

2

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-3.191107	-0.258349	0.016137
2	6	0	-5.421575	-0.706624	-0.361946
3	6	0	-2.953267	-1.603870	0.344349
4	6	0	-5.273165	-2.063202	-0.071122
5	1	0	-6.395338	-0.307100	-0.642414
6	6	0	-4.005545	-2.513152	0.294691
7	1	0	-1.966204	-1.932134	0.650638
8	1	0	-6.123271	-2.736512	-0.123060
9	1	0	-3.837593	-3.557052	0.546099
10	6	0	-2.451815	2.133976	0.063664
11	6	0	-1.464479	3.114767	0.090043
12	6	0	-2.110106	0.766593	0.037008
13	6	0	-0.117657	2.754439	0.083287
14	1	0	-1.745992	4.163776	0.116372
15	6	0	-0.758593	0.412966	0.021584
16	6	0	0.237793	1.400818	0.046105
17	1	0	-0.438268	-0.620864	-0.029401
18	7	0	-4.420614	0.175171	-0.323255
19	7	0	1.631641	1.136634	0.028109
20	7	0	1.940478	-0.085030	-0.006534
21	6	0	3.334607	-0.346684	-0.025633
22	6	0	3.690546	-1.701439	-0.061890
23	6	0	4.335887	0.639974	-0.010831
24	6	0	5.033486	-2.074210	-0.082579
25	1	0	2.895862	-2.441299	-0.073455
26	6	0	5.673055	0.261659	-0.031695
27	1	0	4.041729	1.683146	0.016756
28	6	0	6.026712	-1.093542	-0.067397
29	1	0	5.304441	-3.125992	-0.110774
30	1	0	6.448948	1.022712	-0.020392
31	1	0	7.074851	-1.380140	-0.083646
32	1	0	0.673855	3.497257	0.101576

33	1	0	-3.502219	2.402048	0.060811

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.829379	0.051009	0.001438
2	6	0	5.848110	-1.028871	-0.280462
3	6	0	4.490882	1.260546	0.277262
4	6	0	6.585884	0.131258	-0.038178
5	1	0	6.355502	-1.967214	-0.500872
6	6	0	5.881909	1.298485	0.252138
7	1	0	3.929643	2.153663	0.528718
8	1	0	7.670964	0.113479	-0.068913
9	1	0	6.406990	2.225962	0.464728
10	6	0	1.745484	-1.325917	0.109548
11	6	0	0.362058	-1.452866	0.124715
12	6	0	2.347366	-0.060973	0.003594
13	6	0	-0.459473	-0.321279	0.025837
14	1	0	-0.111785	-2.425819	0.214024
15	6	0	1.512161	1.069808	-0.104777
16	6	0	0.130934	0.948732	-0.094352
17	1	0	1.947177	2.057503	-0.224339
18	1	0	-0.509873	1.818426	-0.185436
19	7	0	4.515459	-1.078906	-0.264183
20	7	0	-1.852517	-0.569521	0.051224
21	7	0	-2.575665	0.459958	-0.048673
22	6	0	-3.970863	0.210956	-0.021707
23	6	0	-4.785212	1.345465	-0.140201
24	6	0	-4.556864	-1.060135	0.113125

25	6	0	-6.173071	1.218334	-0.125517
26	1	0	-4.304670	2.313768	-0.242727
27	6	0	-5.941312	-1.179825	0.127392
28	1	0	-3.911340	-1.926449	0.204021
29	6	0	-6.753343	-0.044218	0.008322
30	1	0	-6.799961	2.100885	-0.217993
31	1	0	-6.396567	-2.161282	0.231710
32	1	0	-7.835085	-0.147638	0.020355
33	1	0	2.383903	-2.199056	0.179092

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.952367	-0.113814	0.017676
2	6	0	7.908270	0.877657	0.735322
3	6	0	6.679901	-1.135964	-0.617012
4	6	0	8.708068	-0.106191	0.152172
5	1	0	8.362727	1.704543	1.279734
6	6	0	8.069521	-1.131744	-0.543142
7	1	0	6.170570	-1.912547	-1.176923
8	1	0	9.789616	-0.061956	0.235636
9	1	0	8.644651	-1.915277	-1.029489
10	6	0	3.804907	1.134054	0.322061
11	6	0	2.418455	1.216192	0.295992
12	6	0	4.466903	-0.059637	-0.011107
13	6	0	1.627061	0.107654	-0.055434
14	1	0	1.937390	2.147828	0.580267
15	6	0	3.679541	-1.170555	-0.354762
16	6	0	2.291203	-1.088610	-0.376054

17	1	0	4.146337	-2.120586	-0.596480
18	1	0	1.713884	-1.961278	-0.667498
19	7	0	6.575608	0.883214	0.677207
20	6	0	0.148793	0.195952	-0.081997
21	6	0	-0.651690	-0.900435	0.304347
22	6	0	-0.500139	1.373933	-0.491619
23	6	0	-2.035952	-0.828610	0.283822
24	1	0	-0.171926	-1.810812	0.652503
25	6	0	-1.888032	1.453026	-0.514629
26	1	0	0.089613	2.224070	-0.821114
27	6	0	-2.670448	0.356425	-0.128931
28	1	0	-2.647094	-1.669876	0.591022
29	1	0	-2.393995	2.357326	-0.839119
30	7	0	-4.070554	0.549215	-0.192021
31	7	0	-4.758991	-0.447931	0.161146
32	6	0	-6.161800	-0.253838	0.097990
33	6	0	-6.789925	0.933418	-0.317998
34	6	0	-6.938118	-1.353341	0.488711
35	6	0	-8.177628	1.005711	-0.338003
36	1	0	-6.173550	1.773974	-0.616430
37	6	0	-8.329477	-1.274128	0.466417
38	1	0	-6.425824	-2.256802	0.805485
39	6	0	-8.951566	-0.094810	0.053084
40	1	0	-8.665156	1.922526	-0.659239
41	1	0	-8.926613	-2.129348	0.770553
42	1	0	-10.036153	-0.029069	0.034341
43	1	0	4.401794	1.991736	0.610979

A2

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	77	0	1.342436	0.052654	0.025724
2	6	0	1.026496	1.497989	2.685175
3	6	0	1.730273	2.830159	0.880401
4	6	0	1.053659	2.570702	3.562460
5	1	0	0.737275	0.506231	3.009073
6	6	0	1.770155	3.947129	1.731405
7	6	0	1.434289	3.823791	3.070866
8	1	0	0.780064	2.423691	4.601713
9	1	0	2.068273	4.908407	1.329056
10	1	0	1.466376	4.689762	3.725889
11	6	0	3.323314	-0.533706	0.364895
12	6	0	3.760308	-1.601179	-0.466609
13	6	0	4.251988	-0.056758	1.307463
14	6	0	5.049869	-2.152227	-0.349608
15	6	0	5.532802	-0.600054	1.426857
16	1	0	3.974182	0.764257	1.966130
17	6	0	5.936739	-1.653483	0.597473
18	1	0	5.370339	-2.969559	-0.991447
19	1	0	6.224812	-0.201737	2.166541
20	1	0	6.933486	-2.076709	0.688624
21	6	0	-0.900287	-1.528495	1.367106
22	6	0	1.164002	-2.312323	2.158418
23	6	0	-1.561473	-2.481949	2.161027
24	6	0	0.562129	-3.270563	2.964165
25	1	0	2.241736	-2.197600	2.113688
26	6	0	-0.832633	-3.352551	2.960142
27	1	0	-2.643483	-2.536618	2.145942
28	1	0	1.172026	-3.930797	3.571732
29	1	0	-1.345982	-4.088564	3.572894
30	6	0	-0.723068	0.318956	-0.268699
31	6	0	-1.376915	1.242747	-1.108763
32	6	0	-1.570668	-0.555064	0.486037

33	6	0	-2.763969	1.307371	-1.204313
34	1	0	-0.779829	1.927542	-1.705439
35	6	0	-2.964633	-0.495390	0.394548
36	6	0	-3.573909	0.437685	-0.454599
37	1	0	-3.616675	-1.151061	0.961590
38	6	0	0.598545	-1.808977	-2.281248
39	6	0	2.779442	-2.079777	-1.444167
40	6	0	0.774743	-2.808796	-3.226833
41	1	0	-0.330564	-1.259549	-2.199228
42	6	0	3.001637	-3.100510	-2.383245
43	6	0	2.005023	-3.468818	-3.275162
44	1	0	-0.035135	-3.056435	-3.904504
45	1	0	3.964770	-3.596442	-2.408810
46	1	0	2.184117	-4.257489	-4.000624
47	6	0	1.949020	1.550060	-1.173561
48	6	0	2.255524	1.501831	-2.546871
49	6	0	2.060472	2.819729	-0.538394
50	6	0	2.645614	2.640766	-3.249253
51	1	0	2.187975	0.557977	-3.080762
52	6	0	2.455826	3.966777	-1.250550
53	6	0	2.748392	3.881390	-2.604885
54	1	0	2.874537	2.565834	-4.310423
55	1	0	2.533992	4.929013	-0.750129
56	1	0	3.053847	4.766082	-3.156609
57	7	0	0.461176	-1.464994	1.385497
58	7	0	1.353848	1.612157	1.382574
59	7	0	1.563326	-1.448954	-1.410380
60	7	0	-4.966155	0.583618	-0.626268
61	7	0	-5.681678	-0.219091	0.037113
62	6	0	-7.078586	-0.054528	-0.145809
63	6	0	-7.890817	-0.955427	0.556901
64	6	0	-7.671748	0.926355	-0.960446
65	6	0	-9.279144	-0.885053	0.449338
66	1	0	-7.407280	-1.701964	1.180027

67	6	0	-9.056884	0.992599	-1.062782
68	1	0	-7.029241	1.616352	-1.495883
69	6	0	-9.865748	0.089337	-0.360698
70	1	0	-9.901848	-1.587885	0.996372
71	1	0	-9.514725	1.751511	-1.692311
72	1	0	-10.947559	0.148403	-0.446437
73	1	0	-3.255358	2.025361	-1.856292

A3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	1.202387	-0.067934	-0.069536
2	6	0	1.188347	-0.349563	-3.101513
3	6	0	0.446773	-2.229825	-1.901606
4	6	0	0.989647	-0.977586	-4.321135
5	1	0	1.562621	0.664550	-3.040461
6	6	0	0.226589	-2.905571	-3.113316
7	6	0	0.496231	-2.286344	-4.324005
8	1	0	1.213692	-0.449401	-5.241694
9	1	0	-0.157565	-3.918879	-3.091768
10	1	0	0.324290	-2.812164	-5.258865
11	6	0	3.176312	-0.705458	0.191607
12	6	0	3.738041	-0.347603	1.448227
13	6	0	4.023651	-1.391196	-0.697468
14	6	0	5.069019	-0.660009	1.781755
15	6	0	5.344854	-1.703342	-0.370844
16	1	0	3.644595	-1.695938	-1.671239
17	6	0	5.873973	-1.336727	0.872750
18	1	0	5.485521	-0.379359	2.746396

19	1	0	5.968893	-2.237960	-1.084619
20	1	0	6.901719	-1.580091	1.128706
21	6	0	0.685329	2.786465	-1.028384
22	6	0	2.996840	2.379565	-1.039643
23	6	0	0.921833	4.100880	-1.470834
24	6	0	3.285434	3.666013	-1.478982
25	1	0	3.778653	1.651789	-0.849807
26	6	0	2.218942	4.541590	-1.697165
27	1	0	0.087473	4.773119	-1.632144
28	1	0	4.315064	3.966965	-1.641024
29	1	0	2.397333	5.557707	-2.038432
30	6	0	-0.674516	0.876050	-0.269619
31	6	0	-1.950528	0.350663	-0.000526
32	6	0	-0.641462	2.213831	-0.755242
33	6	0	-3.128484	1.083705	-0.199007
34	1	0	-2.058740	-0.662604	0.377152
35	6	0	-1.827922	2.955959	-0.959870
36	6	0	-3.065591	2.404264	-0.687358
37	1	0	-1.787835	3.975059	-1.336662
38	1	0	-3.983789	2.959471	-0.839931
39	6	0	0.677514	1.251831	2.633004
40	6	0	2.837958	0.364016	2.359375
41	6	0	0.955738	1.684967	3.921332
42	1	0	-0.291961	1.403527	2.176041
43	6	0	3.164863	0.786287	3.658684
44	6	0	2.229594	1.446049	4.442777
45	1	0	0.188223	2.193193	4.495070
46	1	0	4.156363	0.585978	4.047487
47	1	0	2.487458	1.767931	5.447916
48	6	0	0.512299	-1.870546	0.500351
49	6	0	0.286806	-2.347016	1.805843
50	6	0	0.206561	-2.761802	-0.566940
51	6	0	-0.211374	-3.627228	2.040818
52	1	0	0.504311	-1.707779	2.656959

53	6	0	-0.294546	-4.054137	-0.325640
54	6	0	-0.504808	-4.489741	0.975499
55	1	0	-0.373107	-3.961917	3.063540
56	1	0	-0.522850	-4.722151	-1.152633
57	1	0	-0.891585	-5.487420	1.163854
58	7	0	1.742615	1.947298	-0.822565
59	7	0	0.931231	-0.948038	-1.921366
60	7	0	1.583342	0.611265	1.866532
61	7	0	-4.329485	0.407306	0.123962
62	7	0	-5.386387	1.065888	-0.081539
63	6	0	-6.583014	0.379757	0.250496
64	6	0	-7.769648	1.087502	0.014265
65	6	0	-6.640082	-0.919699	0.785018
66	6	0	-9.004182	0.508679	0.305724
67	1	0	-7.695239	2.089157	-0.398529
68	6	0	-7.874091	-1.491027	1.074488
69	1	0	-5.711842	-1.451722	0.961053
70	6	0	-9.058892	-0.781509	0.836868
71	1	0	-9.920538	1.062291	0.119665
72	1	0	-7.919103	-2.495349	1.488037
73	1	0	-10.019107	-1.236001	1.066297

B2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.998079	-0.069276	-0.099620
2	6	0	-0.586730	0.872957	-2.958191
3	6	0	-1.325795	2.520947	-1.449934
4	6	0	-0.571380	1.765825	-4.017994

5	1	0	-0.301771	-0.163513	-3.085953
6	6	0	-1.323648	3.464384	-2.493312
7	6	0	-0.947995	3.089170	-3.774791
8	1	0	-0.268895	1.427699	-5.003180
9	1	0	-1.619059	4.480813	-2.280731
10	1	0	-0.948343	3.821586	-4.576887
11	6	0	-2.979319	-0.676552	-0.376479
12	6	0	-3.448576	-1.573380	0.630283
13	6	0	-3.852466	-0.337111	-1.420332
14	6	0	-4.757062	-2.076073	0.536307
15	6	0	-5.137097	-0.864649	-1.461780
16	1	0	-3.552831	0.346571	-2.209340
17	6	0	-5.619439	-1.742446	-0.495024
18	1	0	-6.623279	-2.146415	-0.538143
19	6	0	1.256842	-1.866181	-1.089488
20	6	0	-0.798181	-2.785367	-1.748983
21	6	0	1.926509	-2.950572	-1.682288
22	6	0	-0.187330	-3.877010	-2.352355
23	1	0	-1.876113	-2.666555	-1.743293
24	6	0	1.207129	-3.955734	-2.314327
25	1	0	3.008011	-3.000483	-1.641143
26	1	0	-0.790244	-4.639673	-2.833642
27	1	0	1.727164	-4.793112	-2.771303
28	6	0	1.059735	0.242338	0.184409
29	6	0	1.699734	1.302101	0.856190
30	6	0	1.916870	-0.747731	-0.392818
31	6	0	3.085714	1.388054	0.955718
32	1	0	1.095553	2.080659	1.314742
33	6	0	3.309872	-0.664741	-0.301070
34	6	0	3.906315	0.406585	0.376011
35	1	0	3.969957	-1.405283	-0.739786
36	6	0	-0.319590	-1.500663	2.501211
37	6	0	-2.498650	-1.892165	1.699202
38	6	0	-0.517318	-2.311337	3.609150

39	1	0	0.617618	-0.986726	2.330741
40	6	0	-2.743630	-2.725461	2.805543
41	6	0	-1.756703	-2.935033	3.758901
42	1	0	0.282884	-2.442203	4.329529
43	1	0	-3.710702	-3.194295	2.905203
44	1	0	-1.955315	-3.577413	4.612179
45	6	0	-1.614898	1.616915	0.801740
46	6	0	-1.955408	1.782633	2.154262
47	6	0	-1.694537	2.755559	-0.059593
48	6	0	-2.354531	3.025044	2.624125
49	1	0	-1.918228	0.956585	2.855251
50	6	0	-2.107961	3.985217	0.478044
51	6	0	-2.441719	4.152509	1.809995
52	1	0	-2.757101	5.114118	2.194861
53	7	0	-0.104624	-1.807393	-1.138578
54	7	0	-0.952307	1.227270	-1.710562
55	7	0	-1.271470	-1.291676	1.569297
56	7	0	5.297281	0.590733	0.529647
57	7	0	6.022297	-0.290611	-0.011273
58	6	0	7.416976	-0.091711	0.153006
59	6	0	8.239787	-1.051608	-0.452410
60	6	0	7.997509	0.974028	0.863407
61	6	0	9.627113	-0.953674	-0.354080
62	1	0	7.765657	-1.864316	-0.994684
63	6	0	9.381571	1.066039	0.958673
64	1	0	7.346917	1.707816	1.325859
65	6	0	10.201341	0.105338	0.351881
66	1	0	10.258487	-1.701268	-0.826633
67	1	0	9.829980	1.889932	1.508088
68	1	0	11.282250	0.185279	0.431239
69	1	0	3.567077	2.211719	1.476867
70	9	0	-2.194881	5.085641	-0.313508
71	9	0	-2.675474	3.161539	3.927796
72	9	0	-5.243434	-2.936106	1.470647

73	9	0	-5.961117	-0.524871	-2.475562

B3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.985313	-0.199176	-0.142931
2	6	0	-0.917814	-0.133598	-3.176376
3	6	0	-0.234794	1.849896	-2.110715
4	6	0	-0.713863	0.403910	-4.437392
5	1	0	-1.271908	-1.147855	-3.042431
6	6	0	-0.008832	2.437647	-3.368595
7	6	0	-0.248327	1.718088	-4.530111
8	1	0	-0.913204	-0.197135	-5.318029
9	1	0	0.352973	3.453870	-3.413980
10	1	0	-0.072726	2.176826	-5.498895
11	6	0	-2.971582	0.424040	0.031172
12	6	0	-3.554692	0.134092	1.301637
13	6	0	-3.773151	1.043654	-0.939201
14	6	0	-4.897708	0.478207	1.528086
15	6	0	-5.095796	1.363019	-0.658665
16	1	0	-3.381633	1.294813	-1.920972
17	6	0	-5.689938	1.089149	0.570200
18	1	0	-6.722270	1.343160	0.776341
19	6	0	-0.387975	-3.096444	-0.882196
20	6	0	-2.707648	-2.745697	-0.960300
21	6	0	-0.588230	-4.445482	-1.226777
22	6	0	-2.960228	-4.067766	-1.304559
23	1	0	-3.509726	-2.025724	-0.839852
24	6	0	-1.871029	-4.932230	-1.438654

25	1	0	0.263418	-5.108360	-1.322859
26	1	0	-3.979979	-4.403860	-1.459066
27	1	0	-2.021155	-5.975162	-1.703781
28	6	0	0.914502	-1.105947	-0.242776
29	6	0	2.171336	-0.529647	0.006049
30	6	0	0.920297	-2.474931	-0.631559
31	6	0	3.369824	-1.244625	-0.123182
32	1	0	2.250389	0.510049	0.311990
33	6	0	2.127291	-3.199433	-0.764973
34	6	0	3.346595	-2.597763	-0.515304
35	1	0	2.117886	-4.243053	-1.069347
36	1	0	4.280569	-3.138423	-0.614902
37	6	0	-0.496505	-1.330606	2.641529
38	6	0	-2.672654	-0.507469	2.279999
39	6	0	-0.785749	-1.691132	3.949419
40	1	0	0.483632	-1.486514	2.209847
41	6	0	-3.012856	-0.860266	3.598466
42	6	0	-2.072725	-1.450269	4.432129
43	1	0	-0.016537	-2.144813	4.565000
44	1	0	-4.012213	-0.660428	3.954099
45	1	0	-2.342486	-1.716041	5.450376
46	6	0	-0.341589	1.646508	0.321219
47	6	0	-0.161016	2.185556	1.605451
48	6	0	-0.035064	2.469531	-0.806969
49	6	0	0.301695	3.484337	1.755635
50	1	0	-0.376833	1.610363	2.498742
51	6	0	0.427011	3.777144	-0.586985
52	6	0	0.606096	4.311486	0.676292
53	1	0	0.964175	5.324010	0.813607
54	7	0	-1.467048	-2.268505	-0.757366
55	7	0	-0.692096	0.558536	-2.042531
56	7	0	-1.403060	-0.758910	1.823600
57	7	0	4.548667	-0.514333	0.163990
58	7	0	5.623863	-1.159360	0.021232

59	6	0	6.799465	-0.421417	0.312628
60	6	0	8.004736	-1.116950	0.143486
61	6	0	6.819482	0.916506	0.745368
62	6	0	9.221852	-0.487698	0.401281
63	1	0	7.958433	-2.148846	-0.191502
64	6	0	8.036304	1.538016	1.001755
65	1	0	5.877316	1.438329	0.870239
66	6	0	9.239841	0.840678	0.831088
67	1	0	10.153077	-1.031433	0.267755
68	1	0	8.053352	2.571984	1.336613
69	1	0	10.186426	1.334716	1.033660
70	9	0	-5.494671	0.214453	2.721240
71	9	0	-5.849703	1.959231	-1.606783
72	9	0	0.724147	4.585574	-1.637350
73	9	0	0.468721	3.982026	2.999000

A4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-2.276688	-0.106685	0.087429
2	6	0	-2.381101	0.285689	3.103370
3	6	0	-1.289795	-1.661892	2.367890
4	6	0	-2.148940	-0.018375	4.435671
5	1	0	-2.909162	1.183947	2.809335
6	6	0	-1.027414	-2.009575	3.703333
7	6	0	-1.454026	-1.193642	4.739846
8	1	0	-2.502432	0.653082	5.210793
9	1	0	-0.486518	-2.924657	3.915443
10	1	0	-1.249278	-1.465599	5.771404

11	6	0	-4.123356	-1.076477	-0.051989
12	6	0	-4.672766	-1.089681	-1.363646
13	6	0	-4.902225	-1.672029	0.956750
14	6	0	-5.928140	-1.664548	-1.636028
15	6	0	-6.148230	-2.243328	0.691202
16	1	0	-4.527560	-1.695975	1.978547
17	6	0	-6.667389	-2.240508	-0.609450
18	1	0	-6.336668	-1.666847	-2.643929
19	1	0	-6.720557	-2.697677	1.497878
20	1	0	-7.636570	-2.685832	-0.817711
21	6	0	-2.231932	2.936861	0.355844
22	6	0	-4.456428	2.194384	0.447431
23	6	0	-2.679087	4.266073	0.469106
24	6	0	-4.950701	3.487527	0.565174
25	1	0	-5.113819	1.331689	0.430080
26	6	0	-4.035252	4.543082	0.574619
27	1	0	-1.960420	5.077159	0.470235
28	1	0	-6.019510	3.656185	0.643570
29	1	0	-4.376227	5.571218	0.661404
30	6	0	-0.567138	1.134460	0.091864
31	6	0	0.781671	0.756951	-0.015070
32	6	0	-0.824468	2.527619	0.241142
33	6	0	1.846751	1.675461	0.013526
34	1	0	1.017985	-0.300759	-0.097221
35	6	0	0.228969	3.461269	0.276335
36	6	0	1.546416	3.044303	0.162645
37	1	0	0.031499	4.524886	0.384716
38	1	0	2.345293	3.780067	0.159813
39	6	0	-1.823981	0.655603	-2.835882
40	6	0	-3.844573	-0.465554	-2.398425
41	6	0	-2.104039	0.753054	-4.191222
42	1	0	-0.907962	1.047329	-2.412362
43	6	0	-4.170746	-0.387983	-3.762658
44	6	0	-3.306080	0.218937	-4.661909

45	1	0	-1.393167	1.234700	-4.853996
46	1	0	-5.105384	-0.813043	-4.109229
47	1	0	-3.562849	0.273455	-5.716202
48	6	0	-1.297957	-1.857419	-0.054029
49	6	0	-0.944043	-2.570266	-1.215762
50	6	0	-0.904133	-2.427763	1.189951
51	6	0	-0.239867	-3.771307	-1.150803
52	1	0	-1.224684	-2.182117	-2.190969
53	6	0	-0.193663	-3.640516	1.251330
54	6	0	0.140754	-4.313997	0.084406
55	1	0	0.015941	-4.295210	-2.069679
56	1	0	0.101537	-4.060582	2.209799
57	1	0	0.689768	-5.250397	0.130168
58	7	0	-3.143626	1.920869	0.348814
59	7	0	-1.970391	-0.504865	2.091895
60	7	0	-2.661444	0.067756	-1.957583
61	6	0	3.251900	1.221658	-0.110358
62	6	0	4.292375	1.874267	0.587486
63	6	0	3.593546	0.128277	-0.927090
64	6	0	5.611174	1.461615	0.476254
65	1	0	4.048745	2.702061	1.247371
66	6	0	4.914188	-0.290284	-1.044419
67	1	0	2.817417	-0.381292	-1.489420
68	6	0	5.936903	0.369304	-0.348118
69	1	0	6.404877	1.960777	1.020944
70	1	0	5.183534	-1.127898	-1.680889
71	7	0	7.240723	-0.138649	-0.545256
72	7	0	8.148522	0.458076	0.097815
73	6	0	9.454639	-0.053756	-0.107049
74	6	0	9.771572	-1.129736	-0.955278
75	6	0	10.473142	0.592342	0.607395
76	6	0	11.093222	-1.543149	-1.077818
77	1	0	8.971121	-1.617673	-1.500041
78	6	0	11.796573	0.172679	0.480690

79	1	0	10.199289	1.420133	1.254595
80	6	0	12.109288	-0.895639	-0.362236
81	1	0	11.339370	-2.374485	-1.733492
82	1	0	12.581498	0.677458	1.037238
83	1	0	13.139724	-1.225644	-0.464147

B4

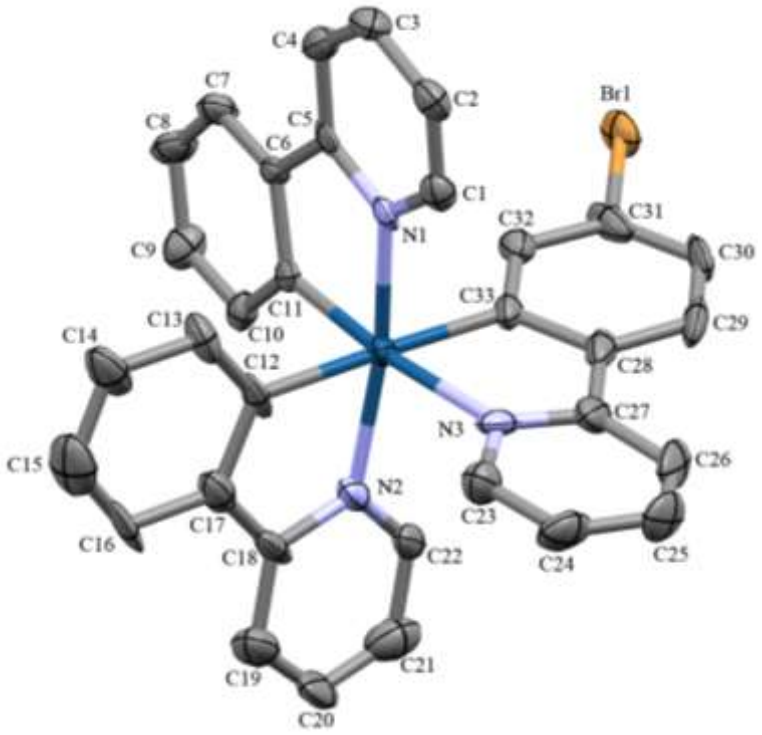
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-2.036483	0.183613	0.118349
2	6	0	-2.119586	0.569465	3.126827
3	6	0	-1.092557	-1.417273	2.395225
4	6	0	-1.904426	0.259366	4.460315
5	1	0	-2.614550	1.484914	2.829116
6	6	0	-0.848678	-1.773912	3.733919
7	6	0	-1.253694	-0.938945	4.765073
8	1	0	-2.237792	0.943380	5.233296
9	1	0	-0.343594	-2.704563	3.945420
10	1	0	-1.063397	-1.219449	5.797025
11	6	0	-3.903225	-0.744121	-0.017272
12	6	0	-4.453878	-0.734897	-1.334507
13	6	0	-4.660383	-1.322063	1.012520
14	6	0	-5.721132	-1.303376	-1.545611
15	6	0	-5.908923	-1.869575	0.745339
16	1	0	-4.289931	-1.363090	2.032772
17	6	0	-6.469413	-1.873541	-0.528981
18	1	0	-7.443481	-2.304333	-0.724807
19	6	0	-1.914731	3.216800	0.401275
20	6	0	-4.156965	2.528424	0.495171

21	6	0	-2.329275	4.555735	0.521769
22	6	0	-4.619062	3.832368	0.619714
23	1	0	-4.836175	1.683065	0.478081
24	6	0	-3.677931	4.865187	0.631396
25	1	0	-1.590889	5.348787	0.525423
26	1	0	-5.683119	4.026597	0.701920
27	1	0	-3.993609	5.900788	0.723548
28	6	0	-0.296643	1.375640	0.125441
29	6	0	1.040316	0.963108	0.009671
30	6	0	-0.518746	2.773665	0.281190
31	6	0	2.128899	1.853906	0.035559
32	1	0	1.250409	-0.099468	-0.079320
33	6	0	0.558529	3.679462	0.315105
34	6	0	1.864120	3.228917	0.192581
35	1	0	0.388922	4.747236	0.428417
36	1	0	2.681699	3.943707	0.188842
37	6	0	-1.572181	0.958237	-2.791471
38	6	0	-3.622951	-0.120021	-2.372909
39	6	0	-1.843119	1.077723	-4.146563
40	1	0	-0.648344	1.321757	-2.360381
41	6	0	-3.942360	-0.017859	-3.739071
42	6	0	-3.055601	0.578970	-4.624701
43	1	0	-1.117178	1.548142	-4.800948
44	1	0	-4.883170	-0.414530	-4.089125
45	1	0	-3.308418	0.650491	-5.678834
46	6	0	-1.105889	-1.587687	-0.041511
47	6	0	-0.782133	-2.273098	-1.224325
48	6	0	-0.735149	-2.180239	1.206028
49	6	0	-0.120954	-3.490693	-1.164218
50	1	0	-1.039544	-1.875616	-2.199614
51	6	0	-0.069357	-3.416548	1.198196
52	6	0	0.251860	-4.093720	0.035416
53	1	0	0.766739	-5.045778	0.062657
54	7	0	-2.851255	2.223264	0.391374

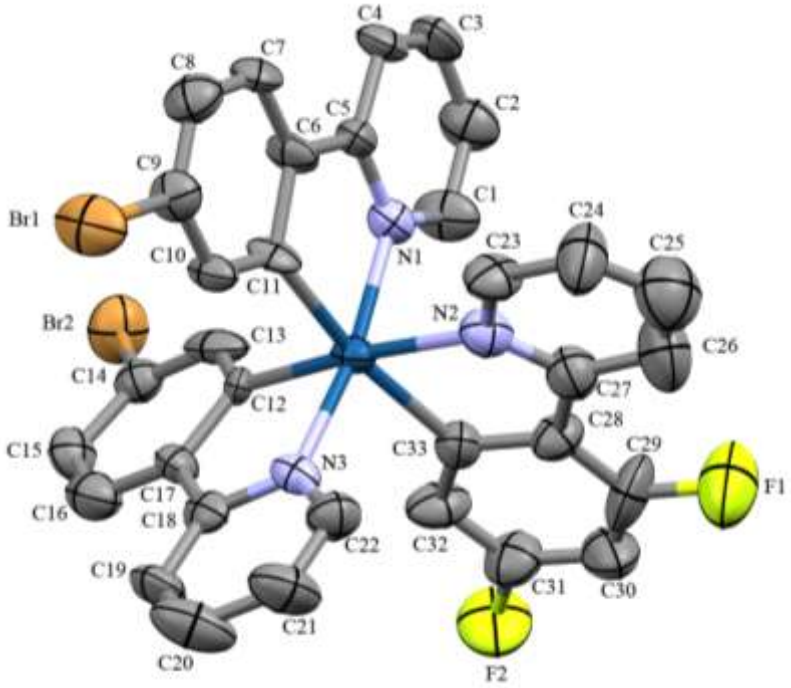
55	7	0	-1.732924	-0.236069	2.118411
56	7	0	-2.427364	0.381806	-1.923137
57	6	0	3.521175	1.364820	-0.099618
58	6	0	4.580854	1.983691	0.599520
59	6	0	3.830106	0.271411	-0.928883
60	6	0	5.887947	1.537670	0.477982
61	1	0	4.361819	2.811036	1.268580
62	6	0	5.138873	-0.180593	-1.056359
63	1	0	3.039066	-0.211102	-1.494488
64	6	0	6.181102	0.445402	-0.358356
65	1	0	6.696907	2.010384	1.023756
66	1	0	5.383434	-1.018359	-1.702472
67	7	0	7.470782	-0.094972	-0.566108
68	7	0	8.396635	0.476384	0.073802
69	6	0	9.688366	-0.067270	-0.138965
70	6	0	10.727067	0.556001	0.566630
71	6	0	9.972650	-1.153285	-0.986014
72	6	0	12.038946	0.103918	0.431837
73	1	0	10.477952	1.391939	1.213331
74	6	0	11.282857	-1.599276	-1.116259
75	1	0	9.156803	-1.623334	-1.523593
76	6	0	12.319311	-0.974328	-0.409832
77	1	0	12.839923	0.590935	0.981225
78	1	0	11.504091	-2.438553	-1.770613
79	1	0	13.340597	-1.329830	-0.517712
80	9	0	0.295015	-4.006398	2.365695
81	9	0	0.182023	-4.130543	-2.313623
82	9	0	-6.285028	-1.313298	-2.783053
83	9	0	-6.621040	-2.419942	1.751604

X-Ray Crystal Structure

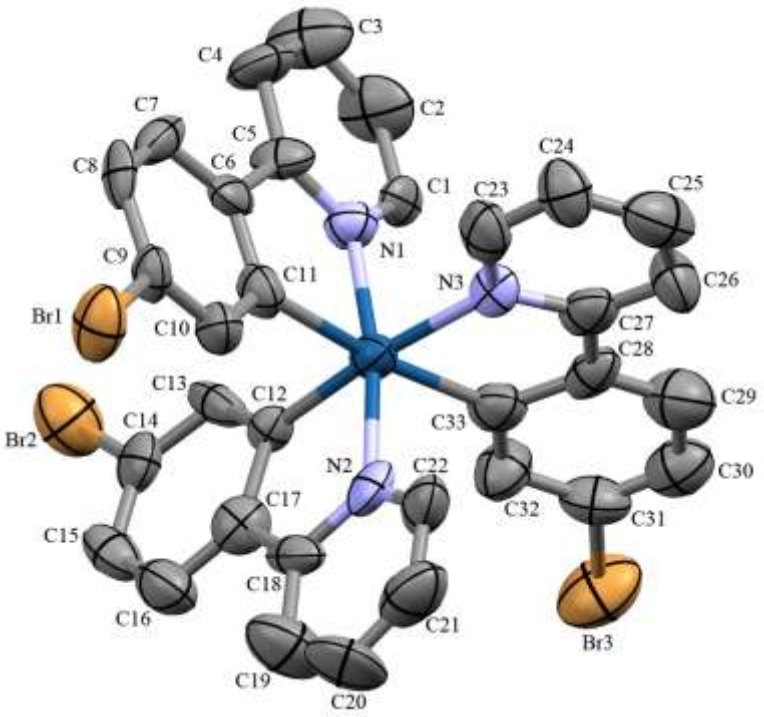
[Ir(ppy)$_2$((5-bromo-2-pyridyl)phenyl)], **C:**



[Ir((5-bromo-2-pyridyl)phenyl)$_2$(Fppy)], **F-Fppy:**



[Ir((5-bromo-2-pyridyl)phenyl)$_3$], **H:**



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