

# Spectroscopic and crystallographic studies on the stability of self-assembled coordination nanotubes

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## Supplementary information for the NMR data of $2b\cdot 3^{14+}$ and $2a\cdot 4^{20+}$

**Figure S1.**  $^1\text{H}$  NMR of  $2b\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)

**Figure S2.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $2b\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)

**Figure S3.** Relational  $^1\text{H}$ - $^1\text{H}$  COSY of  $2b\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)

**Figure S4.** NOESY of  $2b\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)

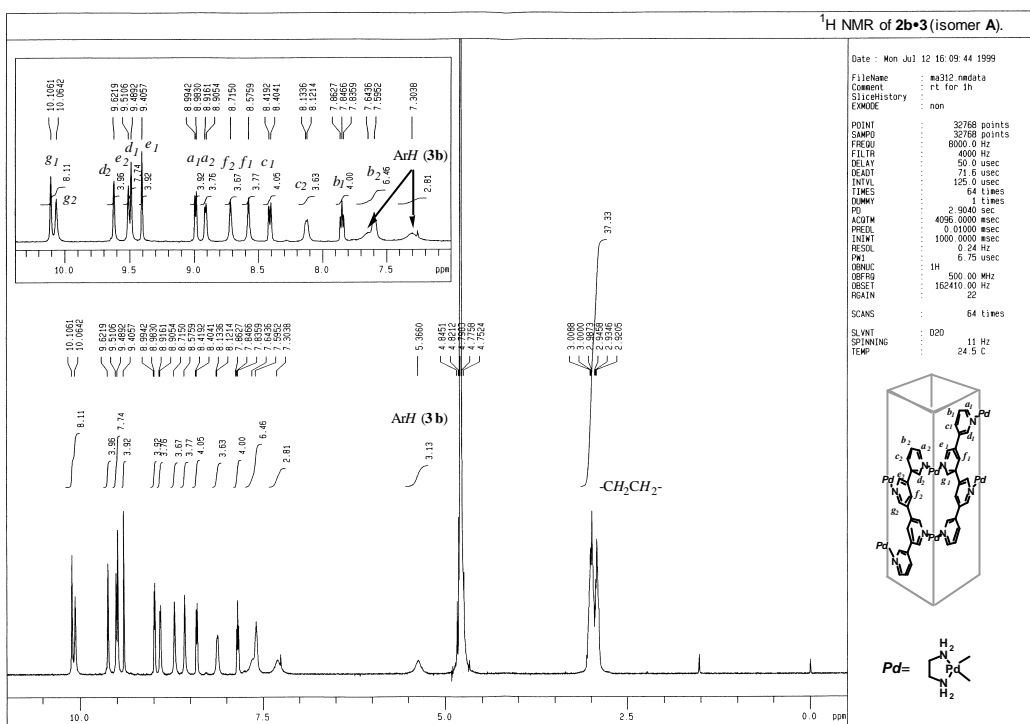
**Figure S5.**  $^1\text{H}$  NMR of  $2a\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

**Figure S6.**  $^{13}\text{C}$  NMR of  $2a\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

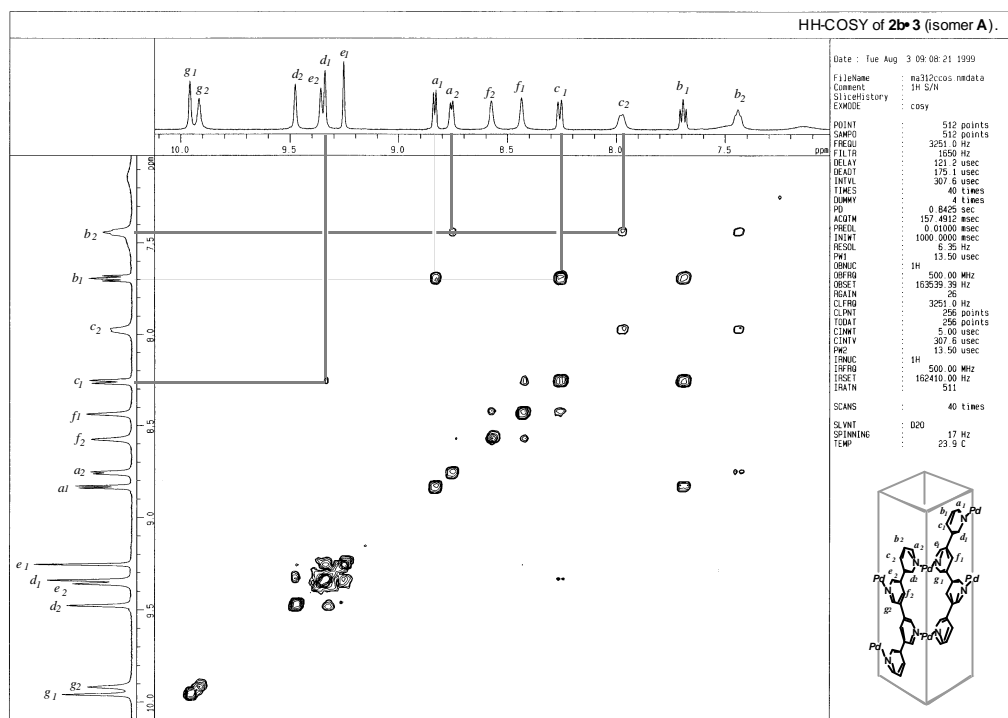
**Figure S7.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $2a\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

**Figure S8.** NOESY of  $2a\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

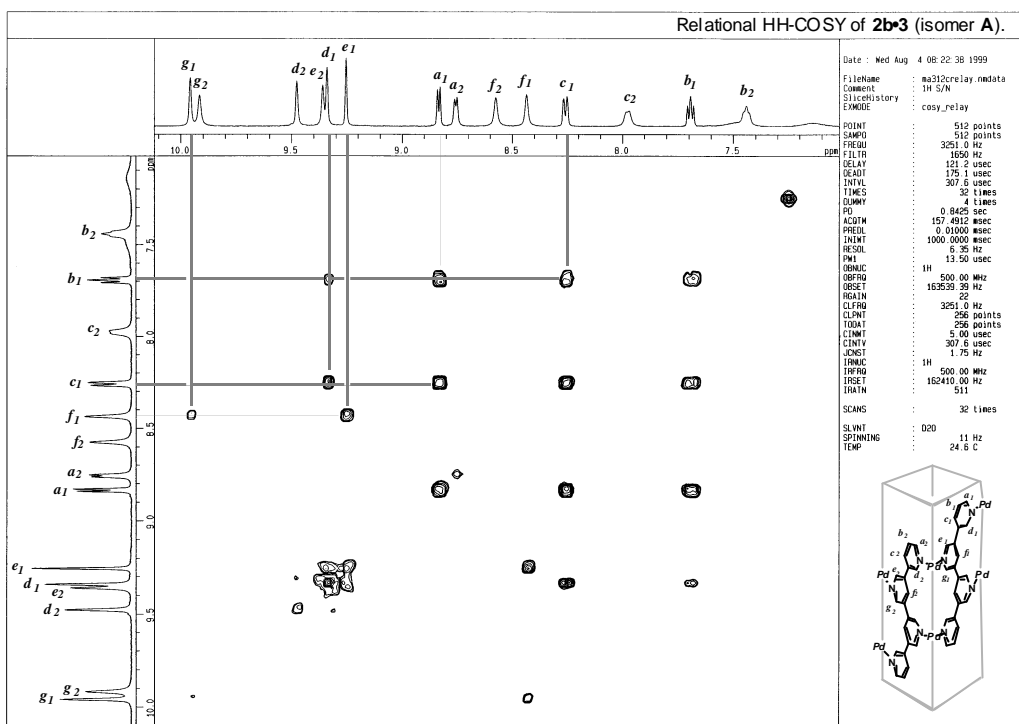
**Figure S9.**  $^{13}\text{C}$ - $^1\text{H}$  COSY of  $2a\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)



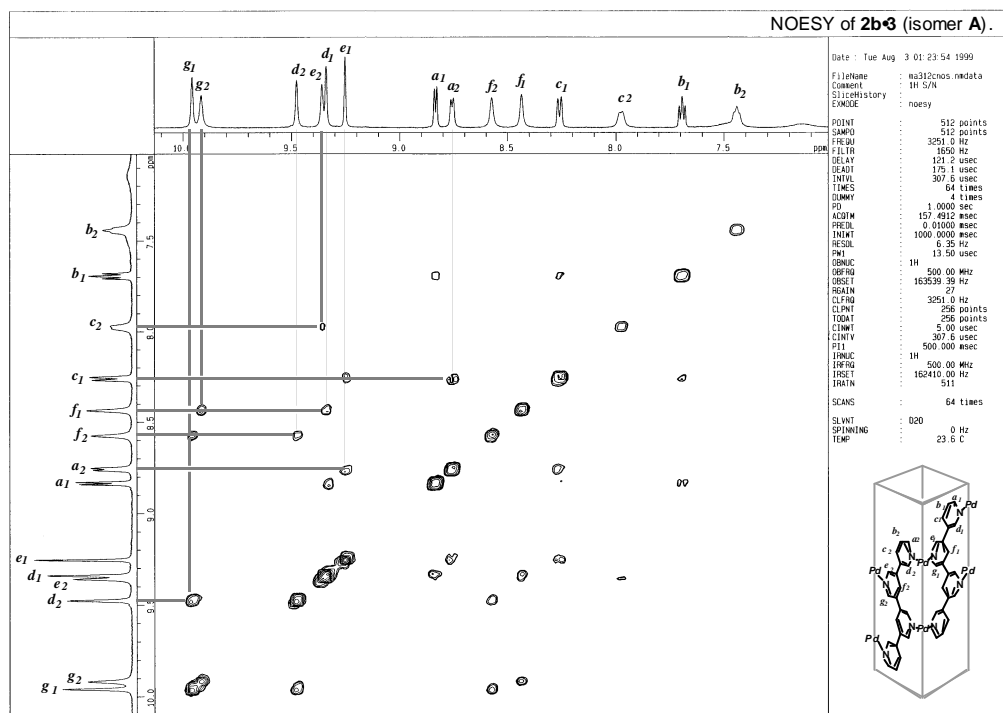
**Figure S1.** <sup>1</sup>H NMR of 2b•3<sup>14+</sup> (D<sub>2</sub>O, 25 °C)



**Figure S2.** <sup>1</sup>H-<sup>1</sup>H COSY of 2b•3<sup>14+</sup> (D<sub>2</sub>O, 25 °C)



**Figure S3.** Relational  $^1\text{H}$ - $^1\text{H}$  COSY of  $2\text{b}\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)



**Figure S4.** NOESY of  $2\text{b}\cdot 3^{14+}$  ( $\text{D}_2\text{O}$ , 25 °C)

<sup>1</sup>H NMR of 2a•4

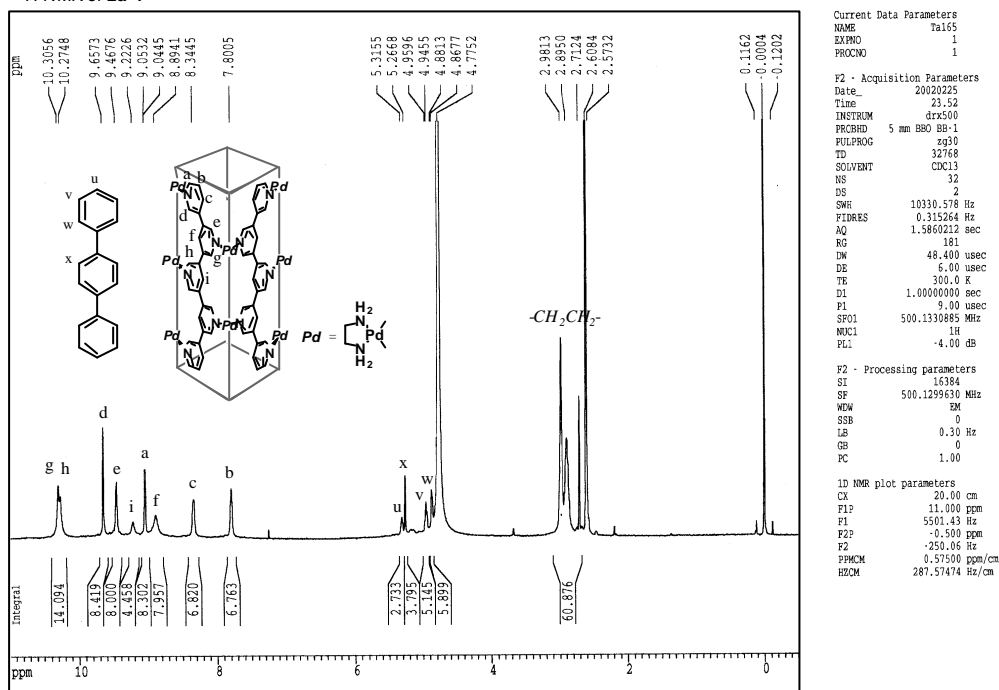


Figure S5. <sup>1</sup>H NMR of 2a•4<sup>20+</sup> (D<sub>2</sub>O, 27 °C)

<sup>13</sup>C NMR of 2a•4

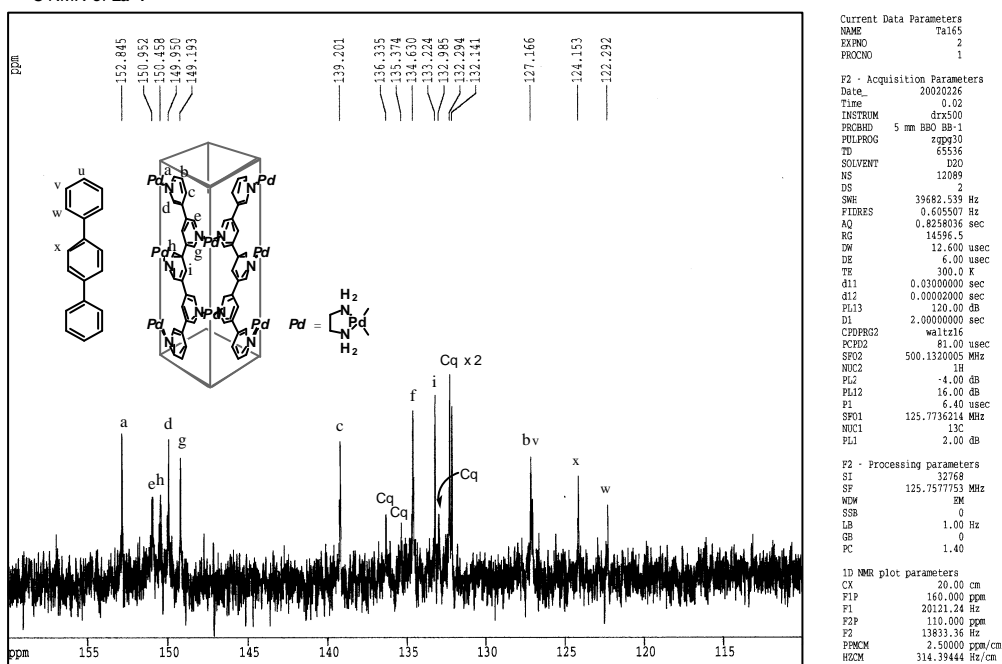
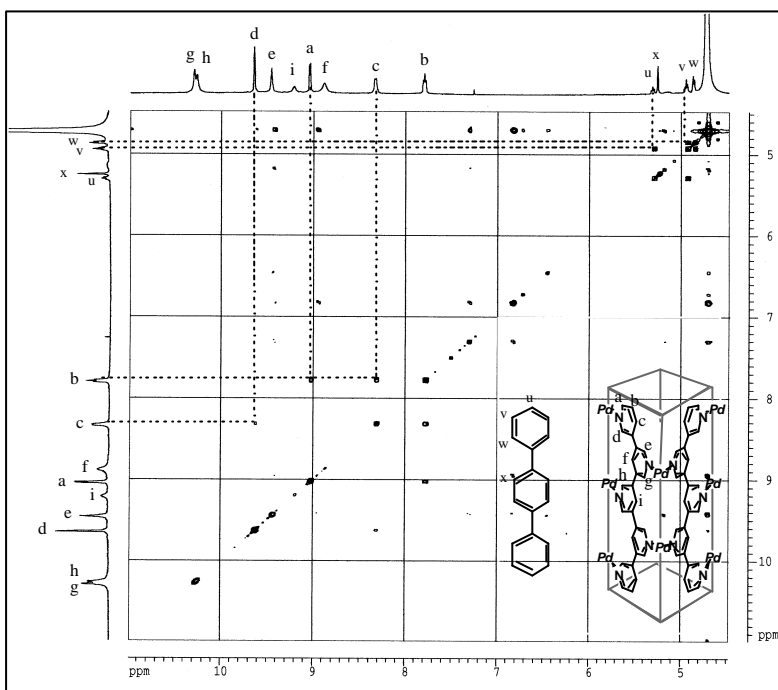


Figure S6. <sup>13</sup>C NMR of 2a•4<sup>20+</sup> (D<sub>2</sub>O, 27 °C)

HH-COSY of 2a•4



COSYGE

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Current Data Parameters
NAME          2a4
EXPNO        16
PROCNO       1

F2 - Acquisition Parameters
Date_        20020913
Time         16:51
INSTRUM     drx500
PROBHD      5 mm BBO 5B-1
PULPROG     coeppg0
TD           2488
SOLVENT     D2O
NS           4
DS           4
SWH          3355.208 Hz
F2RES       1.529457 Hz
AQ           0.3146248 sec
RG           4206
DM           153.650 usec
DE           4.20 usec
TE           300.2 K
SF           0.00000000 sec
D1           2.00000000 sec
F1           9.20 usec
SFO1        500.133844 MHz
NUC1         1H
P1          4.00 usec
RG1         0.00000000 sec

F1 - Acquisition parameters
NUC1         1H
SF1         500.1338 MHz
PT1RES      13.715857 Hz
SW          10.98 ppm

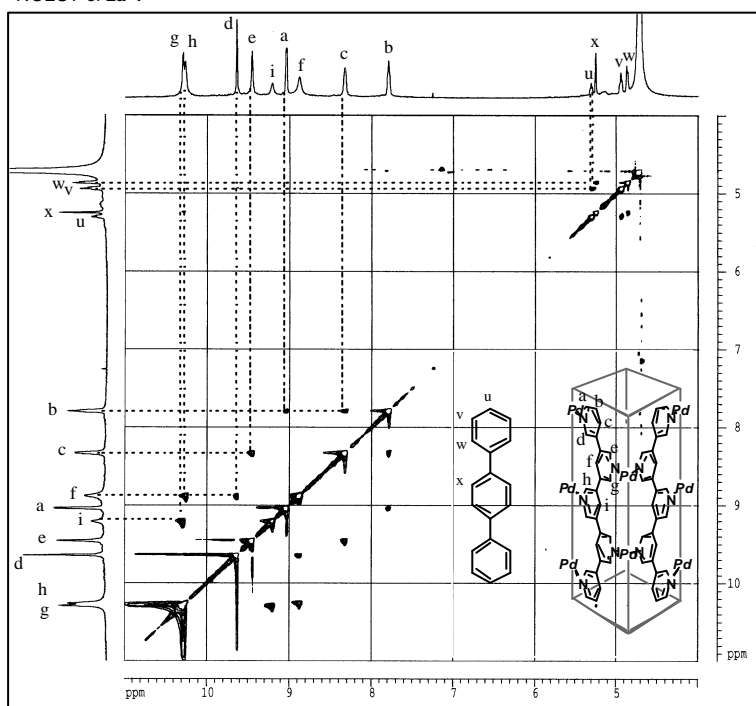
F2 - Processing parameters
SI          1024
SF          500.130000 MHz
WDW         EM
SSB         0
GB          0.00 Hz
CB          0
PC          1.00

F1 - Processing parameters
SI          1024
MC1         67
SF          500.130000 MHz
WDW         EM
SSB         0
GB          0.00 Hz
CB          0

2D NMR plot parameters
CX2         15.00 cm
CY2         15.00 cm
F2F2C0     10.985 ppm
F2F2C1     5493.0 Hz
F2F2H1     4.476 ppm
F2F2H2     2196.7 Hz
F1F1C0     10.985 ppm
F1F1C1     5493.0 Hz
F1F1H1     4.476 ppm
F1F1H2     2196.7 Hz
F2F2PCMC   0.4339 ppm/cm
F1F2PCMC   217.0199 Hz/cm
F1F2PCMC   0.4339 ppm/cm
F1F2PCMC   217.0199 Hz/cm
    
```

Figure S7.  $^1\text{H}$ - $^1\text{H}$  COSY of  $2\text{a}\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

NOESY of 2a•4



COSYGE

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Current Data Parameters
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EXPNO        6
PROCNO       1

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Time         6:18
INSTRUM     drx500
PROBHD      5 mm BBO 5B-1
PULPROG     coeppg0
TD           2048
SOLVENT     D2O
NS           4
DS           4
SWH          6311.131 Hz
F2RES       1.196278 Hz
AQ           0.1822514 sec
RG           4104
DM           79.200 usec
DE           8.20 usec
TE           300.2 K
SF           0.00000000 sec
D1           8.40 usec
F1           9.20 usec
SFO1        500.133844 MHz
NUC1         1H
P1          4.00 usec
RG1         0.30000000 sec
WDW         EM
GB          0.00 Hz
CB          0

F1 - Acquisition parameters
NUC1         1H
SF1         500.1332 MHz
PT1RES      12.110135 Hz
SW          10.98 ppm

F2 - Processing parameters
SI          1024
SF          500.130000 MHz
WDW         EM
SSB         0
GB          0.00 Hz
CB          0
PC          1.00

F1 - Processing parameters
SI          1024
MC1         677
SF          500.130000 MHz
WDW         EM
SSB         0
GB          0.00 Hz
CB          0

2D NMR plot parameters
CX2         15.00 cm
CY2         15.00 cm
F2F2C0     10.984 ppm
F2F2C1     5496.0 Hz
F2F2H1     4.492 ppm
F2F2H2     2196.7 Hz
F1F1C0     10.984 ppm
F1F1C1     5496.0 Hz
F1F1H1     4.492 ppm
F1F1H2     2196.7 Hz
F2F2PCMC   0.46673 ppm/cm
F1F2PCMC   233.45454 Hz/cm
F1F2PCMC   0.46673 ppm/cm
F1F2PCMC   233.45454 Hz/cm
    
```

Figure S8. NOESY of  $2\text{a}\cdot 4^{20+}$  ( $\text{D}_2\text{O}$ , 27 °C)

CH-COSY of **2a•4**

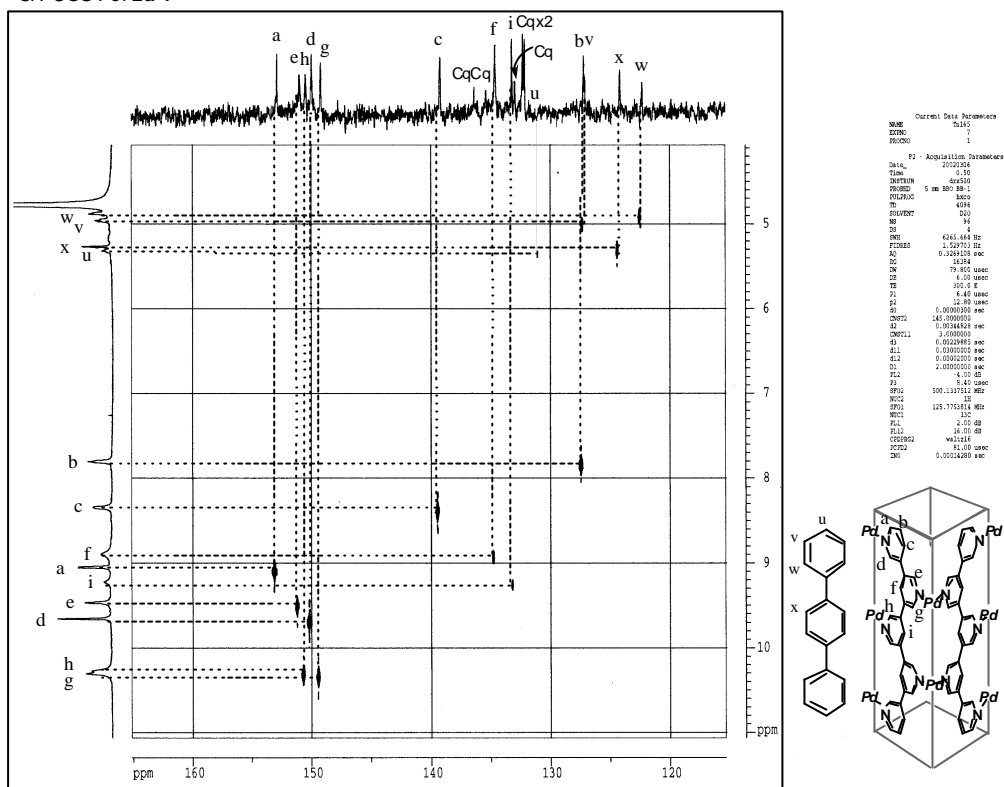


Figure S9.  $^{13}\text{C}$ - $^1\text{H}$  COSY of **2a•4**<sup>20+</sup> ( $\text{D}_2\text{O}$ , 27 °C)