

Dynamic aspects in host–guest complexation by coordination nanotubes

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Supplementary information for the NMR data of 2a•3a, 2a•3b and 2b•3a

Figure S1. ^1H NMR of $2\mathbf{a}\cdot\mathbf{3a}^{19+}$ (D_2O , 27 °C)

Figure S2. ^1H - ^1H COSY of $2\mathbf{a}\cdot\mathbf{3a}^{19+}$ (D_2O , 27 °C)

Figure S3. NOESY of $2\mathbf{a}\cdot\mathbf{3a}^{19+}$ (D_2O , 27 °C)

Figure S4-8. VT-NMR($[\text{H}]/[\text{G}]=1/1, 1/1.1, 1/1.2, 1/1.5, 1/2$ of $2\mathbf{a}\cdot\mathbf{3a}^{19+}$). (D_2O)

Figure S9. ^1H NMR of $2\mathbf{a}\cdot\mathbf{3b}^{20+}$ (D_2O , 27 °C)

Figure S10. ^1H - ^1H COSY of $2\mathbf{a}\cdot\mathbf{3b}^{20+}$ (D_2O , 27 °C)

Figure S11. NOESY of $2\mathbf{a}\cdot\mathbf{3b}^{20+}$ (D_2O , 27 °C)

Figure S12. VT-NMR($[\text{H}]/[\text{G}]=1/1$ of $2\mathbf{a}\cdot\mathbf{3b}^{20+}$). (D_2O)

Figure S13. ^1H NMR of $2\mathbf{b}\cdot\mathbf{3a}^{11+}$ (D_2O , 15 °C)

Figure S14. ^1H - ^1H COSY of $2\mathbf{b}\cdot\mathbf{3a}^{11+}$ (D_2O , 15 °C)

Figure S15. VT-NMR($[\text{H}]/[\text{G}]=1/1$ of $2\mathbf{b}\cdot\mathbf{3a}^{11+}$). (D_2O)

NOESY of 2a•3a

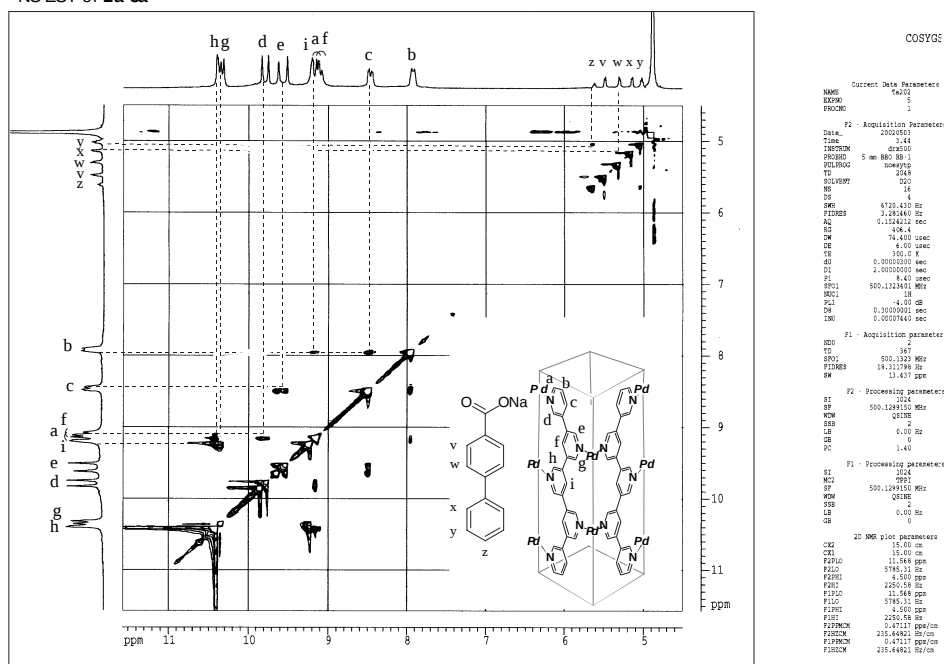


Figure S3. NOESY of 2a•3a¹⁹⁺ (D₂O, 27 °C)

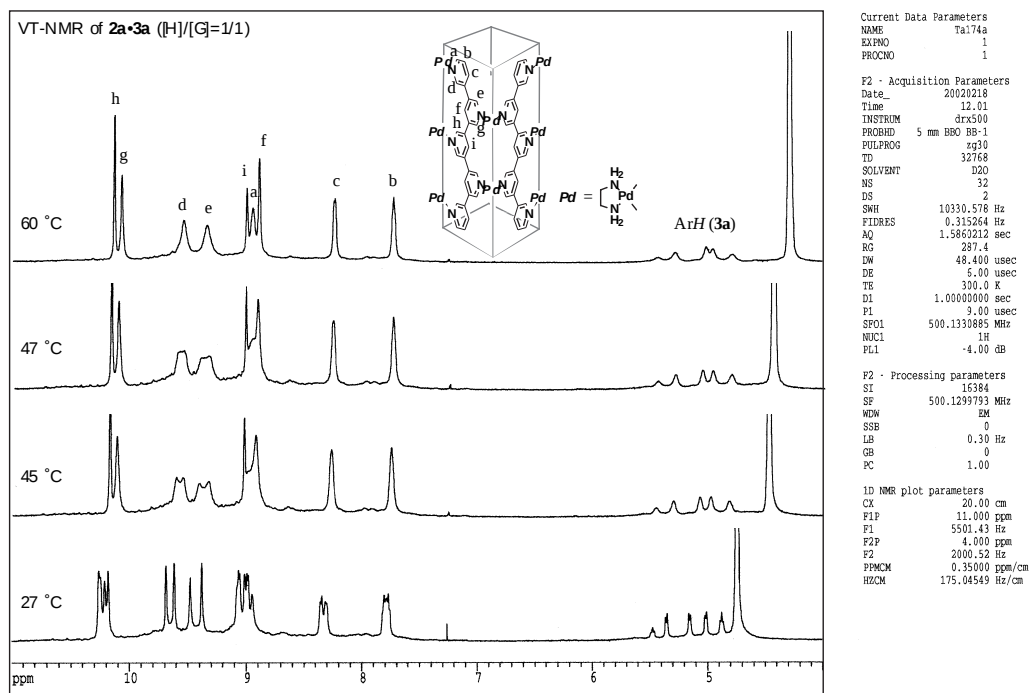


Figure S4. VT-NMR([H]/[G]=1/1 of 2a•3a¹⁹⁺). (D₂O)

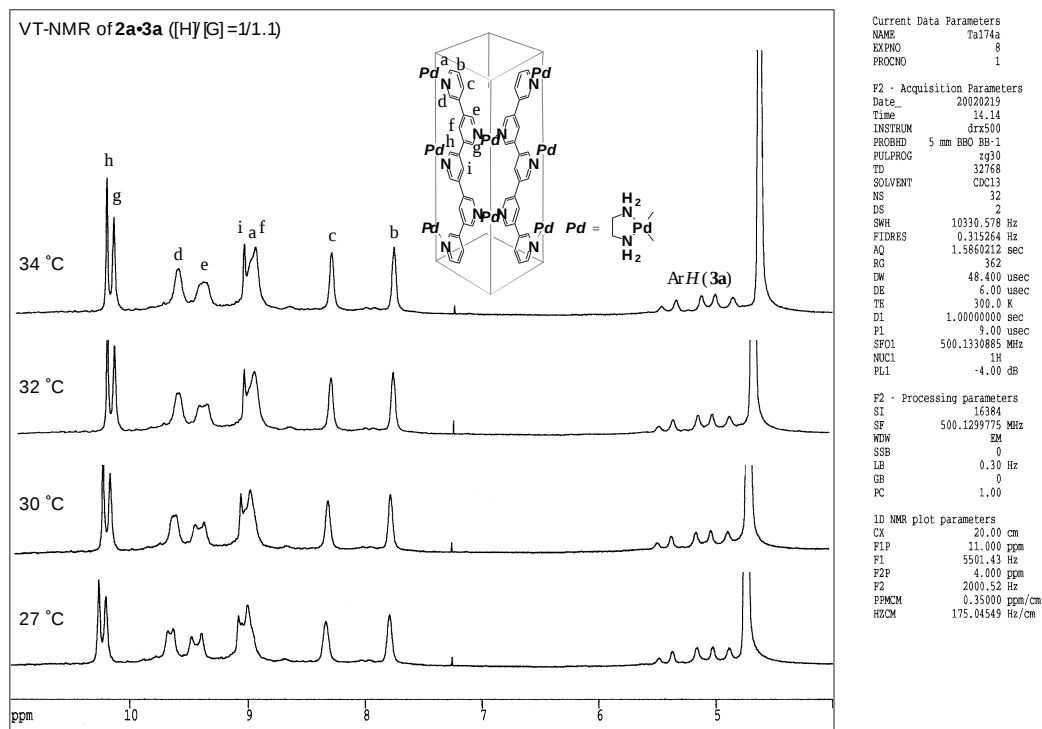


Figure S5. VT-NMR([H]/[G]=1/1.1 of **2a•3a**¹⁹⁺). (D₂O)

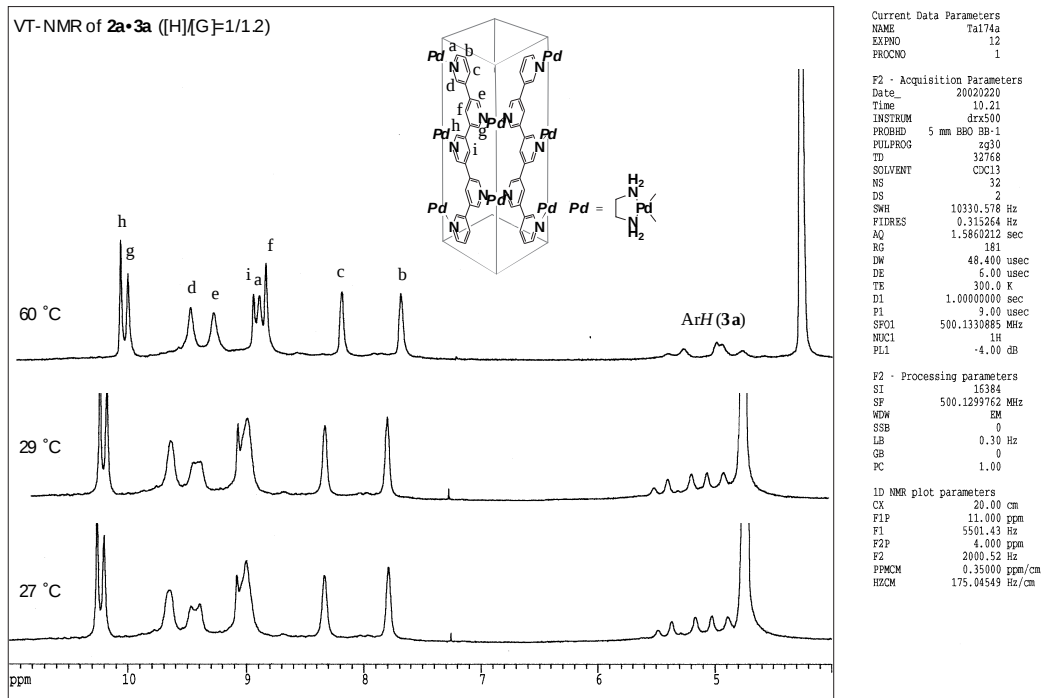


Figure S6. VT-NMR([H]/[G]=1/1.2 of **2a•3a**¹⁹⁺). (D₂O)

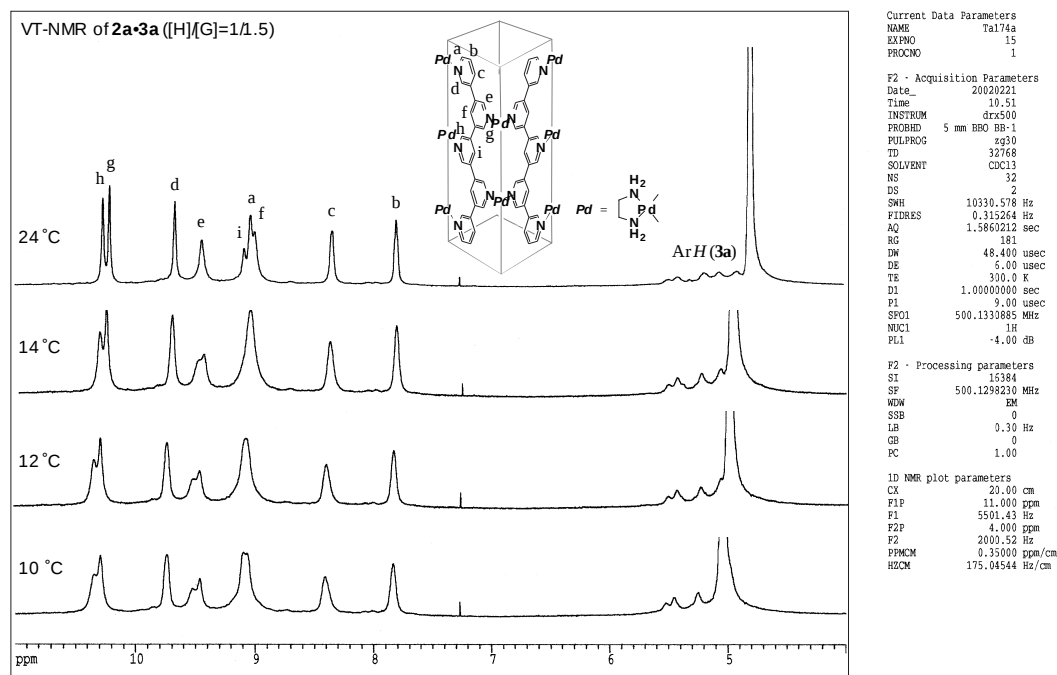


Figure S7. VT-NMR([H]/[G]=1/1.5 of **2a•3a**¹⁹⁺). (D₂O)

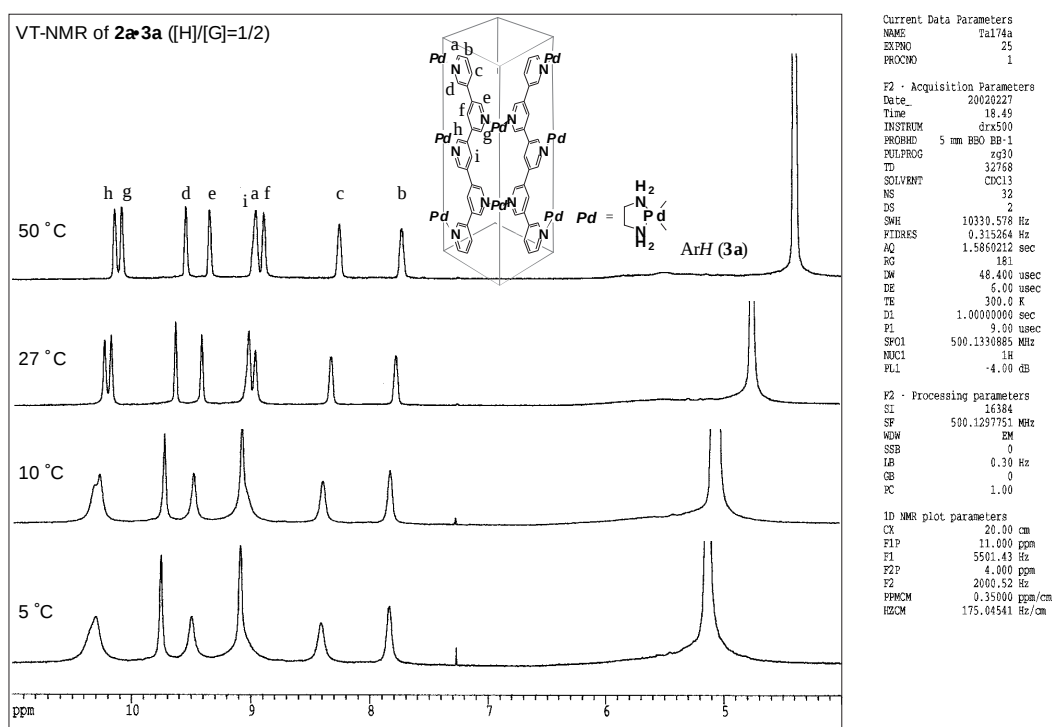
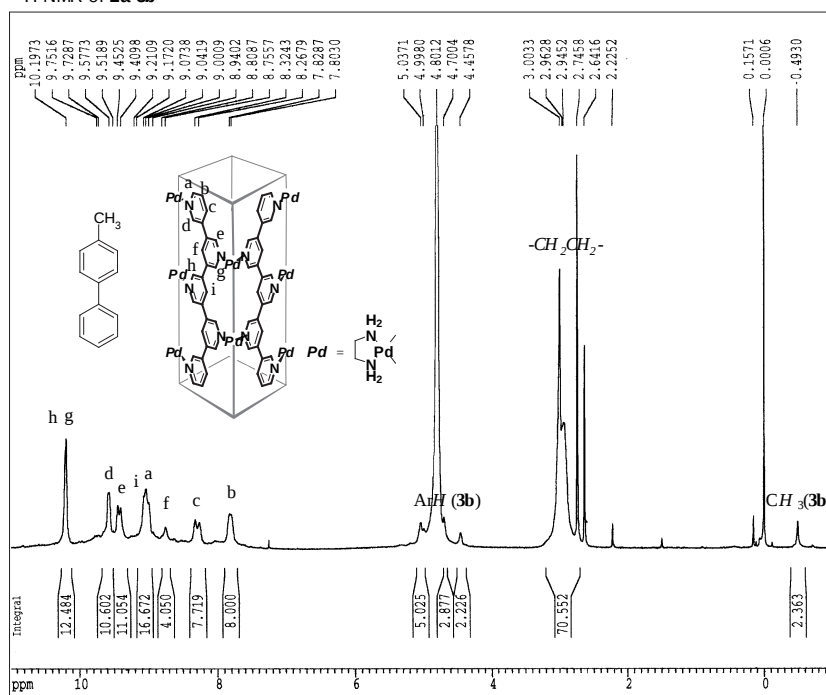


Figure S8. VT-NMR([H]/[G]=1/2 of **2a•3a**¹⁹⁺). (D₂O)

¹H NMR of 2a•3b



Current Data Parameters
NAME Ta176
EXPNO 7
PROCNO 1

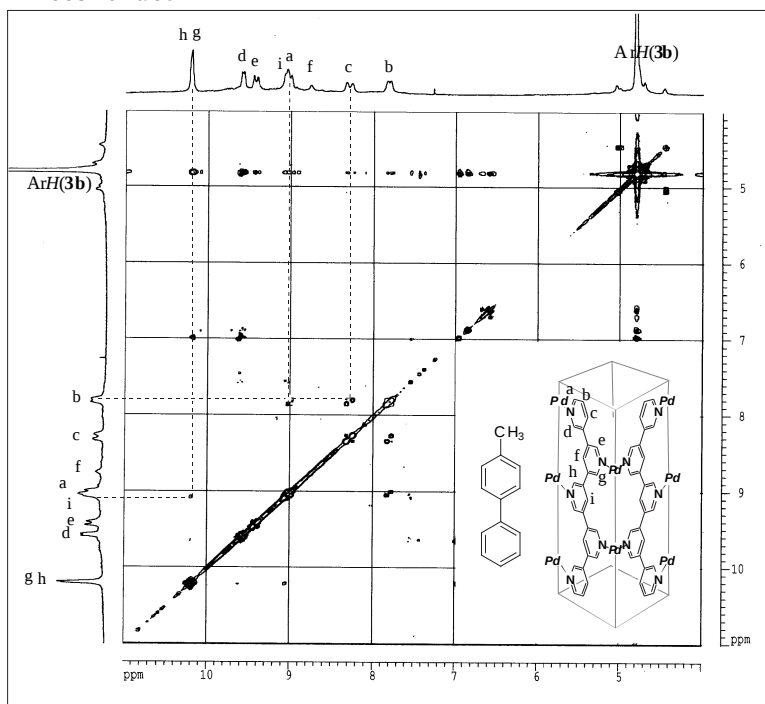
F2 - Acquisition Parameters
Date_ 20020223
Time 13.02
INSTRUM drx500
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.00 usec
SFO1 500.1330885 MHz
NUC1 1H
FL1 -4.00 dB

F2 - Processing parameters
SI 16384
SF 500.1299510 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FLP 11.000 ppm
FI 5501.43 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPNMC 0.60000 ppm/cm
HZCM 300.07797 Hz/cm

Figure S9. ¹H NMR of 2a•3b²⁰⁺ (D₂O, 27 °C)

HH-COSY of 2a•3b



COSYGE

Current Data Parameters
NAME Ta176
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020226
Time 17.12
INSTRUM drx500
PULPROG zgpg30
TD 2048
SOLVENT D₂O
NS 16
DS 4
SWH 3901.401 Hz
FIDRES 1.709468 Hz
AQ 0.2945044 sec
RG 4096
DW 142.800 usec
DE 6.00 usec
TE 300.0 K
D1 0.00000100 sec
D11 2.00000000 sec
P1 9.00 usec
SFO1 500.1337907 MHz
NUC1 1H
FL1 -4.00 dB
LNO 0.00125560 sec

F1 - Acquisition parameters
SI 256
SF 500.1299543 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1536
SF 500.1299439 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
FLP2 10.999 ppm
FLP1 5497.14 Hz
FIDRES 1.990 ppm
F2P1 1995.74 Hz
F1P2 11.014 ppm
F1P1 5858.95 Hz
F1L2 4.233 ppm
F1L1 2097.13 Hz
F1P2M 0.44672 ppm/cm
F1S2CM 133.44671 Hz/cm
F1P1M 0.44672 ppm/cm
F1S1CM 233.44671 Hz/cm

Figure S10. ¹H-¹H COSY of 2a•3b²⁰⁺ (D₂O, 27 °C)

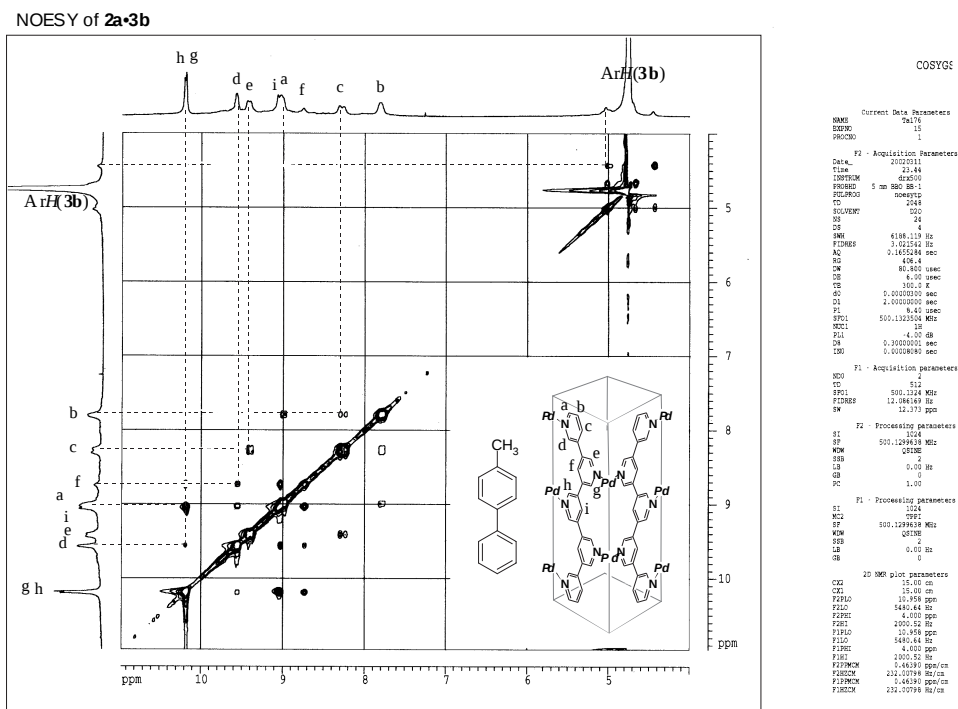


Figure S11. NOESY of **2a•3b**²⁰⁺ (D₂O, 27 °C)

VT-NMR of **2a•3b** ([H]/[G]=1/1)

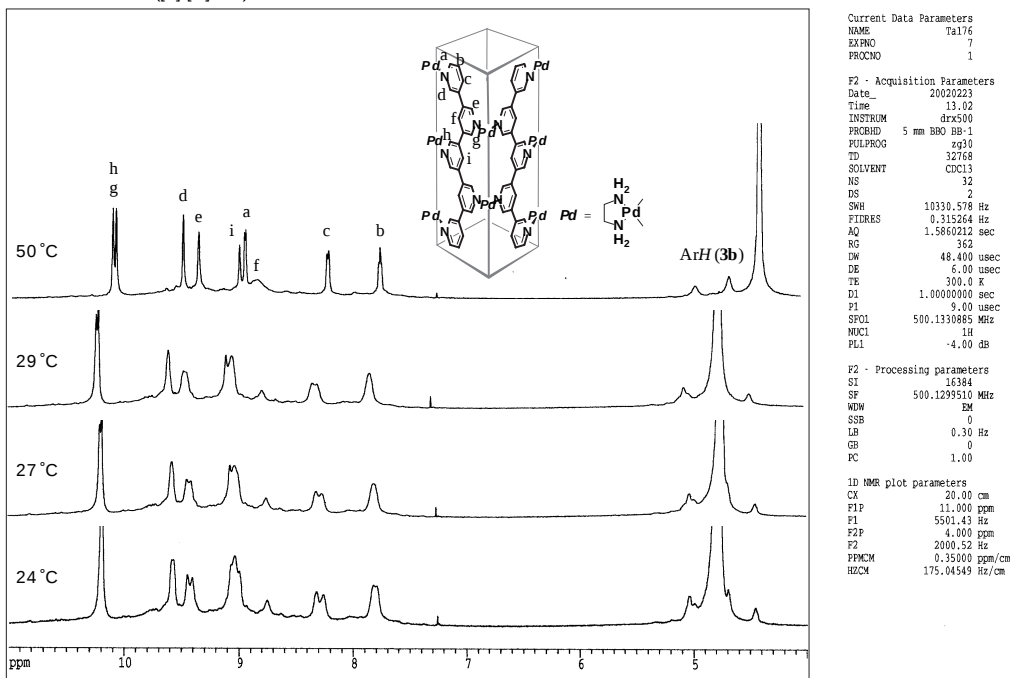


Figure S12. VT-NMR([H]/[G]=1/1 of **2a•3b**²⁰⁺). (D₂O)

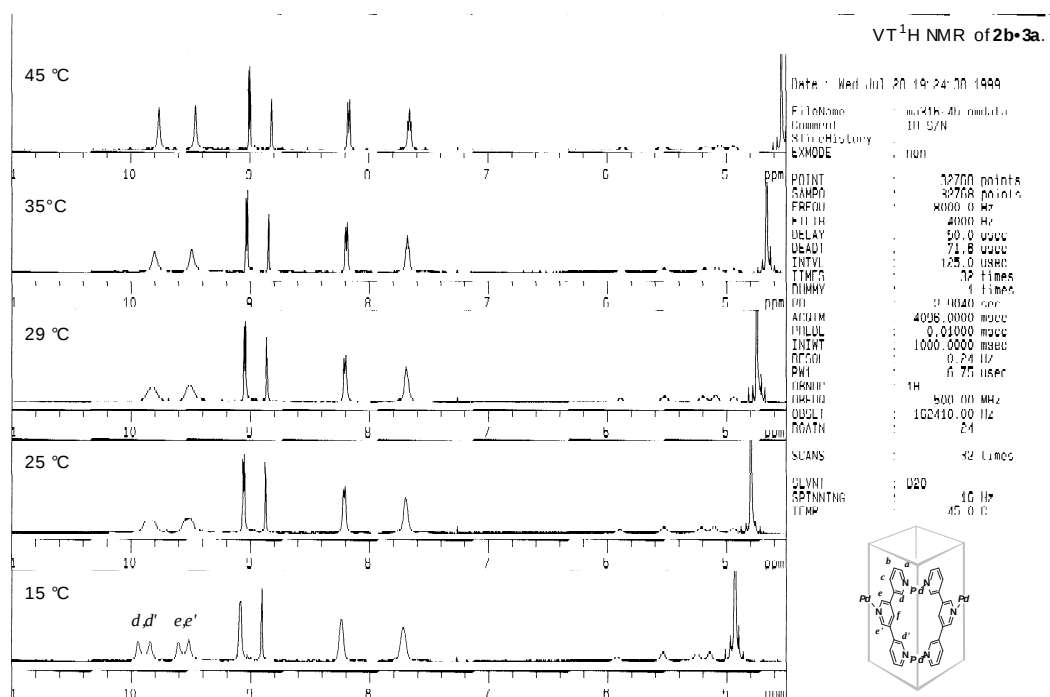


Figure S15. VT-NMR([H]/[G]=1/1 of 2b•3a¹¹⁺). (D₂O)