Supplementary Material (ESI) for Chemical Communications

Supplemental Information for:

Isolation of an [SNS]Pd(II) Pincer with a Water Ladder and its Suzuki Coupling Activity in Water

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1. **Materials and Physical Measurements**: All the starting chemicals were used as purchased. Elemental analyses (C, H, N) were performed on a Perkin–Elmer PE 2400 CHNS Elemental Analyzer. Infrared spectra were obtained from running the sample in KBr discs on the Shimadzu IR–470 spectrometer. The NMR spectra were measured at 25°C using a Bruker ACF 300 NMR spectrometer. Thermogravimetric analysis was carried out in a nitrogen stream using TA instrument 2960 equipment with a heating rate of 10 °C/min. Suzuki-Miyaura coupling reaction results were processed and analyzed by a HP 6890/5973 GC-MS equipment.

2. **Table S1** Hydrogen bonds parameters in complexes **1** and **2**.

D–H···A[a]	D–H	D···A	H···A	∠D–H···A
		Complex **1**		
O2W–H4W[b]···O1W	0.83(3)	2.820(10)	2.11(3)	144(4)
O2W–H3W[b]···O1WA	0.85(4)	2.900(9)	2.12(3)	153(5)
O1W–H2W[b]···O2WB	0.86(7)	2.940(9)	2.32(7)	129(7)
O1W–H1W[b]···Cl2C	0.86(5)	3.114(6)	2.32(6)	152(8)
N1–H1N[b]···Cl2	0.89(4)	3.141(4)	2.25(4)	175(3)
C3–H···Cl1C	0.98	3.812(5)	2.84	170
C9–H···Cl1C	0.98	3.785(5)	2.82	169
C1–H···Pd1C	0.98	3.867(5)	3.07	139
C7–H···Pd1C	0.98	3.898(5)	3.08	142
C11–H···Cl1F	0.97	3.767(6)	2.83	162
C2–H···Cl2G	0.98	3.641(5)	2.80	145
[a] Symmetry codes: A, 1–x, 1–y, 1–z; B, 2–x, 1–y, 1–z; C, 1+x, y, z; F, –x, 1–y, –z; G, 1–x, –y, 1–z. [b] H atoms H1N, H1W, H2W, H3W, H4W were located from difference map, the positions were refined with constraints DFIX 0.90(2) for N–H, DFIX 0.85(2) for O–H, and DFIX 1.20(2) for H···H of water, with thermal parameter at –1.2000 of the relevant N or O.				
		Complex **2**		
N1–H1N···Cl2	0.87	3.120(2)	2.26	167
C2–H···Cl2	0.98	3.577(2)	2.85	132
C11–H···Cl2A	0.98	3.643(2)	2.84	139
C1–H···Cl2B	0.98	3.630(2)	2.74	152
C1–H···Pd1B	0.98	3.978(2)	3.21	136
C10–H···Pd1B	0.98	3.979(2)	3.18	140
C3–H···Cl1C	0.98	3.581(2)	2.79	138
C17–H···Cl2D	0.94	3.729(2)	2.87	152
[a] Symmetry codes: A, 1–x, –y, –z; B, x, 1+y, z; C, 1.5–x, 0.5+y, 0.5–z; D, 1+x, y, z.				

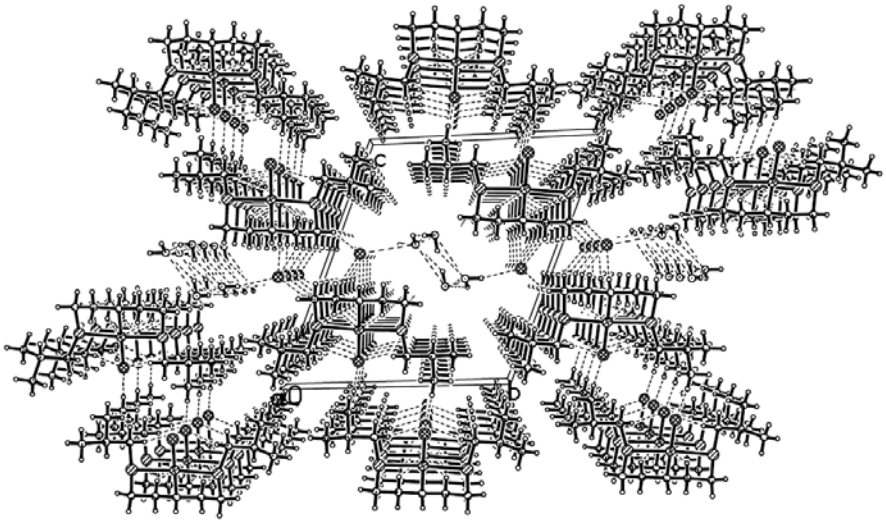

Figure S1 Molecular packing of **1** along the *a* direction, in which indicated the supramolecular network of the cationic pincers and the water ladder connected by the anionic Cl^- ions.

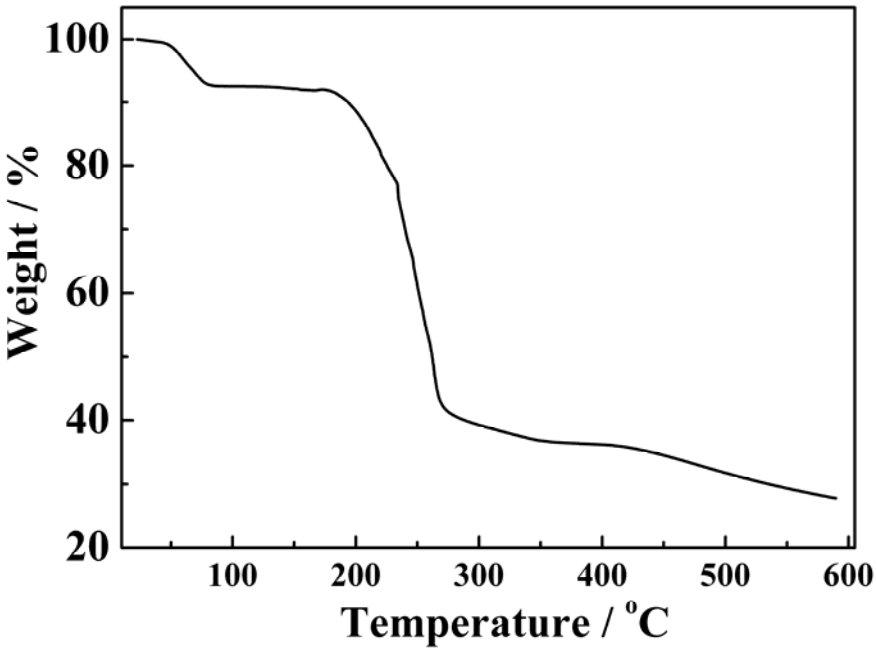

Figure S2 TGA diagram of complex **1**.