

Supporting Information

for

Pd₂L₂ metallacycles as molecular container for small molecules

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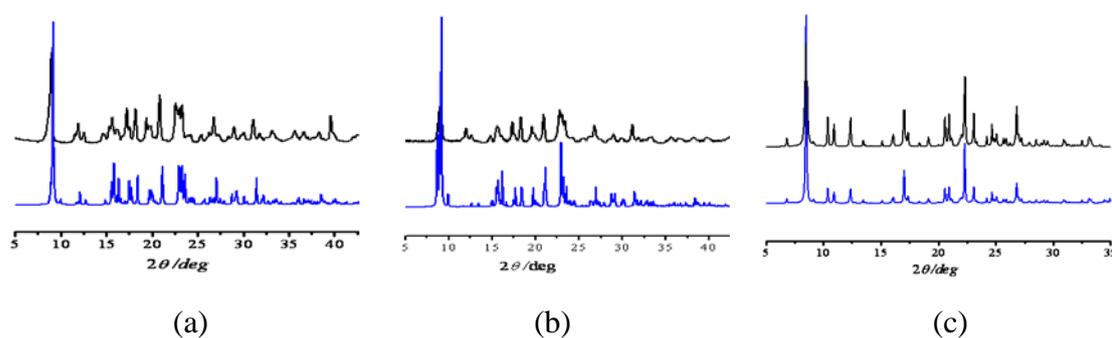


Figure S1. The simulated X-ray powder diffraction patterns (lower) and the measured ones (upper) for: (a) **1**, (b) **2** and (c) **5**.

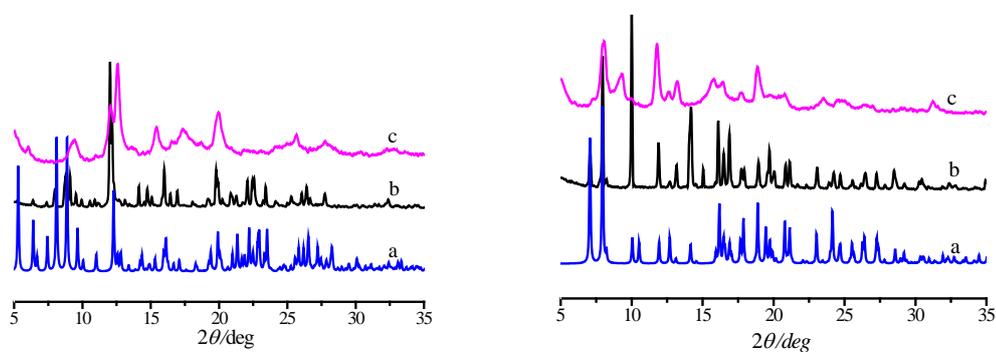


Figure S2. The simulated X-ray powder diffraction patterns and the measured ones for **3** (left) and **4** (right): (a) simulated pattern, (b) measured for the freshly synthesized crystals, and (c) measured for the grinded crystals or long air exposed crystals.

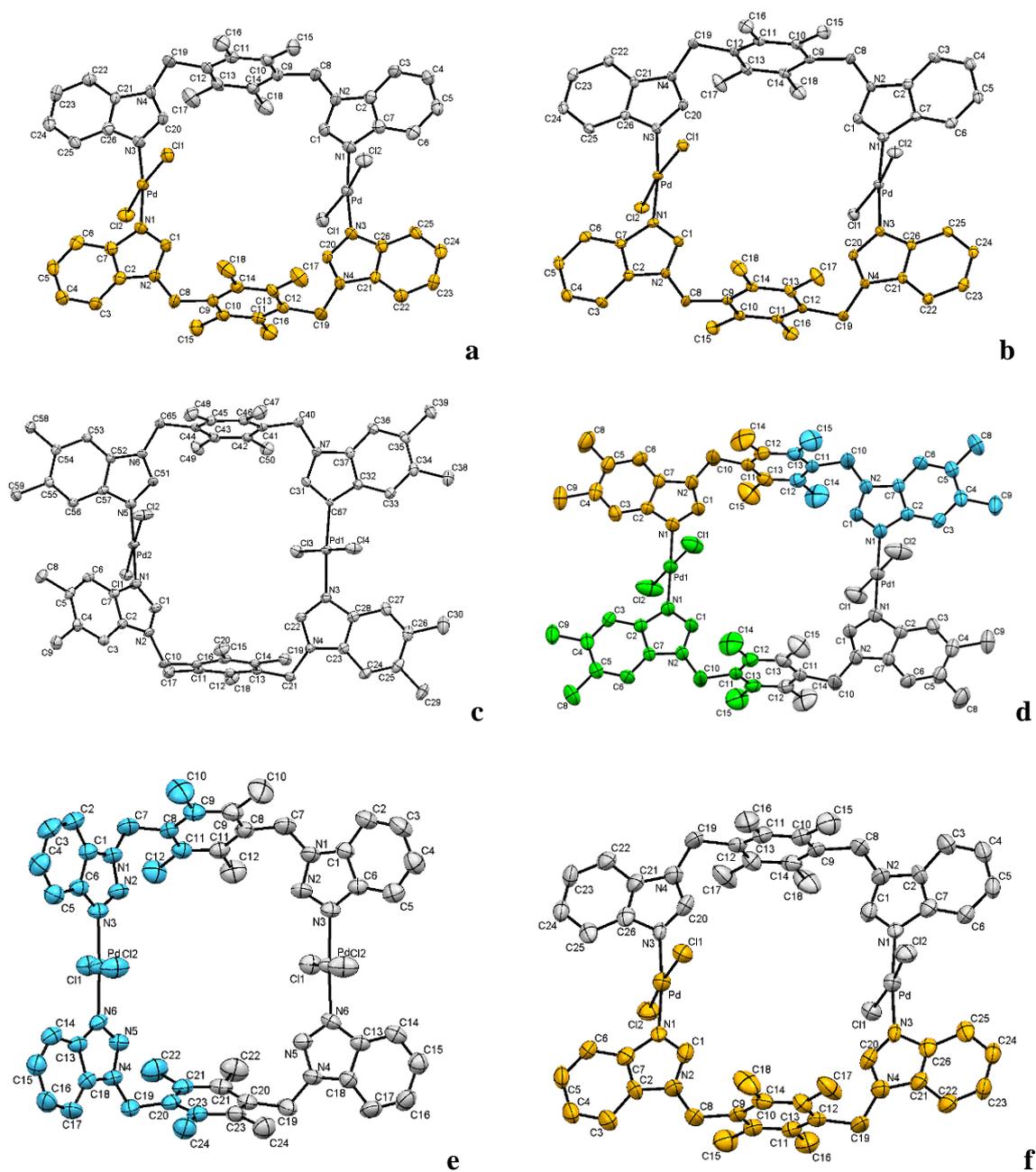


Figure S3 Ortep view of crystal structures showing atomic labeling scheme and asymmetric unit differentiated by colors: (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5** and (f) **1'**. H atoms and solvated molecules are omitted for clarity.

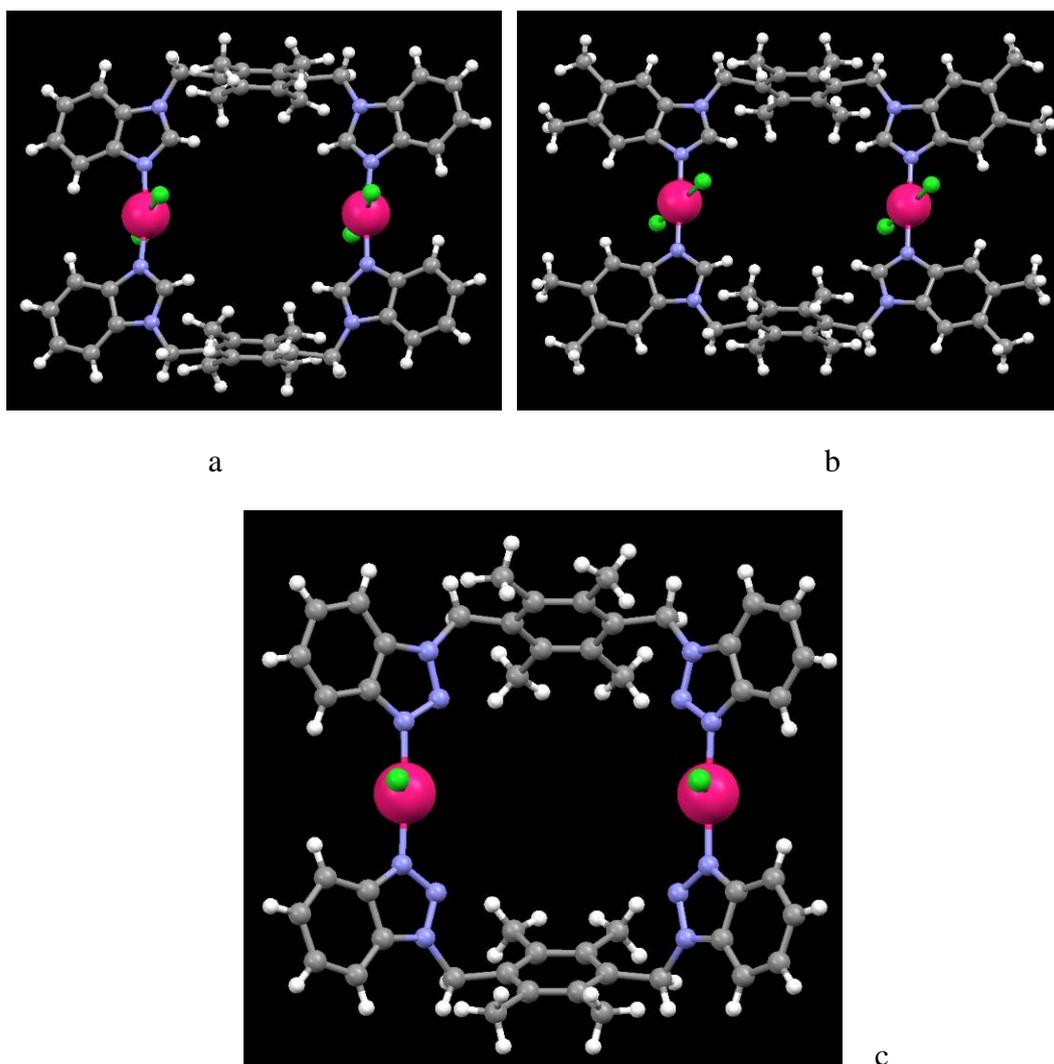


Figure S4 Crystal structures showing orientation relationship between the benzimidazole rings and the bridging phenyl ring in **1** (a) and **4** (b), and between the benzotriazole rings and the bridging phenyl ring in **5** (c).

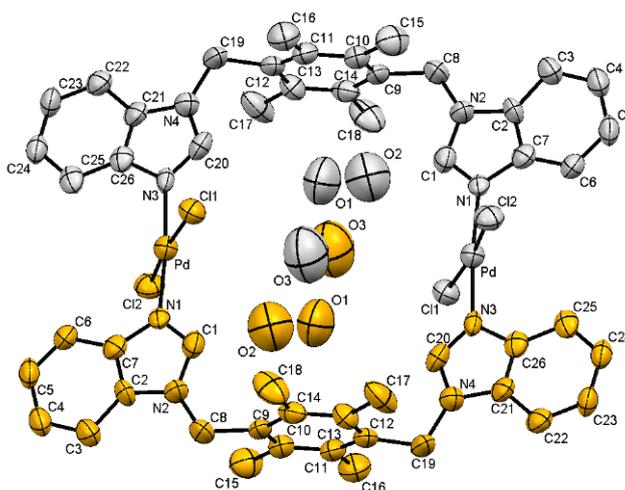


Figure S5 Crystal structure of **1a** showing rectangular box where water molecules are located. The asymmetric units are differentiated by colors

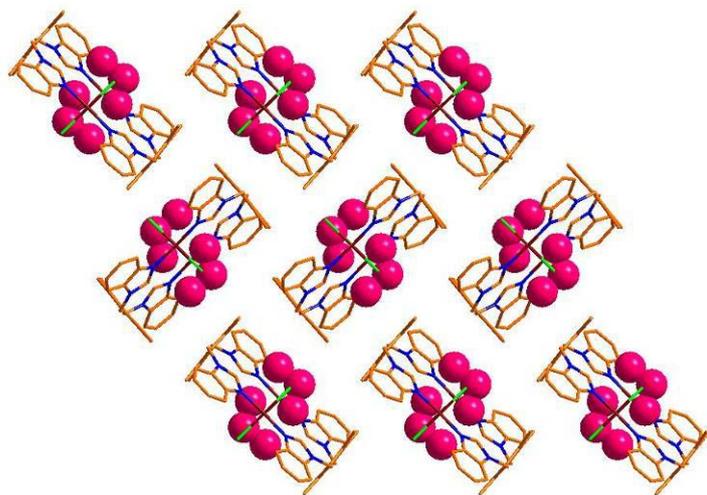


Figure S6. Crystal packing viewed along *c*-axis for **1**.

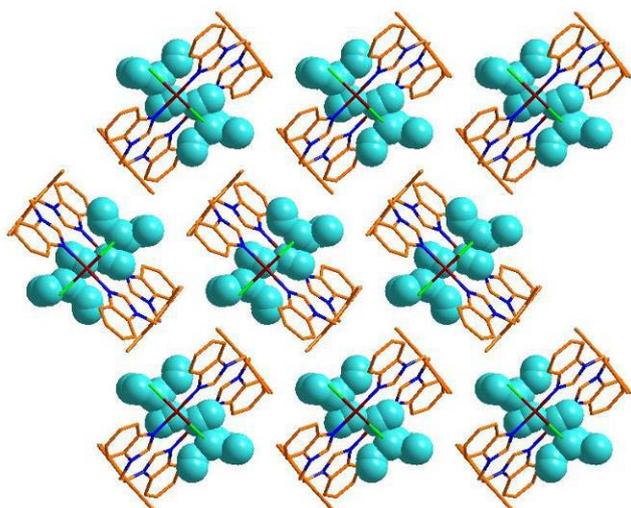


Figure S7. Crystal packing viewed along *c*-axis for **2**.

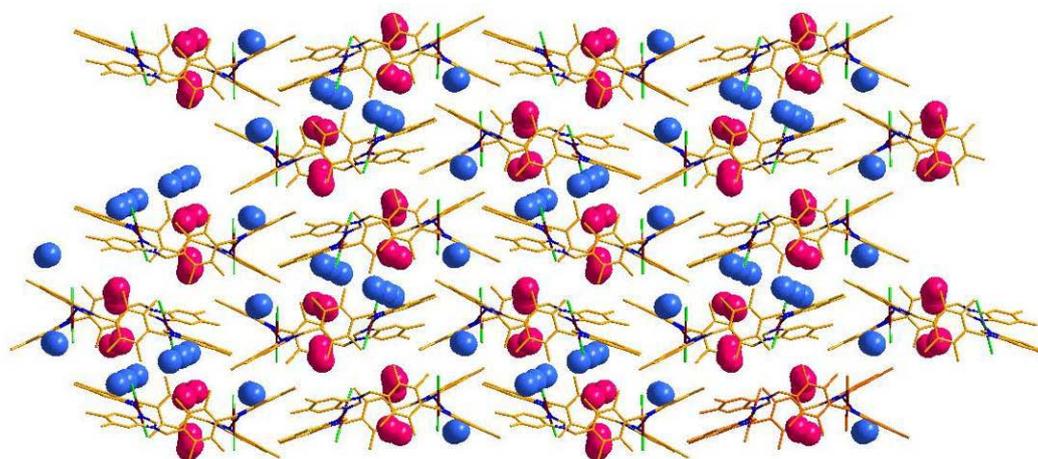
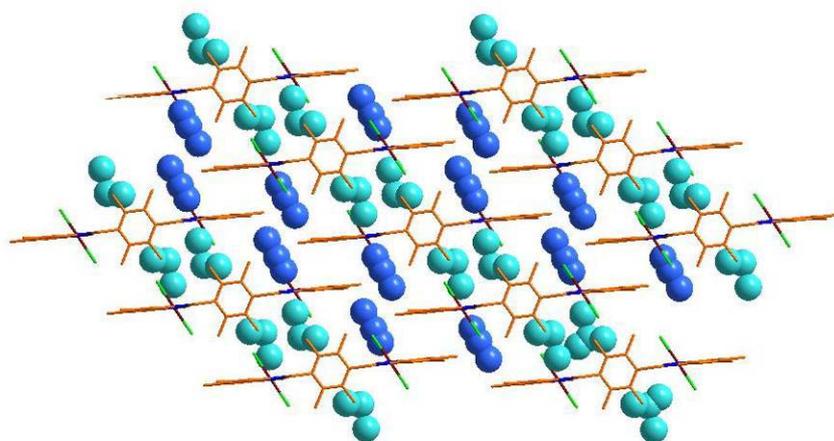
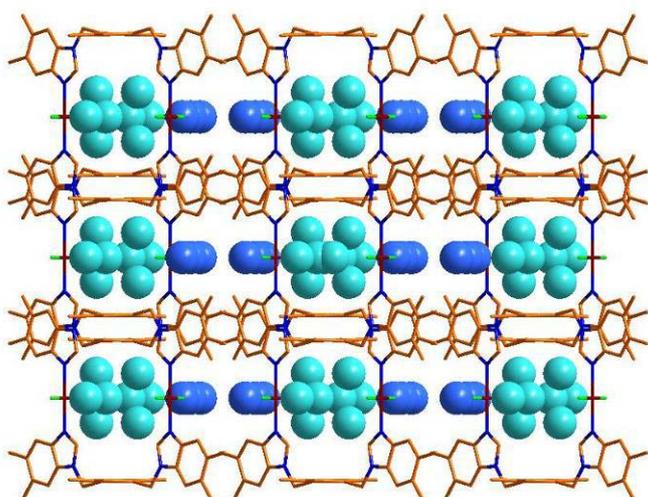


Figure S8. Crystal packing viewed along *a*-axis for **3**.



a



b

Figure S9. Crystal packing viewed along *b*-axis (a) and *a*-axis (b) for **4**.

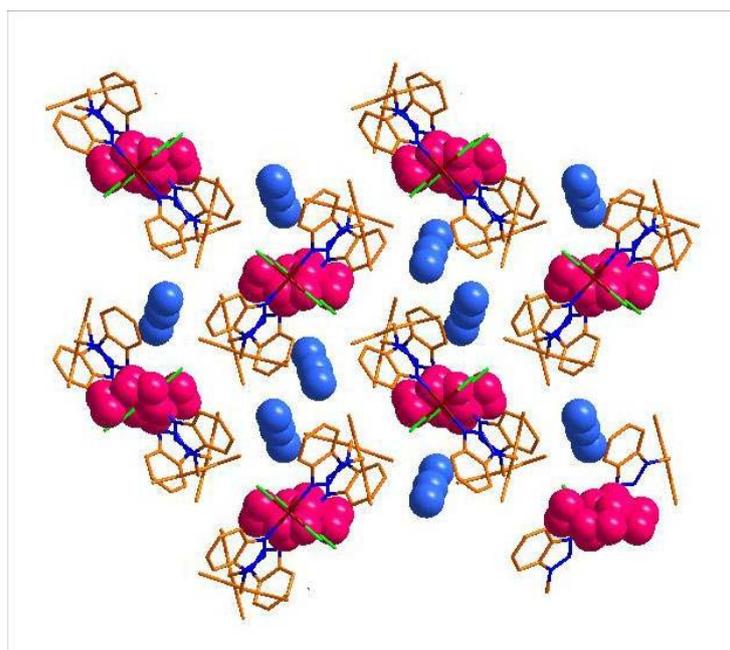


Figure S10. Crystal packing viewed along *b*-axis for **5**.

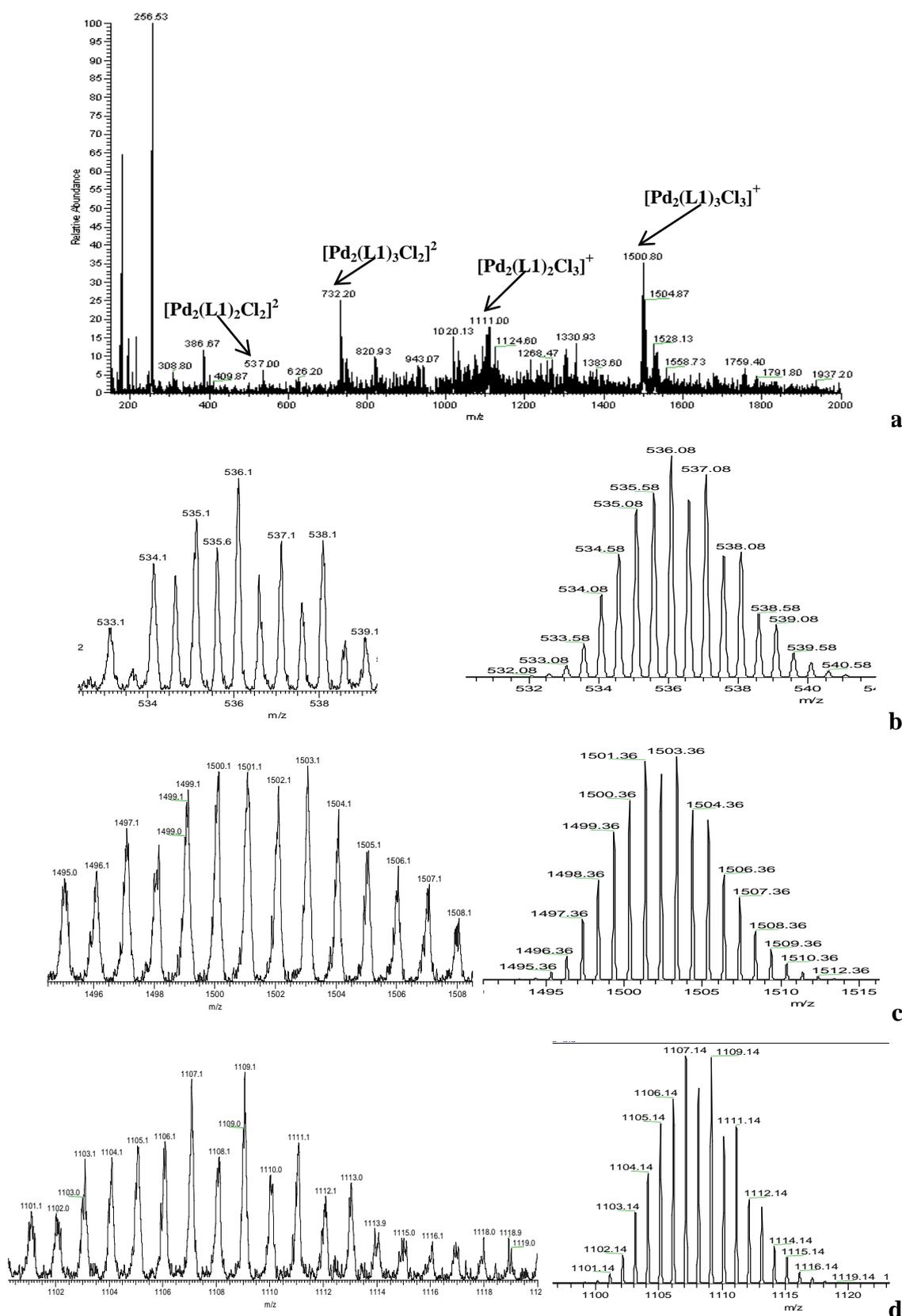


Figure S11. ESI-MS spectrum of **1** (a) and isotopic distributions of selected peaks shown together with simulations for $[\text{Pd}_2(\text{L}1)_2\text{Cl}_2]^{2+}$ (b), $[\text{Pd}_2(\text{L}1)_3\text{Cl}_3]^+$ (c) and $[\text{Pd}_2(\text{L}1)_2\text{Cl}_3]^+$ (d).

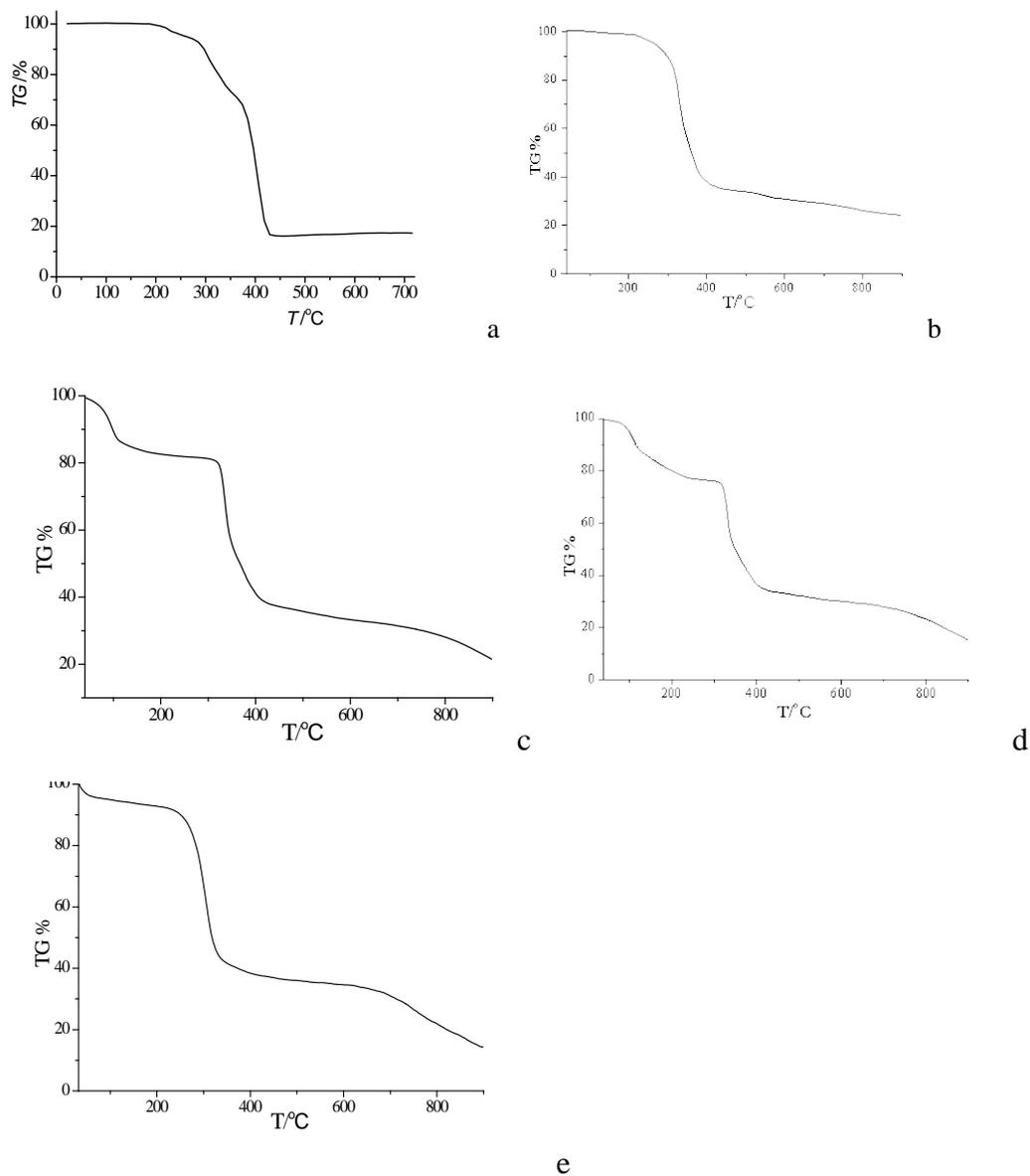


Figure S12. TG curves for a) 1, b) 2, c) 3, d) 4 and e) 5.

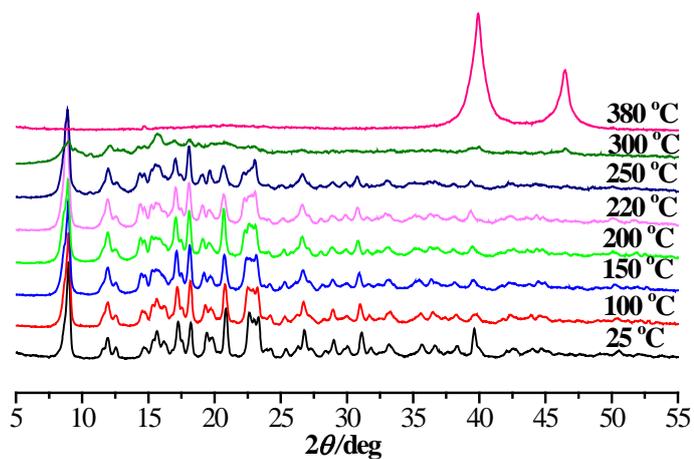


Figure S13. Variable-temperature PXRD spectra of 1.