

**Supplementary Information for
Self-Assembled Coordination Cage Enhances Reactivity of Confined
Amides via Mechanical Bond-Twisting**

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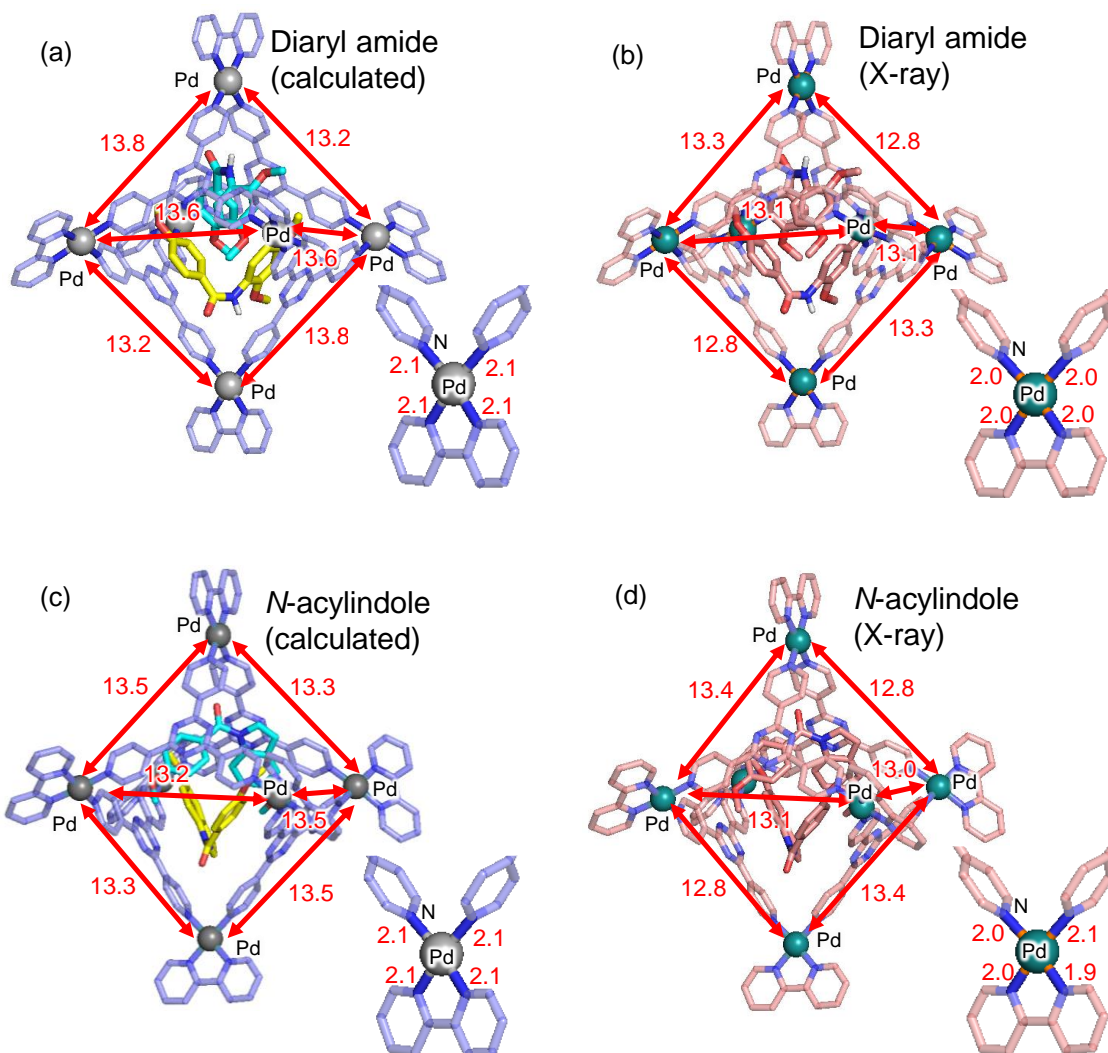


Fig. S1. Pd-Pd and Pd-N distances (\AA) in the octahedral coordination cage which encapsulates (a)(b) two diaryl amides and (c)(d) two *N*-acylindole (a)(c) as calculated by DFT-(B3LYP-D3)-QM/MM/PCM and (b)(d) as determined by X-ray diffraction.

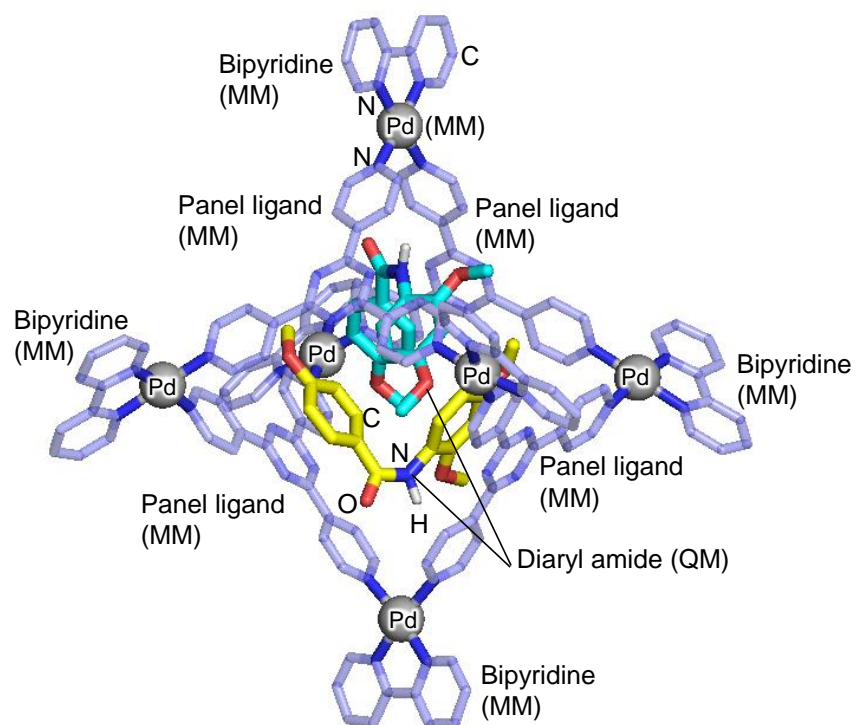


Fig. S2. QM and MM regions of the amide-confined cage. The amide molecules are included in the QM regions. The panel ligands, bipyridine, and Pd are included in the MM region.