Reaction-network-based analysis and prediction on the coordination self-assembly of Pd_3L_6 double-walled triangle

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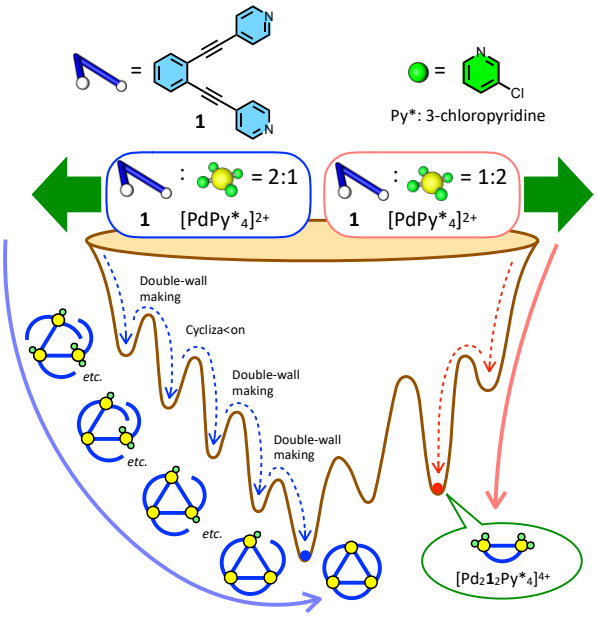
The self-assembly process of the $[Pd_3\mathbf{1}_6]^{6+}$ double-walled triangle (DWT)[1] was analyzed by our developed numerical analysis of self-assembly system (NASAP), which has already succeeded in obtaining detailed information of several coordination self-assemblies[2-6]. The self-assembly of the DWT, which takes place in a complicated reaction network consisting of multiple inter- and intramolecular reactions (oligomerization, cyclization, and double-wall making), is a good example not only to reveal general principles underlying complicated molecular self-assembly but also *to demonstrate the power of numerical simulation to predict a suitable reaction condition under which a new molecular self-assembly is produced under kinetic control.* The reaction network for the DWT composed of 161 chemical species that are connected by total 896 elementary reactions classified into 9 types of reversible reactions was established by the numerical search of 18-dimensional parameter space so that the time-development of the species would reproduce the corresponding experimental data obtained by quantitative analysis of self-assembly system (QASAP)[7]. NASAP led to the dominant reaction pathways, which are determined by the balance between inter- and intramolecular reactions. Besides, the numerical simulation predicted the formation of $[Pd_2\mathbf{1}_2Py^*_4]^{4+}$ as a major product (#%) from **1** and $[PdPy^*_4]^{2+}$ in a 1:2 ratio under kinetic control, which was consistent with the experimental result (#%).



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