Supplementary Information

A Highly Efficient Supramolecular Adsorbent for Precious Metal: Adsorption Behavior of PdII by Melamine Cyanurate

D. Nagai,* and T. Kimoto

The XRD pattern of the separated Pd was consistent with that in the literature,[1] although the crystallinity decreased (Figure S1).
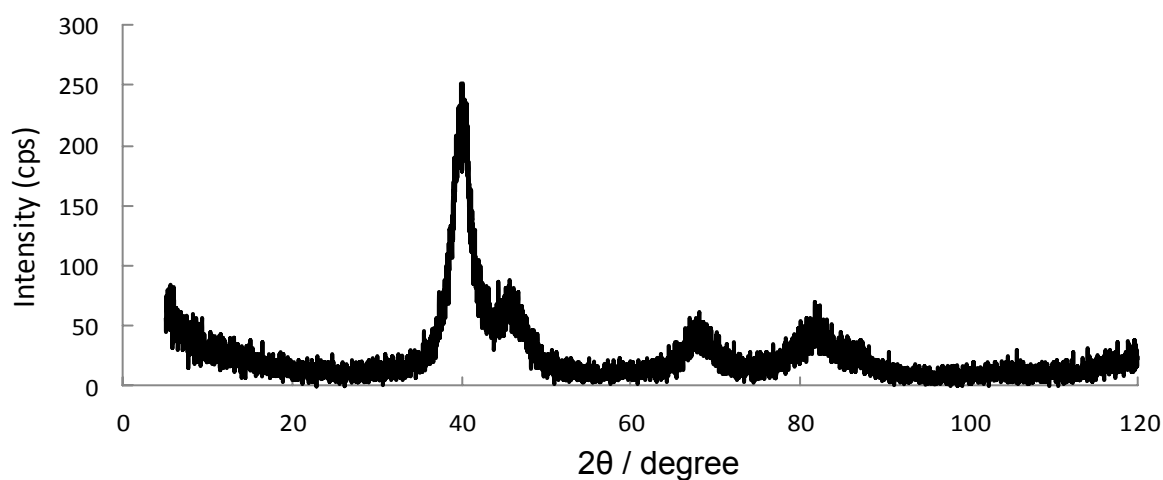

Figure S1. XRD spectrum of the separated Pd.

Reference

1. C. C. Tseng, Y. H. Lin, Y. Y. Shu, C. J. Chen, and M. D. Ger *J. Taiwan Inst. Chem. E.* 2011, **42**, 989-995.

After adsorption of Pd^{II} by M-CA, the filtrate was concentrated by reduced pressure. The residue (10 mg) and 1,4-dioxane (2 μL) were dissolved in DMSO-d_6, and its ^{1}H NMR measurement was carried out. Based on the integral ratio of CA and 1,4-dioxane, the amount of CA in the residue was estimated. From the amount of CA and adsorption amount, the amount of M in the residue was estimated.
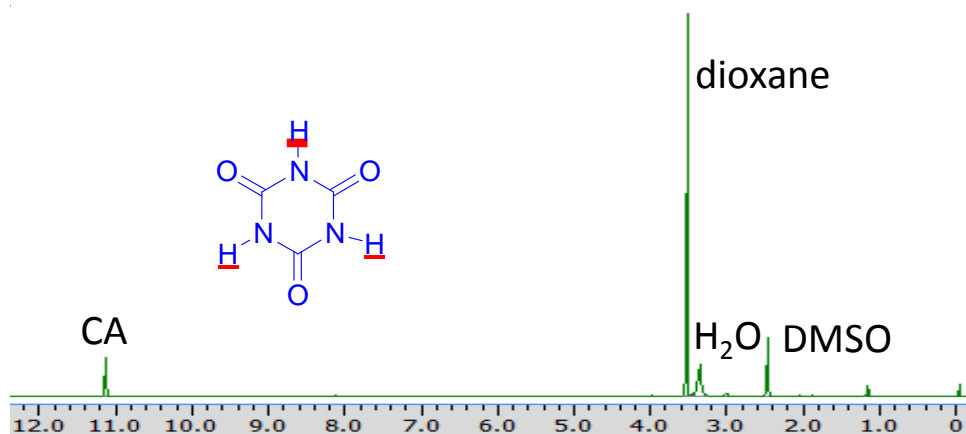

Figure S2. ^{1}H NMR spectrum (DMSO-d_6, rt) of the eluted residue in the filtrate obtained from Table 5, entry 4.

Table S1. Comparison of calculated potential energies and bond energies for M-CA, PdCl$_2$-M complex, and PdCl$_2$-CA complex.

	Basis set		potential energy (Hartree)	bond energy	
				(Hartree)	(kcal/mol)
M	6-31G		-446.51115	–	–
CA	6-31G		-506.13728	–	–
M-CA	6-31G		-952.68208	-0.03365	-21.1
PdCl$_2$	6-31G	SDD	-1048.29707	–	–
PdCl$_2$-M	6-31G	SDD	-1494.90257	-0.09435	-59.2
PdCl$_2$-CA	6-31G	SDD	-1554.49037	-0.05602	-35.2