

Addition/Correction

A Palladium-Oxo Complex. Stabilization of This Proposed Catalytic Intermediate by an Encapsulating Polytungstate Ligand [*J. Am. Chem. Soc.* 2005, 127, 11948–11949].

Travis M. Anderson, Rui Cao, Elena Slonkina, Britt Hedman, Keith O. Hodgson, Kenneth I. Hardcastle, Wade A. Neiwert, Shaoxiong Wu, Martin L. Kirk, Sushilla Knottenbelt, Ezra C. Depperman, Bineta Keita, Louis Nadjjo, Djamaladdin G. Musaev, Keiji Morokuma, and Craig L. Hill

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A Palladium-Oxo Complex. Stabilization of This Proposed Catalytic Intermediate by an Encapsulating Polytungstate Ligand [*J. Am. Chem. Soc.* **2005**, *127*, 11948–11949]. Travis M. Anderson, Rui Cao, Elena Slonkina, Britt Hedman, Keith O. Hodgson, Kenneth I. Hardcastle, Wade A. Neiwert, Shaoxiong Wu, Martin L. Kirk, Sushilla Knottenbelt, Ezra C. Depperman, Bineta Keita, Louis Nadjo, Djamaladdin G. Musaev, Keiji Morokuma, and Craig L. Hill*

In the originally submitted crystallographic file (CIF, Supporting Information) of the complex $K_{10}Na_3[Pd(O)(OH)P_2W_{19}O_{69}(OH_2)] \cdot 16H_2O$ (**2**), one of the potassium cations, K9, had short distances to K10 and four oxygens (O29, O34, O39, and O40) on the polyanion unit. We have now collected a new X-ray single-crystal diffraction dataset, and in our new refinement the original K9 is assigned as the positionally disordered W19B (Figure 1). Here we submit the new CIF file with the corrected assignment of the K9 site.

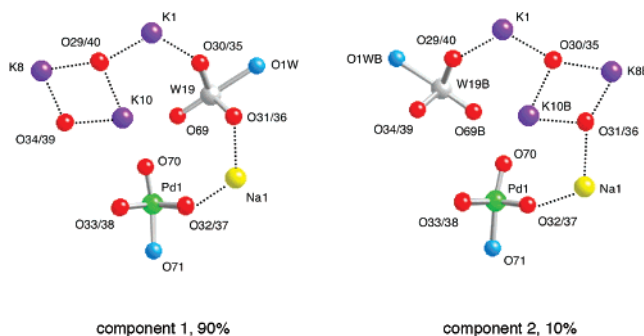


Figure 1. Atomic arrangement in the central belt of the polyanion in **2**, illustrating that the bridging $[O=W^{VI}(OH_2)]^{4+}$ unit, W19, is disordered between two sites, component 1 (left, 90%) and component 2 (right, 10%).

Importantly, as noted in the original publication, only one peak is observed in the ^{31}P NMR spectrum, strongly suggesting that the two components are equivalent in solution because of fast cation exchange. This positional disorder of W19 does not change the central conclusions in this publication, including the existence of the terminal Pd-oxo unit and its corroboration by Pd EXAFS, ^{17}O NMR, and other techniques.

Supporting Information Available: New CIF file for **2** with corrected assignment of the K9 site. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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