

2005, Volume 44

Patrick Frank,* Maurizio Benfatto, Robert K. Szilagyi, Paola D'Angelo, Stefano Della Longa, and Keith O. Hodgson: The Solution Structure of $[\text{Cu}(\text{aq})]^{2+}$ and Its Implications for Rack-Induced Bonding in Blue Copper Protein Active Sites

Pages 1922–1933. In the original document, one set of transverse angles for the final MXAN structure of $[\text{Cu}(\text{H}_2\text{O})_5]^{2+}$ was misreported as 17° . The correct angle is 5° . Therefore, in the abstract, in Table 1, in the legend to Figure 4, on p 1926, column 1, and on p 1928, column 2, where “ 17° ” or “ $\pm 17^\circ$ ” appears, the correct rendering should be $+5^\circ$, -17° .

In the table “CuW5 B38HFP86/BS5 MXAN Structure” in the Supporting Information, describing the final MXAN structure of $[\text{Cu}(\text{H}_2\text{O})_5]^{2+}$, the *xyz* coordinates for one of the hydrogen atoms is missing. The complete coordinates are as follows:

Table 1

Cu	0.000000	0.000000	0.000000
O	-0.093900	1.899980	-0.563090
O	0.114110	-1.886460	-0.605540
O	-1.940070	-0.104210	0.166850
O	1.936070	0.087390	0.226640
O	-0.050180	-0.068240	2.353310
H	0.933910	-2.300070	-0.911450
H	2.357460	0.093800	1.098330
H	-2.382200	-0.171950	1.025660
H	-0.632810	-2.398060	-0.947310
H	-0.904170	2.371250	-0.802590
H	0.663660	2.466810	-0.766450
H	-2.618230	-0.091060	-0.524310
H	2.623120	0.214890	-0.444000
H	0.034420	-0.858720	2.903390
H	-0.178410	0.675690	2.957130

Note that this listing differs from the published table only in the last set of hydrogen coordinates.

We thank Dr. Vyacheslav Bryantsev, Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA, for bringing these errors to our attention.

Neither error materially affects the science or the conclusions of the work.

IC701524X

10.1021/ic701524x

Published on Web 08/08/2007