

**Correction to Photochemistry of *trans*-Cr(cyclam)(ONO)<sub>2</sub><sup>+</sup>, a Nitric Oxide Precursor** [*Inorganic Chemistry* 2011, 50, 4453–4462 DOI: 10.1021/ic200094x]. Alexis D. Ostrowski, Ryan O. Absalonsen, Malcolm A. De Leo, Guang Wu, James G. Pavlovich, Janet Adamson, Bilal Azhar, Alexei V. Iretskii, Ian L. Megson, and Peter C. Ford\*

Pages 4459 and 4461. The crystal structure reported in Figure 5 of this manuscript and in Tables S-1–S-6 and Figure S-1 of the accompanying Supporting Information as the *trans*-dioxo complex *trans*-[Cr(cyclam)(O)<sub>2</sub>](ClO<sub>4</sub>)·H<sub>2</sub>O (cyclam is 1,4,8,11-tetraazacyclotetradecane) is apparently incorrect.

Discrepancies in the structure were pointed out to us by Professor John T. Groves of Princeton University, who suggested that our reported structure was more consistent with the *trans*-difluoro analogue. The material for which this structure was determined was isolated after exhaustive photolysis of the *trans*-Cr(cyclam)(ONO)<sub>2</sub><sup>+</sup> cation. Crystals formed by the addition of sodium perchlorate and a slow evaporation of the solution. This material, when redissolved in acetonitrile, displayed a strong room temperature electron paramagnetic resonance spectrum consistent with the presence of a 3d<sup>1</sup> Cr(V) complex, and a crystal chosen from this product gave the structure reported. We did not consider the possibility of the difluoro complex but agree with Professor Groves' suggestion that fluorides might have originated with the BF<sub>4</sub><sup>-</sup> present as counterions to the *trans*-Cr(cyclam)(ONO)<sub>2</sub><sup>+</sup> cation.

In these contexts, we recalculated the structure by replacing the putative oxides by fluorides and found that the final *R* indices [*I* > 2σ(*I*)] improved from *R*1 = 0.0668 and *wR*2 = 0.1960 to *R*1 = 0.0595 and *wR*2 = 0.1716 (details are shown in the Supporting Information). Furthermore, the newly calculated structure gives Cr–F bonds nearly identical with those reported for the analogous *trans*-[Cr([15]aneN<sub>4</sub>)F<sub>2</sub>](ClO<sub>4</sub>)·H<sub>2</sub>O ([15]aneN<sub>4</sub> = 1,4,8,12-tetraazacyclopentadecane).<sup>1</sup> In this context, we conclude that the structure reported in Figure 5 and refined in the attached Supporting Information is indeed that of *trans*-[Cr(cyclam)F<sub>2</sub>](ClO<sub>4</sub>)·H<sub>2</sub>O.

## ■ ASSOCIATED CONTENT

**S Supporting Information.** Two figures and six tables describing the structure solved as the difluoro complex. This material is available free of charge via the Internet at <http://pubs.acs.org>.

## ■ ACKNOWLEDGMENT

We thank Professor John T. Groves and his co-workers at Princeton University for pointing out the discrepancies in the reported structure.

## ■ REFERENCES

(1) Choi, J. H.; Oh, I.-G.; Ryoo, K. S.; Lim, W.-T.; Park, Y. C.; Habibi, M. H. *Spectrochim. Acta A* 2006, 65, 1138–1143.

DOI: 10.1021/ic200888n

Published on Web 05/16/2011