Inorg. Chem. **2004**, *43*, 6858

Inorganic Chemistry
Additions and Corrections

2003, Volume 42

Tiqing Liu,* Timothy Lovell,* Wen-Ge Han, and Louis Noodleman*: DFT Calculations of Isomer Shifts and Quadrupole Splitting Parameters in Synthetic Iron–Oxo Complexes: Applications to Methane Monoxygenase and Ribonucleotide Reductase

Page 5248. There are errors in the third column [quadrupole splitting (QS) parameter comparisons] in Table 2. The SD (standard deviation of the fitting) and the error bar for α and *C* require modification. The fitting for QS comparisons was originally done with an older version of ORIGIN (data analysis and graphing software from OriginLab Corporation). It has since been found that there are discrepancies between the fittings made by ORIGIN 5.0 or later and those made by the older version used for this paper. The published and corrected fitting parameters are listed in the table below. The standard deviation for the linear fitting of the experimental quadrupole splitting parameters (QS) vs the calculated QS stated in this paper should be corrected from 0.12 to 0.30 mm s^{-1}. This correction and others comparing the "published" and "old ORIGIN" columns are due to copying errors. There are no corrections for the second column (IS fittings) of Table 2. The IS fitting was redone with ORIGIN 5.0 or later. We thank Dr. Victor Nemykin for finding these errors.

Corrections for QS Comparisons in Table 2

parameter	published	old ORIGIN	ORIGIN 5.0
α	0.96 ± 0.03	0.96 ± 0.06	0.93 ± 0.05
C	0.12 ± 0.02	0.12 ± 0.09	0.04 ± 0.09
r	0.95	0.95	0.95
SD	0.12	0.30	0.30
N	36	36	36

IC0401041

10.1021/ic0401041
Published on Web 09/22/2004