Inorganic Chemistry

ADDITION/CORRECTION

pubs.acs.org/IC

Correction to Density Functional Theory Calculations on Mössbauer Parameters of Nonheme Iron Nitrosyls [*Inorganic Chemistry* **2009**, *48*, 9155–9165 DOI: 10.1021/ic9008784]. Kathrin H. Hopmann, Abhik Ghosh,* and Louis Noodleman*

Page 9163. In Table 4, the $\{FeNO\}^7$ and $\{Fe(NO)_2\}^9$ labels to the rows for $[Fe(NO)_2\{Fe(NO)(N(CH_2CH_2S)_3)\}$-*S*,*S*′] were inadvertently reversed. Thus, it is the $\{FeNO\}^7$ unit that possesses an experimental isomer shift of 0.37 mm s^{-1} at 77 K (and predicted values of 0.39−0.40 mm s^{-1}). Likewise, the $\{Fe(NO)_2\}^9$ unit actually possesses an experimental isomer shift of 0.18 mm s^{-1} at 77 K (and a predicted value of 0.19 mm s^{-1}).

DOI: 10.1021/ic200575z
Published on Web 03/31/2011