Additions and Corrections

1999, Volume 38

Takafumi Yoshida, Takayoshi Suzuki, Kan Kanamori, and Sumio Kaizaki*: Synthesis, Magnetic Properties, and Electronic Spectra of Octahedral Mixed-Ligand $(\beta$ -Diketonato)nickel(II) Complexes with a Chelated Nitronyl Nitroxide Radical.

Pages 1064, 1066, and 1067. We made reverse assignments to two doublet-doublet MLCT, because the formulation for the MLCT transition energies should be $30(\chi(\text{Ni}) - \chi(\text{NIT})) +$ (5/3)D + (6/5)D' for $E(t_{2g} \rightarrow \pi^*)$ and $30(\chi(\text{Ni}) - \chi(\text{NIT})) - \Delta$ + (5/3)D + (6/5)D' for $E(e_g \rightarrow \pi^*)$.

Page 1064. The last paragraph continuing on the next page should be replaced with the following, though the first sentence remains unchanged:

There are three possible MLCT transitions: two $t_{2g} \rightarrow \pi^*$ transitions (doublet-doublet and quartet-quartet) and one eg $\rightarrow \pi^*$ doublet-doublet transition (Scheme 1). In the doubletdoublet MLCT for octahedral Ni(II) complexes, the transition energy is estimated to be $30(\chi(\text{Ni}) - \chi(\text{NIT})) + (5/3)D + (6/5)D'$ for $E(t_{2g} \rightarrow \pi^*)$ and $30(\chi(\text{Ni}) - \chi(\text{NIT})) - \Delta + (5/3)D$ + (6/5)D' for $E(e_g \rightarrow \pi^*)$, where $\chi(Ni)$ and $\chi(NIT)$ refer to the optical electronegativity for nickel(II) and the NIT2-py ligand, respectively: Δ is the energy splitting between the t_{2g} and e_g orbitals; (5/3)D is the change in the spin pairing energies from the $d^8(S=1)$ to the $d^7(S=1/2)$ electron configurations, and (6/5)D' corresponds to that from the $p^1(S=1/2)$ to $p^2(S=0)$ one.^{36,37} The energy difference between two doublet-doublet MLCT $(E(t_{2g} \rightarrow \pi^*) - E(e_g \rightarrow \pi^*))$ is given by Δ and approximated to ca. 9800 and 10500 cm⁻¹ for the bis(acac) and mono(acac) complexes, respectively, since Δ are estimated from the first spin-allowed band position. Therefore, the lower energy MLCT components around 16.0–19.0 \times 10³ cm⁻¹ and the shoulder around 25.0×10^3 cm⁻¹ are due to the e_g $\rightarrow \pi^*$ and the $t_{2g} \rightarrow \pi^*$ MLCT transitions, respectively.

Page 1066. The assignments to the MLCT in Figure 11 should be corrected in such a way that the $t_{2g} \rightarrow \pi^*$ and $e_g \rightarrow \pi^*$ are exchanged as shown in the revised Figure 11.

Page 1067. As a result, "the $t_{2g}-\pi^*$ in line 6 should read "the $e_g-\pi^*$ ".

This correction for the MCLT assignment could give no change of the subsequent discussion.

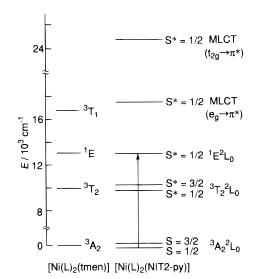


Figure 11. Energy levels of the spin-allowed and spin-forbidden d-d transitions in the β -diketonato Ni(II) complexes with NIT2-py.

IC9907415

10.1021/ic9907415 Published on Web 12/13/1999

1999, Volume 38

James Bourassa, Brian Lee, Stefan Bernhard, Jon Schoonover, and Peter C. Ford*: Flash Photolysis Studies of Roussin's Black Salt Anion: $Fe_4S_3(NO)_7^-$.

Page 2947. There was a spelling error in the name of one of the authors (Stefan Bernhard). The correct list of authors should be as follows: James Bourassa, Brian Lee, Stefan Bernhard, Jon Schoonover, and Peter C. Ford.

IC991193Y

10.1021/ic991193y Published on Web 11/12/1999