

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 (β -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 $e_g \rightarrow \pi^*$ doublet–doublet transition (Scheme 1). In the doublet–doublet 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 $\chi(\text{Ni})$ and $\chi(\text{NIT})$ 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 $\times 10^3 \text{ cm}^{-1}$ and the shoulder around 25.0 $\times 10^3 \text{ cm}^{-1}$ 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 $t_{2g} \rightarrow \pi^*$ in line 6 should read “the $e_g \rightarrow \pi^*$ ”.

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

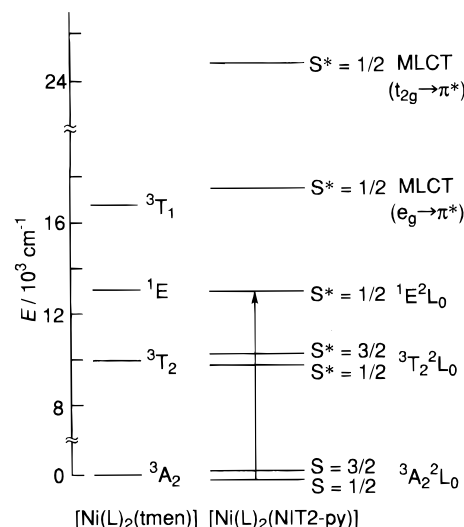


Figure 11. Energy levels of the spin-allowed and spin-forbidden d–d transitions in the β -diketonato Ni(II) complexes with NIT2-py.

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: $\text{Fe}_4\text{S}_3(\text{NO})_7^-$.

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