

# Additions and Corrections

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**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  $E(e_g \rightarrow \pi^*)$ .

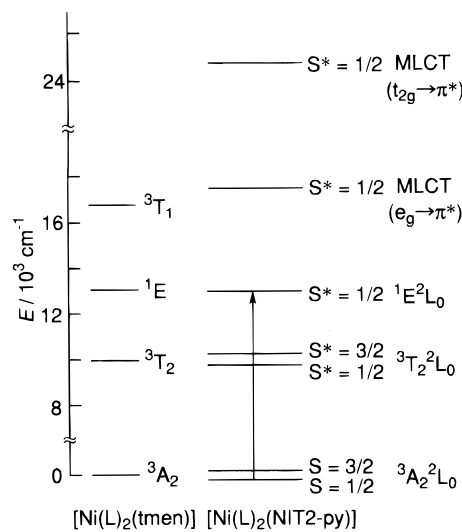
Page 1064. The last paragraph continuing on the next page should be replaced with the following, though the first sentence remains unchanged:

There are three possible MLCT transitions: two  $t_{2g} \rightarrow \pi^*$  transitions (doublet–doublet and quartet–quartet) and one  $e_g \rightarrow \pi^*$  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;  $\Delta$  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.<sup>36,37</sup> The energy difference between two doublet–doublet MLCT ( $E(t_{2g} \rightarrow \pi^*) - E(e_g \rightarrow \pi^*)$ ) is given by  $\Delta$  and approximated to ca. 9800 and 10500  $\text{cm}^{-1}$  for the bis(acac) and mono(acac) complexes, respectively, since  $\Delta$  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  $\beta$ -diketonato Ni(II) complexes with NIT2-py.

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**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.

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