Acetylacetonate Protons.—For these resonances[24] both the $G(\theta,r)$ and $G'(\theta,\Omega,r)$ terms contribute to the dipolar shifts as is indicated in Table II. Inspection of the derived values of $\Delta\nu_{\mathrm{Co}}^{\mathrm{con}}$ shows that they do not even qualitatively agree with the $\Delta\nu_{\mathrm{Ni}}^{\mathrm{iso}}$ values. This implies that the mode of spin delocalization does differ for the acetylacetonato moiety between the cobalt and nickel systems. Such variation with a change in metal has been discussed by Eaton.[25]

Finally, it should be pointed out that a degree of non-Curie behavior is predicted for the dipolar shifts, based on the temperature variations of the principal molecular susceptibilities; however, the predicted deviations from a $1/T$ behavior for $\Delta\nu_{\mathrm{Co}}^{\mathrm{iso}}$ are small for the acac H and CH_3 protons over the temperature range accessible to solution measurements. Complications from the slowing of ligand exchange[26] render an experimental verification impossible for the pyridine nuclei.

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[24] G. N. La Mar, *J. Magn. Resonance*, **1**, 185 (1969).

[25] D. R. Eaton, *J. Amer. Chem. Soc.*, **87**, 3097 (1965).

[26] R. W. Kluiber, R. Kukla, and W. DeW. Horrocks, Jr., *Inorg. Chem.*, **9**, 1319 (1970).

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An Erroneous Conclusion Based on a Misinterpretation of the IUPAC Rules for Designating Absolute Configurations

Sir:

Unfortunately in a recent review article[1] on absolute configurations of transition metal complexes it was concluded that the suggested IUPAC rules for designating absolute configurations[2] did not appear to apply to polydentate ligand complexes. As an example it was pointed out that for the three isomers (+)-Co(en)$_3$$^{3+}$, (+)-Co(en)$_2$(NH$_3$)$_2$$^{3+}$, and (−)-Co(penten)$^{3+}$ (penten = $N,N,',N'$-tetrakis(2′-aminoethyl)-1,2-diaminoethane), shown in Figure 1, which should be configurationally related according to the reviewers,[3] the IUPAC nomenclature indicated that the designations for the three isomers should be Λ, Λ and Δ, respectively. Therefore, the last was not configurationally related to the first two. This is a misinterpretation of the IUPAC rules. The rules simply stated that in a case where a multidentate ligand is involved, all the Δ's and Λ's belonging to all the "skew-line pairs" be given. Thus, (−)-Co(penten)$^{3+}$ should be designated $\Delta\Delta\Lambda$. What, in fact, was referred to in this review article was the "ring-pairing" scheme upon which the IUPAC nomenclature is based.[4] In this scheme the complex would have been designated Δ since Δ pairs predominate over Λ pairs.[5]

More importantly, however, is that experimental evidence, both X-ray[6] and circular dichroism studies,[7] shows clearly that (+)-Co(en)$_3$$^{3+}$ and (+)-Co(en)$_2$(NH$_3$)$_2$$^{3+}$ are *not* configurationally related to (−)-Co(penten)$^{3+}$ as stated by the review article but to (+)-Co(penten)$^{3+}$, Figure 1.

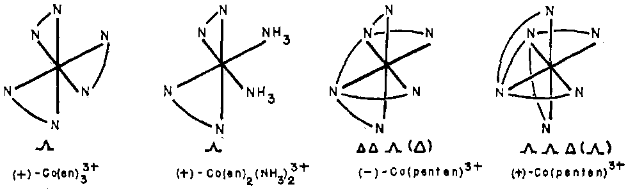

Figure 1.—Absolute configurations of complexes discussed in the text. Designation is that suggested by IUPAC. Designation in parentheses is that obtained by applying the "ring-pairing" scheme. (See text.)

It is important to note, then, that the IUPAC rules still appear to be useful[8] contrary to what was concluded.[1] It is clear that the rules leave something to be desired; but until a better scheme is developed, it is strongly urged that a serious effort be made to follow the IUPAC rules.

[1] R. D. Gillard and P. R. Mitchell, *Struct. Bonding (Berlin)*, **7**, 46 (1970).

[2] *Inorg. Chem.*, **9**, 1 (1970).

[3] The reviewers confused this issue by intermixing nomenclatures at this point and in the review in general although some attempt was made to justify this when nomenclatures were discussed.

[4] J. I. Legg and B. E. Douglas, *J. Amer. Chem. Soc.*, **88**, 2697 (1966).

[5] Note that the suggested IUPAC nomenclature is equivalent to selecting the C_3 axis defined by three chelate rings as in Co(en)$_3$$^{3+}$ whereas ref 4 used the C_2 axis defined by the two chelate rings constituting the ring pair. Designations change in going from one reference axis to the other. See ref 4 for clarification.

[6] F. Muto, F. Marumo, and Y. Saito, *Inorg. Nucl. Chem. Lett.*, **5**, 85 (1969).

[7] S. F. Mason and B. J. Peart, *ibid.*, **5**, 491 (1969).

[8] A recent crystallographic study of $(+)_{5461}$-Co(TRI)$_2$I$_3$ (TRI = tribenzo[b,f,j][1,5,9]triazocycloduodecine), a complex which cannot be "configurationally related" to Co(en)$_3$$^{3+}$ (it has no "ring pairs") but yet has a CD spectrum very similar to that of Co(en)$_3$$^{3+}$ (R. M. Wing and R. Eiss, *J. Amer. Chem. Soc.*, **92**, 1929 (1970)), strongly supports the trigonal twist model (T. S. Piper and A. G. Karipides, *Inorg. Chem.*, **4**, 923 (1965)) and suggests that the "ring-pairing" scheme and consequently the IUPAC rules may be limited to complexes with constraining ligands (*i.e.*, those for which ligand–metal–ligand bond angles are expected to be less than 90° such as for five-membered ring systems which are the most commonly encountered chelates).

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