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Short Communications

Corrigenda and Addenda to "Conformational Analysis of Coordination Compounds. I. Tris-diamine Cobalt(III) Complexes with Three Six-membered Chelate Rings"[1]

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Due to our misinterpretation of Jurnak and Raymond's nomenclature,[2] as put forward in their manuscript made available to us prior to publication, two pairs of conformers were interchanged in the last column of Table 1 (Ref. 1, p. 625). Entries 8 to 11 should read as follows:

8	*anti*-chair$_2$lel	C_2	paδ
9	*syn*-chair$_2$lel	C_2	apδ
10	*anti*-chair$_2$ob	C_2	paλ
11	*syn*-chair$_2$ob	C_2	apλ

For the same reason the conformer mentioned in the fifth line of the *Note added in proof* (Ref. 1, p. 624) should read *syn*-chair$_2$lel instead of *anti*-chair$_2$lel, and consequently, the statement in the conclusion of the same sentence, namely that the conformation of Cr tn$_3$ found by Jurnak and Raymond in [Cr tn$_3$][Ni(CN)$_5$].2H$_2$O corresponds to one of those shown by our conformational calculations to have a low potential energy, is incorrect. In fact, the conformation found (a highly twisted form of the *syn*-chair$_2$lel conformation) is one of the three theoretically possible conformations which we omitted from our calculations partly because molecular models indicated that in their *idealized* forms they would be highly unstable.

Prompted by this apparent disagreement we have submitted also the *syn*-chair$_2$lel conformer to minimization in force field FF-1, starting from two different initial conformations: the experimental (of which the coordinates were kindly supplied by Jurnak and Raymond prior to publication), and the idealized in itself highly unlikely conformation. Although the energy of the former proved very high it minimized with rather small changes in geometry to a value slightly above the energy of the chair$_3$(C_3) conformer, and well below some of the other "mixed" M(tn)$_3$ conformations.[1]

In the idealized *syn*-chair$_2$lel conformation two hydrogen atoms were too close to permit its direct treatment by FF-1. However, omitting the interaction of these two hydrogen atoms from the first few cycles of minimization and subsequently including it (when their distance had grown to make the interaction amenable to the usual treatment) we succeeded in minimizing also the energy of this initial conformation by the method of steepest descent. The convergence of this method, in this case associated with the considerable modification of the initial geometry, was extremely time consuming and in order to obtain a coalescence of the two minimized conformations we resorted to the use of Davidon-Fletcher-Powell and modified Newton minimization methods.*

These findings further support our main conclusion (Ref. 1, p. 640), namely that several conformations (now including a rather twisted *syn*-chair$_2$lel conformation) possess comparable low potential energy so that they could be represented in an equilibrium solution of M(tn)$_3$ species.

We take this opportunity to correct also the following misprints. The value for bending force constants in the second part of Table 2 (Ref. 1, p. 628) are given as $\frac{1}{2}K^\theta$ and not as K^θ as erroneously indicated in the head of the table. Further, in the first four columns of the entries 2 to 5 of Table 3 (p. 629) some numbers have been interchanged. The entries concerned should read as follows:

H···C	3.14	4.20	121.1
H···N	2.81	4.32	99.2
C···C	23.70	4.32	297.8
C···N	21.21	4.44	244.0

These trivial misprints were without consequence to the results and conclusions of Ref. 1.

1. Niketić, S. R. and Woldbye, F. *Acta Chem. Scand. 27* (1973) 621.
2. Jurnak, F. A. and Raymond, K. N. *Inorg. Chem. 11* (1972) 3149.
3. Niketić, S. R. *Force Field Calculations on Coordination Compounds*, Thesis, The Technical University of Denmark, 1974.

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* Details of the continuation of our studies of the conformations of the M(tn)$_3$ system by more powerful computational methods leading to the refinements of the minimized conformations will be made available[3] shortly.