Isomerism in a Macrocyclic Schiff Base Nickel(II) Complex: Structure of the *B*-Isomer

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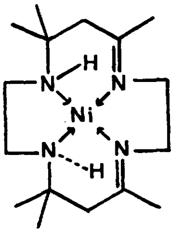
THE Communication by Bailey and Maxwell[1] on the assignment of isomers of the macrocyclic square-planar Ni^{II} complex of hexamethyl-1,4,8,11-tetra-azacyclotetradecadiene prompts us to report briefly on the structure of the *B*-isomer (see refs. 1 and 2 for designation of isomers) as determined by *X*-ray analysis.



Crystals of the perchlorate salt of the *B*-isomers of the diene complex $C_{16}H_{32}N_4Ni^{II}(ClO_4)_2$ are orthorhombic with unit-cell dimensions $a = 10{\cdot}60$, $b = 11{\cdot}11$, $c = 19{\cdot}16$ Å, space group *Pbcn* (No. 60), $Z = 4$. From the Patterson function it was clear that the Ni atoms are situated on the dyad axes, 0, y, 1/4, etc., with $y = 0{\cdot}18$, rather than on the alternative inversion centres of the space group. The positions of all C, N, Cl, O atoms have been determined, and refinement by full-matrix least-squares methods has now led to an *R*-factor of 0·064 for the 1064 reflections for which reliable intensity measurements have been made.

The macrocyclic complex is nickel(II)–5,5,7,12,14,14-hexamethyl-1,4,8,11,-tetra-azacyclotetradeca-7,11-diene (I) corresponding to the "*cis*" arrangement of the imine groups. Since its only symmetric element is the crystallographic dyad axis, it follows that the ligand is chiral with one N–H above, the other below the mean ligand plane. The space group ensures that the crystal is a racemate, containing equal numbers of both enantiomers.

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[1] M. F. Bailey and I. E. Maxwell, preceding Communication.

[2] N. F. Curtis, Y. Curtis, and H. K. J. Powell, *J. Chem. Soc.* (*A*), 1966, 1015.