

## The Structure of the Trinuclear Cation Bis- $[\mu\text{-}(\text{tri-1,2,4-triazolo-}N^1,N^2)\text{-triaquonickel}]$ nickel

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THE COMPLEX bis- $[\mu\text{-}(\text{tri-1,2,4-triazolo-}N^1,N^2)\text{-triaquonickel}]$ nickel hexanitrate dihydrate,  $[(\text{H}_2\text{O})_3(\text{C}_2\text{H}_3\text{N}_3)_3\text{Ni}]_2\text{Ni}(\text{NO}_3)_6(\text{H}_2\text{O})_2$ , has been prepared and has been shown by *X*-ray diffraction techniques to contain a trinuclear cation. This

the structure was solved by the Patterson and electron density Fourier methods. Full matrix isotropic least-squares refinement on all atoms except hydrogen resulted in an *R* value of 0.099. The structure of the complex cation is shown in

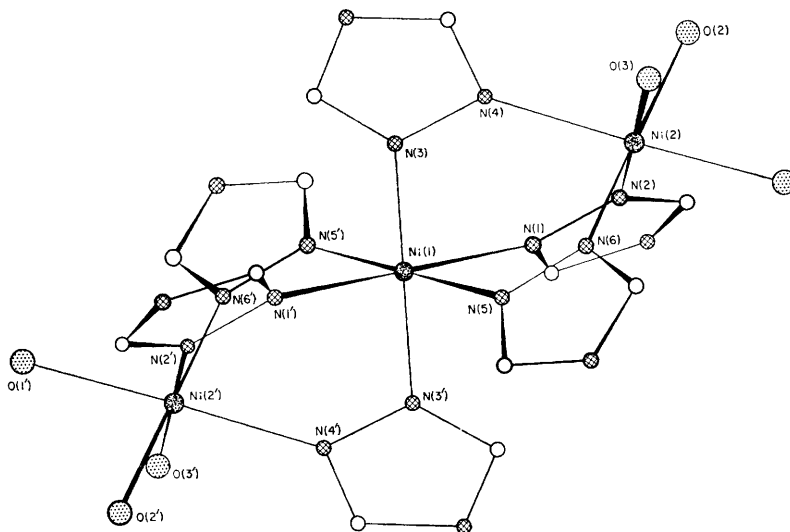


FIGURE. Structure of the bis- $[\mu\text{-}(\text{tri-1,2,4-triazolo-}N^1,N^2)\text{-triaquonickel}]$ nickel cation. The average co-ordination distances are Ni(1)-N = 2.10, Ni(2)-N = 2.05, Ni(2)-O = 2.08 Å.

complex is therefore one of a class of inorganic compounds which contain two or more paramagnetic metal ions per molecule, much studied by magnetic and spectroscopic means.<sup>1,2</sup> Polynuclear species are well suited to detailed study because the exchange coupling between paramagnetic ions in a single molecule is greater than that between ions from neighbouring molecules.

The compound  $[(\text{H}_2\text{O})_3(\text{C}_2\text{H}_3\text{N}_3)_3\text{Ni}]_2\text{Ni}(\text{NO}_3)_6(\text{H}_2\text{O})_2$  separated as purple-blue plates from an aqueous solution (1:2) of  $\text{Ni}(\text{NO}_3)_2$  and 1,2,4-triazole. Crystals of this compound are monoclinic with  $a = 14.26$ ,  $b = 11.75$ ,  $c = 14.95$  Å,  $\beta = 127.9^\circ$ , space group  $P2_1/c$ ,  $D_m = 1.85$ ,  $D_c = 1.84$  g.cm.<sup>-3</sup> and  $Z = 2$ . The intensities of 6885 reflections were measured on a diffractometer and

the Figure, which indicates that the nickel atoms are octahedrally co-ordinated and colinear. The Ni(1)-Ni(2) separation is 3.73 Å. The central nickel atom is co-ordinated by one nitrogen atom from each of six triazole rings while the terminal nickel atoms are co-ordinated by one nitrogen atom from each of three triazole rings, and by three molecules of water. These water molecules are also involved in hydrogen bonding with the nitrate anions as evidenced by the observed O-O distances. At the present time anisotropic refinement, location of hydrogen atoms and the elaboration of the hydrogen bonding network are in progress. Single crystal magnetic and spectroscopic investigations are planned.

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<sup>1</sup> G. J. Bullen, R. Mason, and P. Pauling, *Inorg. Chem.*, 1965, 4, 456.

<sup>2</sup> A. P. Ginsberg, R. L. Martin, and R. C. Sherwood, *Chem. Comm.*, 1967, 856.