X-Ray Crystal Structure of the Pentanitratoaluminate Anion

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Summary *X*-Ray studies show two types of co-ordination between aluminium and NO_3 groups in the $[Al(NO_3)_5]^{2-}$ anion.

STRUCTURES of several transition and heavy metal nitratocomplexes have been studied.[1] Stable nitratocomplexes of boron and aluminium, were first obtained as the salts $Me_4N[B(NO_3)_4]$,[2] $Et_4N[Al(NO_3)_4]$, and $NO_2[Al(NO_3)_4]$.[3] Recently the salt $Cs_2[Al(NO_3)_5]$ which contains the nitratoaluminate anion has been isolated.[4] We now report the crystal structure of this complex.

The caesium pentanitratoaluminate crystallises from nitrate–oleum solution as colourless transparent isometric crystals (m.p. 190°) which readily hydrolyse in air. *Crystal data*: $Cs_2[Al(NO_3)_5]$, $M = 602{\cdot}85$, trigonal, $a = 11{\cdot}16(4)$, $c = 10{\cdot}02(3)$ Å, $U = 1080$ Å^3; $D_m = 2{\cdot}69$, $D_c = 2{\cdot}80$ gcm^{-3}, $Z = 3$; space group $P3_12I$.

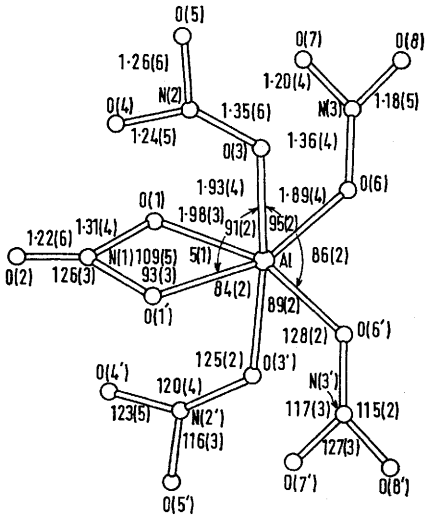

FIGURE. *Structure of pentanitratoaluminate anion*

Intensities of 418 independent non-zero reflections (Mo-K_α radiation) were estimated visually, absorption correction not being applied. The structure was solved by Patterson and Fourier methods. The positional and isotropic thermal parameters were refined by least-squares to an R factor of 0·084.

The $[Al(NO_3)_5]^{2-}$ anion has C_2 symmetry (Figure). The aluminium atom is surrounded by six oxygen atoms which belong to one bidentate and four monodentate nitrato-groups. The oxygen atoms are at the corners of a distorted octahedron. The Al–O distance in the case of the monodentate groups appears to be slightly shorter than in the case of the bidentate group, *i.e.* 1·91 Å (average) compared to 1·98 Å. The differences between the bond-lengths and bond-angles in the nitrato-groups and those of the non-co-ordinate NO_3 ion[5] depend on the mode of co-ordination[1].

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