X-Ray Determination of the Molecular Structure of an Organoaluminium Compound [$Me_2AlOC(Ph)NPh,ONMe_3$]

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Summary The molecular structure of [$Me_2AlOC(Ph)NPh,ONMe_3$] has been determined by *X*-ray structure analysis.

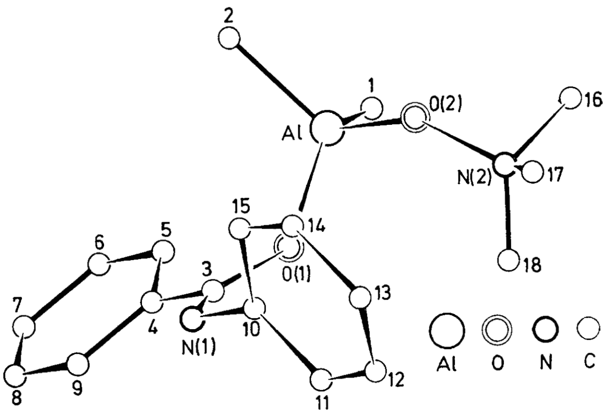
As part of a series of *X*-ray structural studies of organoaluminium compounds related to the highly stereospecific polymerization catalysis of acetaldehyde we report here the molecular structure of [$Me_2AlOC(Ph)NPh,ONMe_3$]. The complex is obtained from an equimolar mixture of [$Me_2AlOC(Ph)NPh$]$_2$ or [$Me_2AlOC(Ph)NPh,MeCHO$]$_2$ and a strong electron donor, $ONMe_3$, in benzene at room temperature. It shows no catalytic activity, unlike the recently reported complexes, [$Me_2AlOC(Ph)NPh$]$_2$,[1] [$Me_2AlOC(Ph)NPh,MeCHO$]$_2$,[2] and [$Me_2AlOC(Ph)NPh,MeCHO,AlMe_3$],[3] which are catalytically active.

Crystal data: [$Me_2AlOC(Ph)NPh,ONMe_3$]: $a = 8{\cdot}517(4)$, $b = 10{\cdot}096(5)$, $c = 12{\cdot}256(5)$ Å, $\alpha = 104{\cdot}67° \pm 0{\cdot}04°$, $\beta = 106{\cdot}97 \pm 0{\cdot}04°$, $\gamma = 98{\cdot}10 \pm 0{\cdot}04°$; space group $P\bar{1}$, $Z = 2$, D_c 1·150, D_m 1·14 g cm^{-3}, $\mu = 1{\cdot}29$ cm^{-1} (for Mo-K_α), Zr-filtered Mo-K_α (0·71069 Å).

The crystal was sealed in a thin-walled glass capillary under argon because the compound decomposes immediately in the air. Intensity data for 2399 independent reflexions were collected on a Rigaku on-line controlled, four-circle, single-crystal diffractometer by the ω–2θ technique. The structure was solved by the symbolic addition method and was refined by block-diagonal least-squares. After applying anisotropic temperature factors for non-hydrogen atoms, the R index is 0·14 for the non-zero reflexions.

The molecular structure is shown in the Figure. The molecule is monomeric; the $ONMe_3$ moiety is connected to the electron-deficient aluminium atom by co-ordination through oxygen. The Al–O(2) distance of 1·815(8) Å is similar to that for related organoaluminium compounds.[1-3] The O(2)–N(2) distance is 1·410(11) Å. The N(2) atom has a typical tetrahedral geometry, and the aluminium atom has a slightly distorted tetrahedral conformation. Angles around the aluminium atom lie between 102·6(0·5)° [O(2)–Al–C(2)] and 117·1(0·6)° [C(1)–Al–C(2)]. Bond angles around the two oxygen atoms are 128·5(0·6)° [Al–O(2)–N(2)] and 138·6(0·6)° [Al–O(1)–C(3)], respectively. The Al–O(1) distance is 1·771(7) Å. The C(3)–O(1) distance [1·313(11) Å] is typical of that of an elongated double bond, whereas C(3)–N(1) [1·277(13) Å] is a localized double bond.

The most remarkable feature is that the Al–O(1)–C(3)–N(1) skeleton has the similar conformation as that of the corresponding fragment in $[Me_2AlOCPhNPh]_2$ except that the two adjacent benzene rings in the amide moiety have a *trans* configuration instead of *cis*. As in the formation of the aldehyde complex $[Me_2AlOCPhNPh,MeCHO]_2$, which is induced by co-ordination of the electron donor MeCHO, co-ordination of the strong electron donor $ONMe_3$ to the aluminium atom induces cleavage of Al–N bonds but not of the Al–O bonds. This is followed by a change in the configuration of two benzene rings from *cis* to the more stable *trans*. Five atoms O(1), C(3), C(4), N(1), and C(10) lie on the same plane within 0·02 Å. The dihedral angle between the best planes through the two benzene rings is 81·1°.



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