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Supporting Information

Role of Scandium precursor decomposition in MOCVD of AlScN and predictions for AlYN

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(EtCp)₂Sc(dtbt)

Sc-N1	2.20 Å
Sc-N2	2.22 Å
N1-N3	1.28 Å
N2-N3	1.28 Å
Sc-C (all)	2.28-2.38 Å

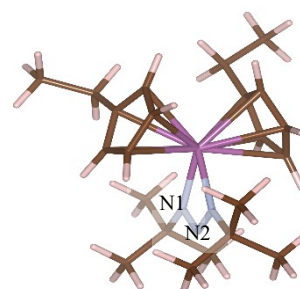


Table S1: Key interatomic distances from DFT relaxations. N1 and N3 are the same by symmetry. Colour scheme is the same as Figure 1.

(EtCp)₂Sc(bdma)

Sc-N1	2.40 Å
Sc-N3	2.22 Å
N1-N2	1.34 Å
N2-C	1.46 Å
C-N3	1.50 Å
N3-N4	1.48 Å
Sc-C (all)	2.28-2.38 Å

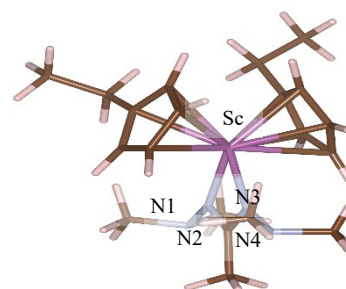


Table S2: Key interatomic distances from DFT relaxations. N1-N4 and N2-N3 are the same by symmetry. Colour scheme is the same as Figure 1.