1,3,2-Diazaalumina-[3]ferrocenophanes with Alkyn-1-yl Substituents at Aluminum

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The 1,3,2-diazaalumina-[3]ferrocenophane-ethyl(dimethyl)amine adduct 2, containing an Al–H function, reacts with terminal alkynes R–C≡C–H [R = "Bu (a), ′Bu (b), Ph (c), SiMe3 (d)] by elimination of H2 to the amine adducts 4a–d containing an Al–C≡C–R function. Addition of pyridine leads to the corresponding pyridine adducts 5a–d, of which the molecular structure of 5d could be determined by single crystal X-ray diffraction. The formation of 4 is accompanied by side reactions such as trimerization of the alkynes to the 1,3,5-trisubstituted benzene derivatives 6a, c, and some polymerization of the alkynes. The solution-state structures of 4 and 5 were confirmed by multinuclear magnetic resonance spectroscopy (1H, 13C, 27Al, 29Si NMR). Structural features and molecular dynamics were investigated by appropriate 1H/1H NOE and magnetization transfer experiments, and particular attention was paid to the correct assignment of 13C(Al–C≡C–R) NMR signals.

Key words: Aluminum, Ferrocenophane, Alkynes, NMR, X-Ray