Preparation, Characterization and Use of Main Group Metal Amidinates

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Five totally new compounds containing NCN amidinato ligand were synthetized in their very pure form. Compounds were prepared applying two methods: 1) a direct nucleophilic addition of metal - containing bases to polarize cumulative CN multiple bonds and 2) a subsequent transmetallation reaction of prepared lithium N,N´-bis(p-tolyl)n-butylamidinate and N,N´-bis(p-tolyl)methylamidinate as precursors with metal halides. Moreover, prepared N,N´-disubstituted methylaluminium amidinates (e.g. Lewis pair consist of aluminium(III) amidinate as Lewis acid and carbonitrile represents Lewis base) could be utilized as initiators in the preparation of biodegradable polymers applicable in medicine and pharmaceutical chemistry. All synthetic procedures were handled using a standard Schlenk technique and vacuum inert line (argon atmosphere). All prepared compounds were identified and characterized with the help of multinuclear NMR spectroscopy (1H, 7Li, 13C as well as 2D NMR - 1H-13C HMBC) or XRD technique of single crystalline materials. Isoquinazolimine derivative (only five derivatives are known yet) was isolated as a by-product from the reaction of lithium amidinate with various metal halides (sequential C-C and C-N coupling reaction) in various molar ratios and reaction temperatures. Isoquinazolimine derivative reveals potential utilization in the treatment of Alzheimer's disease as well as the suppression of tumor growth (based on the DFT calculation on Cdk2). This will be biochemically (in vivo, in vitro) tested and synthetically optimized soon.

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