Beryllium Dichloride Coordination by Nitrogen Donor Molecules

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The reaction of anhydrous beryllium chloride with nitrogen donors L in diethylether as a solvent under mild conditions affords 1:2 complexes of the type L_2BeCl_2 [L = benzonitrile (1), pyridine (2), 3,5-dimethylpyridine, pyrrolidine, piperidine (8), and diethylamine (10)]. Structural studies of compounds 1, 2, 8 (CHCl₃), and 10 have shown that the complexes have the beryllium centers N₂Cl₂tetracoordinated with a distorted tetrahedral geometry of the core unit. In crystals of 8 and 10 these molecules are associated to form helical strings via distinct N-H-Cl hydrogen bonding. The reaction of the weak donor pyrazole (pyz) with (Et₂O)₂BeCl₂ at low temperature gives the mixed complex [(Et₂O)(pyz)BeCl₂] (4), in which one diethylether molecule is retained in the inner coordination sphere of the metal. In tetrahydrofuran (thf) solution, no reaction is observed with pyrazole, indicating that tetrahydrofuran is the stronger donor as compared to pyrazole, and the (thf) BeCl₂ solvate remains intact. By contrast, with the strong base pyrrolidine (pyrr) the same reaction leads to substitution of one chloride ligand to give the ionic product [(pyrr)₃BeCl]⁺Cl⁻, (7). Both products (4, 7) have been structurally characterized. At room temperature the reactions with pyrazole or piperidine lead to ether cleavage as a side-reaction which may even become dominant at long reaction times and more forcing conditions. Dinuclear complexes of the type [LBeCl(μ_2 -OR)]₂ are formed, the structures of which have also been determined. The results suggest that hydrogen bonding may assist in the ether cleavage process, since this reaction is not observed for ligands devoid of N-H functions.

Key words: Beryllium Dichloride Coordination, Nitrogen Donor Molecules