Synthesis and Characterization of Chiral Guanidines und Guanidinium Salts Derived from 1-Phenylethylamine

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The synthesis of two new chiral guanidines **5** and **12** and derived guanidinium salts **6**, **11**, **13** – **15** with one and three N-(1-phenylethyl) substituents is described. In both cases, the well-precedented, reliable route via chloro-formamidines was taken. Since direct attachment of the N-methyl-N-(1-phenethyl)-amino group failed, the two-step protocol – introduction of the primary 1-phenethylamino group first followed by N-methylation – was employed. Crystal structures and NMR data reveal, that the sterically highly congested "tris" salt – with formal C_3 symmetry, albeit unsymmetrical in the crystal – constitutes an intriguing structure with two rotamers present in solution.

Key words: Chiral Guanidine, Chiral Guanidinium Salts, (*R*)- and (*S*)-1-Phenylethylamine, Quaternization, Crystal Structures