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Title: 1,3-Diazolyl functionalized organopropylsilatranes: Synthesis and structural characterization

Authors: Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.)

Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)

Keywords: Silatranes

3,7,10-Trimethylsilatranes Benzimidazole 2-Isopropylimidazole

3-Chloropropyltriethoxysilane

Issue Date: 2014

Publisher:

Elsevier S.A.

Citation: Inorganica Chimica Acta,413, pp.203-207.

Abstract: This work aims at the synthesis of unsubstituted and 3,7,10- trimethylsubstituted organopropylsilatranes by the reaction of 1,3-diazoles, viz. benzimidazole and 2-

isopropylimidazole with 3-chloropropyltriethoxysilane which results in the triethoxysilanes: N-(3-triethoxysilylpropyl)benzimidazole (3) and N-(3-triethoxysilylpropyl)-2-isopropylimidazole (4). In the presence of a base, these silanes undergo transesterification reaction with triethanolamine (1) and tris(isopropanol)amine (2) thus forming the corresponding silatranes, N-(3-silatranylpropyl)benzimidazole (5), N-[3-(3,7,10-trimethylsilatranyl) propyl]benzimidazole (6), N-(3-silatranylpropyl)-2-isopropylimidazole (7), N-[3-(3,7,10-trimethylsilatranyl)propyl]-2-isopropylimidazole (8). Among these novel silatranes, which have been characterized by

isopropylimidazole (8). Among these novel silatranes, which have been characterized by elemental analysis, IR, 1H, 13C NMR spectroscopy, mass spectrometry and thermogravimetric analysis, the structure of silatrane (5) has been deduced by single crystal X-ray diffraction analysis.

Description: Only IISERM authors are available in the record.

 $URI: \\ https://www.sciencedirect.com/science/article/pii/S0020169314000474?via\%3Dihub$

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