Title:	Selective mercury ion recognition using a methyl red (MR) based silatrane sensor
Authors:	Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
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Abstract:	A new methyl red (MR) based silatrane was synthesized in high yield by the transesterification reaction of methyl red-amidopropyltrimethoxysilane 1 (MR-APTMS) and trisisopropanolamine. Single crystal X-ray diffraction analysis was used to deduce the structure of silatrane 2 which was also supported by NMR (1H, 13C) spectroscopy, mass spectrometry, FTIR, UV-Vis and DFT studies. Silatrane 2 when surveyed for cation recognition ability with a library of metal ions in CH3CN/H2O (9:1, v/v) was found to act as an excellent UV-Vis probe for the selective recognition of Hg2+in vitro. Also, quantum mechanical calculations of the interaction complex [MR-APS-Hg]2+3 using DFT at the B3LYP level in conjunction with the LanL2DZ basis set determined the geometric and the stability parameters of the surveyed interaction.
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