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FERROCENYLSILOXANE UREA: SYNTHESIS, STRUCTURE AND PROPERTIES

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The first cyclic ferrocenylsiloxane-urea, {1,1'-ferrocene-diurea-[1,3-bis(propylene)tetramethyldisiloxane]} (FSU), has been formed by reacting 1,1'-ferrocenediisocyanate with 1,3-bis(aminopropyl)-tetramethyldisiloxane in a chloroform-toluene mixture. The ferrocenylsiloxane urea was structurally characterized by FTIR and ^{1}H-NMR spectroscopy, elemental analysis, mass spectrometry (ESI-MS), and single crystal X-ray diffraction. The asymmetric unit contains two conformers packed in one-dimensional supramolecular column through intermolecular interaction between N-H and O-H protons on the one hand with urea oxygen atoms and solvate water molecules on the other hand.

The dynamic of the hydrogen bonds in solid state compound in dependence on temperature was investigated by IR-spectroscopy. ^{1}H-NMR spectra revealed the dependence of the chemical shifts of the groups responsible on the hydrogen bond formation on concentration and solvent polarity. After the loss of crystallization water and retained solvent traces, the compound is stable up to 510 ^{o}C when the organic part is decomposed leaving a large amount of residue consisting in iron and silicon oxides. Due to the co-existence in structure of the polar (ferrocenyl-uree) and nonpolar (bis(propyl)tetramethyldisiloxane) moieties, the compound proved to be able to self-assemble in $CHCl_3$ in quasi-spherical aggregates with vesicle-like aspect. This behavior was less obvious in polar medium (DMSO). The compound showed reversible redox processes and the shape of the voltammogram indicates the presence of essentially noninteracting iron centers in structure.