We are aiming to design and synthesize ferromagnetically coupled organic radicals. According to this goal, crystal structure, magnetic properties and hybrid DF/HF (Density Functional/Hartree-Fock) Gaussian 98 calculations of nitronyl nitroxide radicals containing different substitutions at the 2-position of the imidazole ring are reported. (I) crystallizes in two polymorphic forms. The α form is monoclinic, with four molecules in the asymmetric unit. The β form is monoclinic, with one molecule in the asymmetric unit. In the α form there are three structurally different dimers, while only one dimer presents in the β form. (I) crystallizes in orthorhombic space group. The magnetic measurements have shown that both α and β polymorphs of (I) exhibit antiferromagnetic coupling. The best fitting with the experimental data were obtained using Bleany-Bowers model for the α phase (Jα = 15.0 K) and dimer model (Jβ = 115.2 K) (1) for the β phase. Hybrid DF/HF Gaussian 98 calculations of both single molecules and dimers are in a good agreement with the experimental geometries. The calculated isotropic hyperfine coupling constants and spin densities of nitrogen are very close to the experimental data obtained by ESR measurements for these compounds and polarized neutron diffraction studies of similar nitronyl nitroxide radicals. The J value for both α and β polymorphs of (I) has been calculated to be -110.6 K. The crystal structures were previously determined but never been published in details (1).


Keywords: MAGNETIC PROPERTIES ORGANIC RADICALS

POLYMORPHISM


DENDRIMERS WITH NIобIUM IMIJo COMPLEXES.

MONONUCLEAR MODELS

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An increasing number of reports have been published on the incorporation of transition metals at the core, branches, or periphery of dendrimers. Applications of these macromolecular systems in areas such as catalysis are being widely studied. However, little attention has been paid to dendrimers with metal complexes at their periphery through imido bonds. Imido ligands are very effective as hydrogen bond acceptors and have a strong -donor abilities. Here, we present the synthesis and structural studies of new niobium(V) imido dendrimers obtained by reaction of metal chlorides with the N,N-bis(trimethylsilyl)aniline end-groups of oxygen-free dendrimers. Previous theoretical and X-ray diffraction structural studies on mononuclear models [M–C₆H₄SiMe₃]Nb(N-C₆H₄-4-SiMe₃)Cl₂ and [Nb(N-C₆H₄-4-SiMe₃)Cl₂(NCMe)] are in addition presented.

References


Keywords: DENDRIMERS, ORGANOMETALLIC COMPLEXES, NIобIUM


WATER CLUSTERS IN ORGANIC MOLEClAR CRYSTALS IN THE CSD

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Water clusters have been extensively studied both theoretically and experimentally. However, there are no analyses of the different hydrogen-bonded (H₂O)ₜ clusters present in the solid state. The presence of water molecules in the structure can play an important role in stabilising some supramolecular species since the number of hydrogen bond acceptors and donors can differ significantly from those of the anhydrous compounds. In the present work we have examined more than 1500 hydrated structures retrieved from the CSD. In the first step of our analysis we removed everything other than the water molecules and selected only those structures where the water molecules are H-bonded together, forming patterns either of infinite 1D chains, 2D sheets, 3D networks, or cyclic motifs. The most common motifs are: (a) for isolated clusters (dimension zero) the tetramer motif (b) for 1-dimensional chains and ladders the pattern using 4 molecules to make the repeat in a linear chain (c) for 2-dimensional sheets the motifs forming 4, 5 and 6 membered rings. For 3-dimensional networks there are no predominant patterns. In the case of 1-dimensional ladders the motif is formed by linked rings sharing edges or nodes. The most predominant are a pattern with linked 5-membered rings sharing one edge, and another pattern with linked alternate 4-6 membered rings sharing one edge.

Keywords: WATER CLUSTERS H-BONDING