2-Thiadiazolylnitronylnitroxide – Synthesis, Magnetic Properties and X-ray Structure

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Synthesis of novel molecules with interference of different useful physical properties is an interesting and challenging goal. We suppose nitronylnitroxides with strong donor-acceptor interaction to be a strong candidates to combine non-linear optic and magnetic properties.

Several aldehydes (1) of thiadiazole series with donor groups were prepared according to multi-step procedure that includes nucleophilic substitution, reduction and oxidation. Condensation of 1a (R+R = (CH₂CH₂)₂O) with 3,4-bishydroxylamino-3,4-dimethylbutane followed with oxidation led to nitronylnitroxide 2.

It was found that solid phase of nitronylnitroxide $\mathbf{2}$ demonstrates magnetic behaviour of exchange-coupled dimers with J(Rad-Rad) = -60 cm⁻¹ (strong antiferromagnetic interaction). Magnetic properties and X-ray structure of $\mathbf{2}$ will be discussed in details.

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