Modelling Magnetic Interactions in Sulfur-Nitrogen Radical Chemistry

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Organic radicals have captured the attention of researchers due to their ability to exhibit magnetic order, despite the absence of metal ions. The goal of this study is to gain a better understanding of the electron-electron interactions in one such class of stable radical, known as dithiazolyls (**1**). Such data allows a much improved understanding between structure and magnetic response in these systems, which will assist in the future design process, leading to organic magnets with higher ordering temperatures.

We have employed the 'bottom-up' methodology, pioneered by Novoa *et al.*, to determine appropriate magnetic models based on pair-wise interactions between nearest neighbour molecules in the solid state, in which the strength of the magnetic communication is estimated from the energies (E) and expectation values ($<S^2>$) of the triplet and broken symmetry singlet configurations. Recent calculations and magnetic models for selected dithiazolyl radicals (**1**) will be presented.

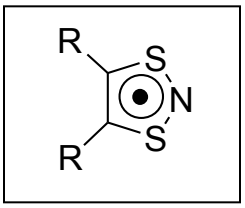

Figure 1: DTA Radical (**1**)