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Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information:

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SYNTHESIS AND CHARACTERISATION OF TETRAFLUOROBENZO-1,3,2-DITHIAZOLYL

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Online publication date: 12 August 2010

To cite this Article Alberola, Antonio , McManus, Gordon D. and Rawson, Jeremy M.(2004) 'SYNTHESIS AND CHARACTERISATION OF TETRAFLUOROBENZO-1,3,2-DITHIAZOLYL', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 179: 4, 979 – 980

To link to this Article: DOI: 10.1080/10426500490429572

URL: <http://dx.doi.org/10.1080/10426500490429572>

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SYNTHESIS AND CHARACTERISATION OF TETRAFLUOROBENZO-1,3,2-DITHIAZOLYL

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(Received August 17, 2003; accepted October 3, 2003)

Keywords: Dithiazolyl radicals; esr

Heterocyclic dithiazolyl (DTA) radicals recently have been shown to exhibit unusual physical properties including high magnetic ordering temperatures, as in the case of benzo-1,3,2-dithiadiazolyl¹ (BDTA) ($T_c = 11$ K) and display of bistability² at room temperature in trithiatriazapentalene (TTTA) among others. A new DTA salt [TFB-DTA]Cl (**1**) was prepared from $C_6F_4(SH)_2$ using standard synthetic methods.² Crystals were grown by sublimation (Figure 1).

The radical was generated in situ by reduction of the salt with Ag powder in CH_2Cl_2 . The X-band EPR spectrum of the radical exhibited a triplet of triplets due to coupling of the unpaired spin to one ^{14}N nucleus ($I = 1$) and two ^{19}F ($I = 1/2$) ($g_{iso} = 2.0044$, $a_{iso}^N = 11.0$ G, $a_{iso}^F = 1.5$ G). Further resolution of coupling to the remaining two F atoms could not be achieved (Figure 2).

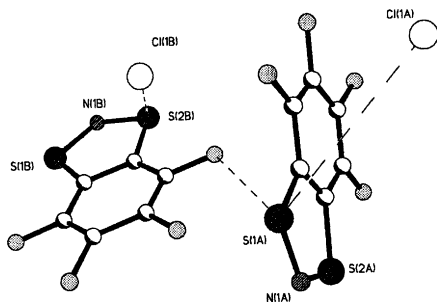


FIGURE 1 The asymmetric unit of [1] Cl.

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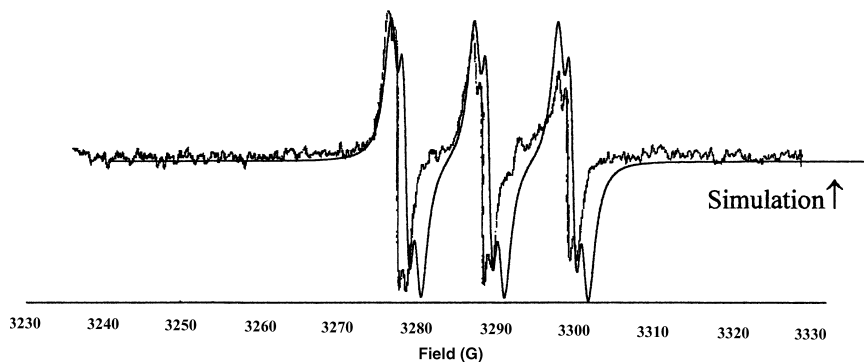


FIGURE 2 Solution EPR spectrum of **1** and simulation using parameters in text.

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