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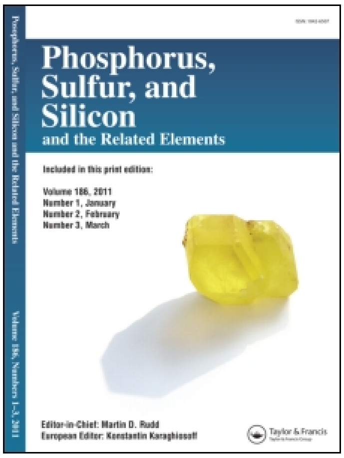

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SMALL MOLECULE FIXATION BY A SULFUR-NITROGEN RADICAL

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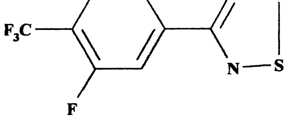
The radical **1**, $CF_3C_6H_3FCNSSN$, crystallizes with a close-packed layer-like structure (triclinic *P*-1) when sublimed under vacuum (Figure 1a). On sublimation under a partial atmosphere of N_2, Ar, CO_2, SO_2, and CH_4, a more open structure with a very similar layer-like pattern is formed (orthorhombic Pbcn), but here the layers are buckled such that channels exist along the *c*-direction (Figure 1b) with the guest molecules accommodated within the channels. In comparison, no inclusion is observed during sublimation in the presence of $CFCl_3$ and CF_2Cl_2 whereas sublimation under O_2 generates the dithiatetrazocine, **2**. It is thought that the reason behind the inclusion behavior of **1** is that favorable intermolecular interactions ($S^{\delta+}\cdots N^{\delta-}$ and $S^{\delta+}\cdots F^{\delta-}$) are maximized and unfavorable ones ($F^{\delta-}\cdots F^{\delta-}$) minimized by adopting the more open inclusion structure.



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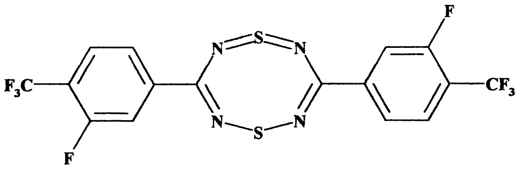

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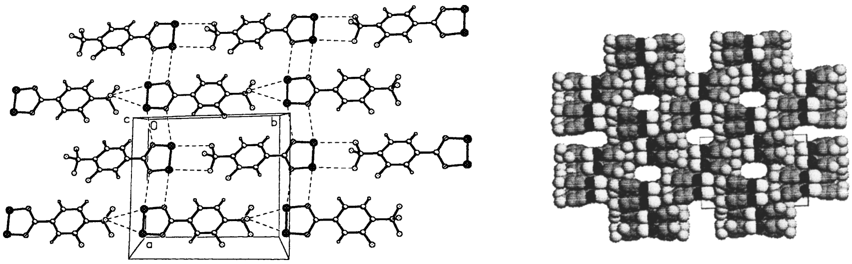

(a) (b)

FIGURE 1 a) Layer-like structure of **1** and b) space-filling diagram of the host-guest structure **1**.N_2.