Supplementary Material (ESI) for Green Chemistry

Supplementary Information

Poly(ethyleneglycol) (PEG): A Versatile Reaction Medium in Gaining Access to 4'-(Pyridyl)-Terpyridines

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X-Ray crystallography

A colourless specimen of **11**, 0.35 × 0.30 × 0.25 mm, obtained from slow evaporation of a $CDCl_3$ solution was used for the single-crystal X-ray diffraction study. The X-ray intensities were measured at 150 K on a Bruker AXS CCD instrument using monochromatized Mo-K_α (λ = 0.71073 Å) X-ray source. Data were corrected for Lorentz and polarization effects and absorption correction applied using multiple symmetry equivalent reflections (μ_{Mo} = 0.344 mm^{-1}, $T_{min/max}$ = 0.889, 0.919). The structure was solved by direct methods and refined on F^2 using the SHELXTL crystallographic package (Bruker ASX).[1] A full matrix least-squares refinement procedure was used, minimising $w(F_o^2-F_c^2)$, with $w = [\sigma^2(F_o^2)+(AP)^2+BP]^{-1}$, where $P= (F_o^2+2F_c^2)/3$. Agreement factors ($R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ and GOOF $= \{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$ are cited, where n is the number of reflections and p is the total number of parameters refined). All hydrogen atoms in molecules were calculated from geometrical considerations and constrained to the bonded carbons during the refinement.

In the disordered thiophene fragments the population parameters of atoms in corresponding rings were refined as x=1-x. The obtained values of the refined parameters are recorded in the CIF file. The values are: x(B) = 0.597(4); x(D) = 0.440(4). The thermal parameters of the thiophene rings containing atoms S1a and S1c (and their carbon atoms) are not perfect and therefore these atoms also exhibit a degree of positional

disorder. However, with the quality of the experimental data at hand we are unable to produce a reasonable disorder model for the atoms in these thiophene rings.

Crystal/refinement details for **11 :** $C_{18}H_{12}N_2S_2$, M = 320.42, F(000) = 1328 e, monoclinic, *Pc* (No. 7), Z = 8, T = 153 K, a = 20.312(3), b = 9.9902(15), c = 15.927(2) Å, β = 108.289(2)°, V = 3068.7(8) Å^3; D_c = 1.387 g cm^{-3}; $\sin\theta/\lambda_{max}$ = 0.683; N(unique) = 14336 (merged from 27936, R_{int} = 0.0242, R_{sig} = 0.0411), N_o ($I > 2\sigma(I)$) = 11766; R = 0.0738, $wR2$ = 0.1835 (A,B = 0.114, 1.4262), GoF = 1.029; $|\Delta\rho_{max}|$ = 1.2(1) e Å^{-3}. CCDC 265089 contains the supplementary crystallographic data for this paper.

1. Bruker (1997). SMART, SAINT, SADABS & SHELXTL. v5.1. Bruker AXS Inc., Madison, Wisconsin, USA.