Molbank 2005, M402

http://www.mdpi.net/molbank/

5-Ferrocnylidene(1,3-diethylthiobarbituric acid)

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Received: 8 April 2004 / Accepted: 20 April 2004 / Published: 1 July 2005

Key Word: ferrocen, knovenagel condensation, dyes

There is considerable interest in the synthesis of new materials with large second-order optical non-linearity because of their potential applications in optical data storage, telecommunications and optical signals processing $^{1-4}$. First and second hyperpolarizability can be observed with molecules which possess an electron donor and acceptor groups connected by a conjugated Π -electron bridge which allow the possibility of intramolecular charge transfer $^{5-6}$.

To a refluxed solution of ferrocenecarboxaldehyde 1 (2.0g, 9.34 mmol) and N,N-diethylthiobarbituric acid 2 (1.87g, 9.34 mmol) in ethanol (50 ml), Piperidine (1 ml) was added. After the addition, the solution became darker and the reflux was continued for six hours, then the solution was left to cool to room temperature and the product 3 was precipitated. The precipitates were filter and washed with cold water and finally with ethanol, dried and recrystallized from ethanol. Deep blue crystal (3g, 81.01%).

Melting point: 164-166 °C (uncorrected).

UV (EtOH; λ_{max} nm; ϵ (dm³.mol⁻¹.cm⁻¹): 374 (16521); 575 (3700).

IR (KBr, cm⁻¹): 1680, 1660 (C=O); 1620 (C=C); 1115 (C=S); 1101, 992, 809.

 1 H-NMR (400 MHz; CDCl₃): δ= 8.46 (1H, s, -CH=C); 5.36 (2H, broad s, H-2, H4, H-5); 4.97 (2H, broad s, H-2, H3, H-4); 4.31 (5H, s, C₅H₅); 4.31 (4H, q, CH₂N); 1.32 (6H, t, <u>CH₃</u>CH₂N).

Elemental Analysis: Calculated for $C_{19}H_{20}N_{2}O_{2}SFe$ (396.19): C, 57.57%; H, 5.05%; N, 7.07%: Found; C, 57.36%; H, 4.88%; N, 7.14%

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