BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

**for**

**Synthesis of photo- and ionochromic *N*-acylated 2-aminomethylenebenzo[*b*]thiophene-3(2*Н*)-ones with a terminal phenanthroline group**

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**X-ray analysis data of 3a**

**Table S1:** Crystal data and structure refinement for compound **3b**.

 CCDC Number 2299603

Empirical formula C24H17N3O2S

Formula weight 411.46

Temperature/K 293(2)

Crystal system triclinic

Space group P-1

a/Å 7.43030(10)

b/Å 9.6398(2)

c/Å 14.3294(3)

α/° 75.731(2)

β/° 82.686(2)

γ/° 78.664(2)

Volume/Å3 971.93(3)

Z 2

ρcalcg/cm3 1.406

μ/mm-1 1.701

F(000) 428.0

Crystal size/mm 0.361 × 0.281 × 0.1

Radiation Cu Kα (λ = 1.54184)

2Θ range for data collection/° 9.61 to 152.768

Index ranges -9 ≤ h ≤ 9, -11 ≤ k ≤ 12, -17 ≤ l ≤ 18

Reflections collected 17777

Independent reflections 4053 [Rint = 0.0201, Rsigma = 0.0153]

Data/restraints/parameters 4053/0/272

Goodness-of-fit on F2 1.054

Final R indexes [I>=2σ (I)] R1 = 0.0307, wR2 = 0.0808

Final R indexes [all data] R1 = 0.0315, wR2 = 0.0813

Largest diff. peak/hole / e Å-3 0.23/-0.35

**Table S2:** Bond lengths for compound **3b**.

Atom Atom Length/Å Atom Atom Length/Å

S1 C8 1.7409(12) C15 C14 1.3606(16)

S1 C1 1.7401(11) C15 C16 1.4292(15)

O1 C2 1.3901(13) C22 C23 1.4972(16)

O1 C22 1.3820(13) C9 C1 1.4491(15)

O2 C22 1.2001(14) C20 C16 1.4147(15)

N3 C14 1.4105(14) C3 C8 1.4072(17)

N3 C9 1.2827(15) C3 C4 1.4028(16)

N2 C20 1.3595(14) C16 C17 1.4086(15)

N2 C19 1.3279(15) C12 C11 1.3737(17)

N1 C21 1.3607(15) C17 C18 1.3687(16)

N1 C10 1.3288(15) C18 C19 1.4046(17)

C13 C21 1.4161(15) C8 C7 1.3992(16)

C13 C14 1.4466(15) C10 C11 1.4016(17)

C13 C12 1.4086(15) C7 C6 1.3833(18)

C2 C3 1.4284(15) C23 C24 1.5224(17)

C2 C1 1.3605(16) C4 C5 1.3811(17)

C21 C20 1.4562(15) C6 C5 1.4003(19)

**Table S3:** Bond angles for compound **3b**.

Atom Atom Atom Angle/˚ Atom Atom Atom Angle/˚

C1 S1 C8 91.11(6) C16 C20 C21 118.29(10)

C22 O1 C2 114.92(8) C8 C3 C2 110.49(10)

C9 N3 C14 117.80(10) C4 C3 C2 129.47(11)

C19 N2 C20 117.38(10) C4 C3 C8 120.03(11)

C10 N1 C21 117.48(10) C20 C16 C15 120.82(10)

C21 C13 C14 120.18(10) C17 C16 C15 121.33(10)

C12 C13 C21 118.09(10) C17 C16 C20 117.84(10)

C12 C13 C14 121.71(10) C11 C12 C13 119.50(10)

O1 C2 C3 123.91(10) C18 C17 C16 119.58(10)

C1 C2 O1 121.64(10) C17 C18 C19 118.33(10)

C1 C2 C3 114.44(10) C3 C8 S1 112.08(8)

N1 C21 C13 122.20(10) C7 C8 S1 126.93(10)

N1 C21 C20 118.31(10) C7 C8 C3 120.99(11)

C13 C21 C20 119.47(10) C2 C1 S1 111.83(8)

C14 C15 C16 121.22(10) C2 C1 C9 126.95(10)

N3 C14 C13 117.43(10) C9 C1 S1 121.21(9)

C15 C14 N3 122.44(10) N2 C19 C18 124.33(10)

C15 C14 C13 119.95(10) N1 C10 C11 124.56(11)

O1 C22 C23 111.09(9) C6 C7 C8 117.89(12)

O2 C22 O1 121.99(10) C22 C23 C24 110.62(10)

O2 C22 C23 126.91(10) C12 C11 C10 118.15(11)

N3 C9 C1 120.05(10) C5 C4 C3 118.80(12)

N2 C20 C21 119.19(10) C7 C6 C5 121.63(11)

N2 C20 C16 122.51(10) C4 C5 C6 120.65(11)

**Table S4:** Torsion angles for compound **3b**.

A B C D Angle/˚ A B C D Angle/˚

S1 C8 C7 C6 179.44(9) C14 C15 C16 C17 -179.41(10)

O1 C2 C3 C8 -179.17(10) C22 O1 C2 C3 -75.26(13)

O1 C2 C3 C4 1.65(19) C22 O1 C2 C1 105.89(12)

O1 C2 C1 S1 177.69(8) C9 N3 C14 C13 -139.08(10)

O1 C2 C1 C9 -1.18(17) C9 N3 C14 C15 45.83(15)

O1 C22 C23 C24 170.73(9) C20 N2 C19 C18 -0.60(17)

O2 C22 C23 C24 -10.02(17) C20 C16 C17 C18 -0.96(16)

N3 C9 C1 S1 10.30(15) C3 C2 C1 S1 -1.26(13)

N3 C9 C1 C2 -170.92(11) C3 C2 C1 C9 179.87(10)

N2 C20 C16 C15 -177.59(10) C3 C8 C7 C6 -1.03(17)

N2 C20 C16 C17 1.57(16) C3 C4 C5 C6 -0.36(18)

N1 C21 C20 N2 -4.53(15) C16 C15 C14 N3 173.51(10)

N1 C21 C20 C16 175.49(10) C16 C15 C14 C13 -1.46(16)

N1 C10 C11 C12 1.50(19) C16 C17 C18 C19 -0.31(17)

C13 C21 C20 N2 177.20(10) C12 C13 C21 N1 1.30(16)

C13 C21 C20 C16 -2.78(15) C12 C13 C21 C20 179.51(10)

C13 C12 C11 C10 -0.33(17) C12 C13 C14 N3 7.48(15)

C2 O1 C22 O2 6.67(14) C12 C13 C14 C15 -177.31(10)

C2 O1 C22 C23 -174.04(9) C17 C18 C19 N2 1.17(18)

C2 C3 C8 S1 1.64(12) C8 S1 C1 C2 1.84(9)

C2 C3 C8 C7 -177.96(10) C8 S1 C1 C9 -179.21(9)

C2 C3 C4 C5 178.52(11) C8 C3 C4 C5 -0.59(17)

C21 N1 C10 C11 -1.20(18) C8 C7 C6 C5 0.07(18)

C21 C13 C14 N3 -174.20(9) C1 S1 C8 C3 -1.99(9)

C21 C13 C14 C15 1.01(16) C1 S1 C8 C7 177.58(11)

C21 C13 C12 C11 -0.97(16) C1 C2 C3 C8 -0.24(14)

C21 C20 C16 C15 2.39(15) C1 C2 C3 C4 -179.43(11)

C21 C20 C16 C17 -178.45(10) C19 N2 C20 C21 179.22(10)

C15 C16 C17 C18 178.20(10) C19 N2 C20 C16 -0.80(16)

C14 N3 C9 C1 -172.99(9) C10 N1 C21 C13 -0.24(16)

C14 C13 C21 N1 -177.08(10) C10 N1 C21 C20 -178.47(10)

C14 C13 C21 C20 1.13(15) C7 C6 C5 C4 0.64(19)

C14 C13 C12 C11 177.39(10) C4 C3 C8 S1 -179.09(9)

C14 C15 C16 C20 -0.28(16) C4 C3 C8 C7 1.31(17)

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