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Supporting information for article:

Structural characterization and theoretical calculations of the monohydrate of the 1:2 cocrystal salt formed from acriflavine and 3,5-dinitrobenzoic acid

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Table S1 Geometric parameters for title compound (Å, º).

Atoms	Length/Å	Atoms	Length/Å
O1W—H2W	0.86 (3)	C18A—C23A	1.387 (4)
O1W—H1W	0.91 (3)	C18A—C19A	1.394 (4)
C1—C2	1.347 (6)	C18A—C24A	1.504 (4)
C1—C11	1.418 (5)	C18B—C19B	1.387 (4)
C1—H1A	0.9300	C18B—C23B	1.388 (4)
C2—C3	1.434 (5)	C18B—C24B	1.513 (4)
C2—H2A	0.9300	C19A—C20A	1.383 (4)
C3—N15	1.350 (5)	C19A—H19A	0.9300
C3—C4	1.393 (5)	C19B—C20B	1.361 (5)
C4—C12	1.376 (5)	C19B—H19B	0.9300
C4—H4A	0.9300	C20A—C21A	1.377 (4)
C5—C14	1.383 (5)	C20A—N27A	1.474 (4)
C5—C6	1.393 (5)	C20B—C21B	1.392 (5)
C5—H5A	0.9300	C20B—N27B	1.471 (4)
C6—N17	1.338 (5)	C21A—C22A	1.379 (4)
C6—C7	1.437 (5)	C21A—H21A	0.9300
C7—C8	1.345 (5)	C21B—C22B	1.378 (4)
C7—H7A	0.9300	C21B—H21B	0.9300
C8—C13	1.428 (5)	C22A—C23A	1.378 (4)
C8—H8A	0.9300	C22A—N30A	1.471 (4)
C9—C11	1.379 (5)	C22B—C23B	1.382 (4)

C9—C13	1.382 (5)	C22B—N30B	1.471 (4)
C9—H9A	0.9300	C23A—H23A	0.9300
N10—C12	1.379 (4)	C23B—H23B	0.9300
N10—C14	1.387 (4)	C24A—O26A	1.238 (3)
N10—C16	1.466 (4)	C24A—O25A	1.272 (3)
C11—C12	1.444 (4)	C24B—O26B	1.213 (4)
C13—C14	1.430 (4)	C24B—O25B	1.296 (4)
N15—H15B	0.85 (3)	O25B—H25B	0.987 (14)
N15—H15A	0.88 (3)	N27A—O28A	1.222 (4)
C16—H16A	0.9600	N27A—O29A	1.228 (4)
C16—H16B	0.9600	N27B—O29B	1.220 (4)
C16—H16C	0.9600	N27B—O28B	1.227 (5)
C16—H16D	0.9600	N30A—O32A	1.220 (3)
C16—H16E	0.9600	N30A—O31A	1.226 (3)
C16—H16F	0.9600	N30B—O31B	1.220 (3)
N17—H17A	0.87 (2)	N30B—O32B	1.225 (3)
N17—H17B	0.96 (2)		

Atoms	angle/°	Atoms	angle/°
H2W—O1W—H1W	110 (5)	H16B—C16—H16F	56.3

C2—C1—C11	122.9 (3)	H16C—C16—H16F	141.1
C2—C1—H1A	118.6	H16D—C16—H16F	109.5
C11—C1—H1A	118.6	H16E—C16—H16F	109.5
C1—C2—C3	119.8 (3)	C6—N17—H17A	120 (3)
C1—C2—H2A	120.1	C6—N17—H17B	111 (2)
C3—C2—H2A	120.1	H17A—N17—H17B	129 (4)
N15—C3—C4	121.2 (3)	C23A—C18A—C19A	119.5 (3)
N15—C3—C2	120.1 (3)	C23A—C18A—C24A	119.5 (2)
C4—C3—C2	118.6 (3)	C19A—C18A—C24A	120.9 (2)
C12—C4—C3	122.0 (3)	C19B—C18B—C23B	119.7 (3)
C12—C4—H4A	119.0	C19B—C18B—C24B	120.7 (3)
C3—C4—H4A	119.0	C23B—C18B—C24B	119.6 (3)
C14—C5—C6	121.7 (3)	C20A—C19A—C18A	118.6 (3)
C14—C5—H5A	119.2	C20A—C19A—H19A	120.7
C6—C5—H5A	119.2	C18A—C19A—H19A	120.7
N17—C6—C5	121.8 (3)	C20B—C19B—C18B	119.5 (3)
N17—C6—C7	119.5 (3)	C20B—C19B—H19B	120.2
C5—C6—C7	118.6 (3)	C18B—C19B—H19B	120.2
C8—C7—C6	120.0 (3)	C21A—C20A—C19A	123.5 (3)
C8—C7—H7A	120.0	C21A—C20A—N27A	117.4 (3)
C6—C7—H7A	120.0	C19A—C20A—N27A	119.0 (3)
C7—C8—C13	122.4 (3)	C19B—C20B—C21B	122.8 (3)

C7—C8—H8A	118.8	C19B—C20B—N27B	119.2 (3)
C13—C8—H8A	118.8	C21B—C20B—N27B	117.9 (3)
C11—C9—C13	122.1 (3)	C20A—C21A—C22A	115.9 (3)
C11—C9—H9A	118.9	C20A—C21A—H21A	122.1
C13—C9—H9A	118.9	C22A—C21A—H21A	122.1
C12—N10—C14	123.7 (3)	C22B—C21B—C20B	116.4 (3)
C12—N10—C16	117.3 (3)	C22B—C21B—H21B	121.8
C14—N10—C16	119.0 (3)	C20B—C21B—H21B	121.8
C9—C11—C1	123.6 (3)	C23A—C22A—C21A	123.3 (3)
C9—C11—C12	119.4 (3)	C23A—C22A—N30A	118.8 (2)
C1—C11—C12	117.1 (3)	C21A—C22A—N30A	117.9 (2)
C4—C12—N10	122.8 (3)	C21B—C22B—C23B	122.7 (3)
C4—C12—C11	119.7 (3)	C21B—C22B—N30B	118.5 (3)
N10—C12—C11	117.5 (3)	C23B—C22B—N30B	118.8 (3)
C9—C13—C8	123.2 (3)	C22A—C23A—C18A	119.1 (2)
C9—C13—C14	119.4 (3)	C22A—C23A—H23A	120.4
C8—C13—C14	117.4 (3)	C18A—C23A—H23A	120.4
C5—C14—N10	122.2 (3)	C22B—C23B—C18B	118.9 (3)
C5—C14—C13	119.9 (3)	C22B—C23B—H23B	120.5
N10—C14—C13	117.8 (3)	C18B—C23B—H23B	120.5
C3—N15—H15B	124 (3)	O26A—C24A—O25A	126.2 (3)
C3—N15—H15A	121 (3)	O26A—C24A—C18A	118.5 (2)

H15B—N15—H15A	113 (4)	O25A—C24A—C18A	115.3 (2)
N10—C16—H16A	109.5	O26B—C24B—O25B	126.9 (3)
N10—C16—H16B	109.5	O26B—C24B—C18B	120.8 (3)
H16A—C16—H16B	109.5	O25B—C24B—C18B	112.4 (2)
N10—C16—H16C	109.5	C24A—O25A—H25B	114.1 (15)
H16A—C16—H16C	109.5	C24B—O25B—H25B	112 (2)
H16B—C16—H16C	109.5	O28A—N27A—O29A	123.7 (3)
N10—C16—H16D	109.5	O28A—N27A—C20A	118.1 (3)
H16A—C16—H16D	141.1	O29A—N27A—C20A	118.2 (3)
H16B—C16—H16D	56.3	O29B—N27B—O28B	124.4 (3)
H16C—C16—H16D	56.3	O29B—N27B—C20B	118.1 (3)
N10—C16—H16E	109.5	O28B—N27B—C20B	117.4 (3)
H16A—C16—H16E	56.3	O32A—N30A—O31A	124.0 (2)
H16B—C16—H16E	141.1	O32A—N30A—C22A	117.9 (2)
H16C—C16—H16E	56.3	O31A—N30A—C22A	118.2 (2)
H16D—C16—H16E	109.5	O31B—N30B—O32B	124.3 (3)
N10—C16—H16F	109.5	O31B—N30B—C22B	118.4 (2)
H16A—C16—H16F	56.3	O32B—N30B—C22B	117.3 (3)

Atoms	angle/°	Atoms	angle/°
C11—C1—C2—C3	1.2 (5)	C18A—C19A—C20A—N27A	−179.2 (2)

C1—C2—C3—N15	176.0 (3)	C18B—C19B—C20B—C21B	0.7 (5)
C1—C2—C3—C4	−2.3 (5)	C18B—C19B—C20B—N27B	178.4 (3)
N15—C3—C4—C12	−177.2 (3)	C19A—C20A—C21A—C22A	2.2 (4)
C2—C3—C4—C12	1.1 (5)	N27A—C20A—C21A—C22A	−179.3 (2)
C14—C5—C6—N17	179.9 (3)	C19B—C20B—C21B—C22B	0.3 (5)
C14—C5—C6—C7	−0.7 (5)	N27B—C20B—C21B—C22B	−177.4 (3)
N17—C6—C7—C8	179.8 (3)	C20A—C21A—C22A—C23A	−1.7 (4)
C5—C6—C7—C8	0.4 (5)	C20A—C21A—C22A—N30A	178.9 (3)
C6—C7—C8—C13	0.1 (5)	C20B—C21B—C22B—C23B	−1.0 (4)
C13—C9—C11—C1	−177.3 (3)	C20B—C21B—C22B—N30B	179.4 (3)
C13—C9—C11—C12	1.5 (5)	C21A—C22A—C23A—C18A	−0.3 (4)
C2—C1—C11—C9	179.9 (3)	N30A—C22A—C23A—C18A	179.1 (2)
C2—C1—C11—C12	1.1 (5)	C19A—C18A—C23A—C22A	1.8 (4)
C3—C4—C12—N10	−178.6 (3)	C24A—C18A—C23A—C22A	−176.4 (3)
C3—C4—C12—C11	1.3 (4)	C21B—C22B—C23B—C18B	0.8 (4)
C14—N10—C12—C4	−179.5 (3)	N30B—C22B—C23B—C18B	−179.6 (2)
C16—N10—C12—C4	−2.0 (4)	C19B—C18B—C23B—C22B	0.2 (4)
C14—N10—C12—C11	0.6 (4)	C24B—C18B—C23B—C22B	−179.3 (2)
C16—N10—C12—C11	178.1 (3)	C23A—C18A—C24A—O26A	6.1 (4)
C9—C11—C12—C4	178.8 (3)	C19A—C18A—C24A—O26A	−172.1 (3)
C1—C11—C12—C4	−2.4 (4)	C23A—C18A—C24A—O25A	−174.6 (3)
C9—C11—C12—N10	−1.3 (4)	C19A—C18A—C24A—O25A	7.2 (4)

C1—C11—C12—N10	177.5 (3)	C19B—C18B—C24B—O26B	−174.9 (3)
C11—C9—C13—C8	179.1 (3)	C23B—C18B—C24B—O26B	4.5 (4)
C11—C9—C13—C14	−0.9 (5)	C19B—C18B—C24B—O25B	4.5 (4)
C7—C8—C13—C9	179.6 (3)	C23B—C18B—C24B—O25B	−176.1 (2)
C7—C8—C13—C14	−0.4 (5)	C21A—C20A—N27A—O28A	180.0 (3)
C6—C5—C14—N10	−179.6 (3)	C19A—C20A—N27A—O28A	−1.5 (4)
C6—C5—C14—C13	0.4 (4)	C21A—C20A—N27A—O29A	1.3 (4)
C12—N10—C14—C5	180.0 (3)	C19A—C20A—N27A—O29A	179.9 (3)
C16—N10—C14—C5	2.5 (4)	C19B—C20B—N27B—O29B	−176.8 (3)
C12—N10—C14—C13	0.0 (4)	C21B—C20B—N27B—O29B	1.0 (5)
C16—N10—C14—C13	−177.5 (3)	C19B—C20B—N27B—O28B	3.8 (5)
C9—C13—C14—C5	−179.9 (3)	C21B—C20B—N27B—O28B	−178.5 (3)
C8—C13—C14—C5	0.1 (4)	C23A—C22A—N30A—O32A	−168.4 (3)
C9—C13—C14—N10	0.1 (4)	C21A—C22A—N30A—O32A	11.0 (4)
C8—C13—C14—N10	−179.9 (3)	C23A—C22A—N30A—O31A	11.1 (4)
C23A—C18A—C19A—C20A	−1.3 (4)	C21A—C22A—N30A—O31A	−169.5 (3)
C24A—C18A—C19A—C20A	176.8 (3)	C21B—C22B—N30B—O31B	174.1 (3)
C23B—C18B—C19B—C20B	−0.9 (4)	C23B—C22B—N30B—O31B	−5.5 (4)
C24B—C18B—C19B—C20B	178.6 (3)	C21B—C22B—N30B—O32B	−6.0 (4)
C18A—C19A—C20A—C21A	−0.8 (4)	C23B—C22B—N30B—O32B	174.3 (3)

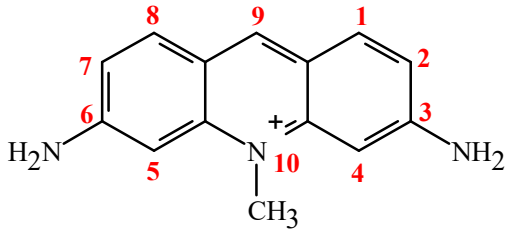
1. NMR measurements

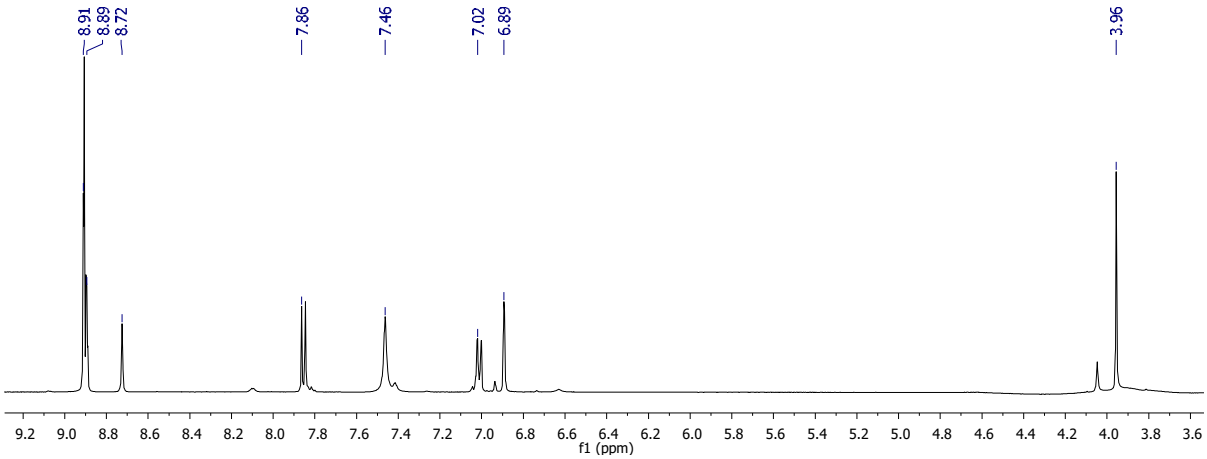
The NMR spectra of Acf-35DBNA complex were recorded on a 500 MHz Bruker spectrometer (Faculty of Chemistry, University of Gdansk, Poland). All NMR measurements were performed in a deuterated

dimethylsulfoxide (DMSO-d_6) at 300 K. Besides standard 1D proton and carbon NMR, the correlation spectroscopy (COSY), the total correlation spectroscopy (TOCSY), the rotating-frame Overhauser enhancement spectroscopy (ROESY), as well as the gradient heteronuclear single quantum coherence (^{1}H-^{13}C gHSQC) technique were used to achieve the proton and carbon assignments. Data were processed and analyzed using MestReNova 6.1. The spectra were calibrated against the DMSO-d_6 signal according to the following equations: δ_{1H} (T) = 2,6725 – 0.000795·T + 0.000000742·T^2 and δ_{13C} (T) = 36.8269 + 0.008792·T, where T [K].

^{1}H NMR (500 MHz, DMSO-d_6) δ=3.96 (s, 3H, CH_3), 6.89 (d, 2H, J=1.5 Hz, $C_{4,5}$-H), 7.01 (dd, 2H, J=1.5 Hz, 8.9 Hz, $C_{2,7}$-H), 7.86 (d, 2H, J=8.9 Hz, $C_{1,8}$-H), 8.73 (s, 1H, C_9-H), 8.91 (d, 4H, J=2.0 Hz, $C_{2,6}$-H DNBA), 8.89 (t, 2H, J=2 Hz, C_4-H DNBA); ^{13}C{H} (NMR 125.7 MHz, DMSO-d_6) δ=35.07, 93.79, 116.63, 133.48, 142.70, 128.53, 120.11, 157.18 ($C_{12,14}$), 143.55 ($C_{3,6}$), 116.67 ($C_{11,13}$), 139.55 (C_1 DNBA), 147.90 ($C_{3,5}$ DNBA) (Fig. S1)

A)





B)

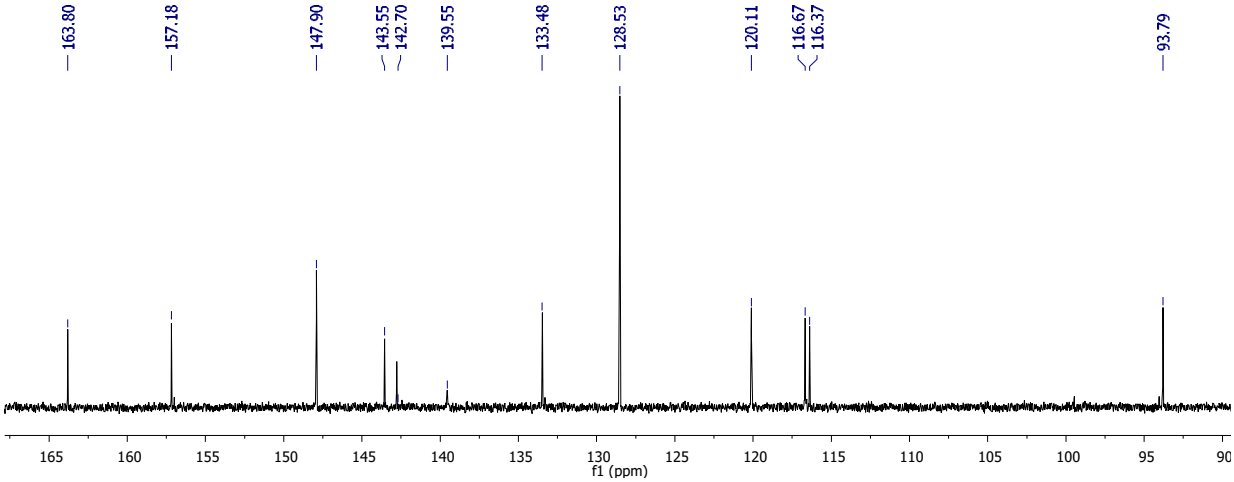


Figure S1 The ^{1}H NMR (a) and ^{13}C NMR (b) spectra of title compound.

2. FTIR measurements

The spectra were recorded at room temperature as average of 16 scans with the spectral resolution of 4 cm^{-1} using a model IFS66 Bruker infrared spectrometer (Faculty of Chemistry, University of Gdansk, Poland). The FTIR spectra were recorded for acriflavine (Acf), 3,5-dinitrbenzoic acid (DNBA) and Acf-DNBA complex. The FTIR of samples were performed on KBr pellets containing 1 mg of sample in 200 mg of KBr. FTIR (KBr) 3423 cm^{-1} (νNH_2), 1705 cm^{-1} ($\nu C{=}O$), 1537 cm^{-1} ($\nu_{as} NO_2$), 1349 cm^{-1} ($\nu_s NO_2$) (Fig. S2).

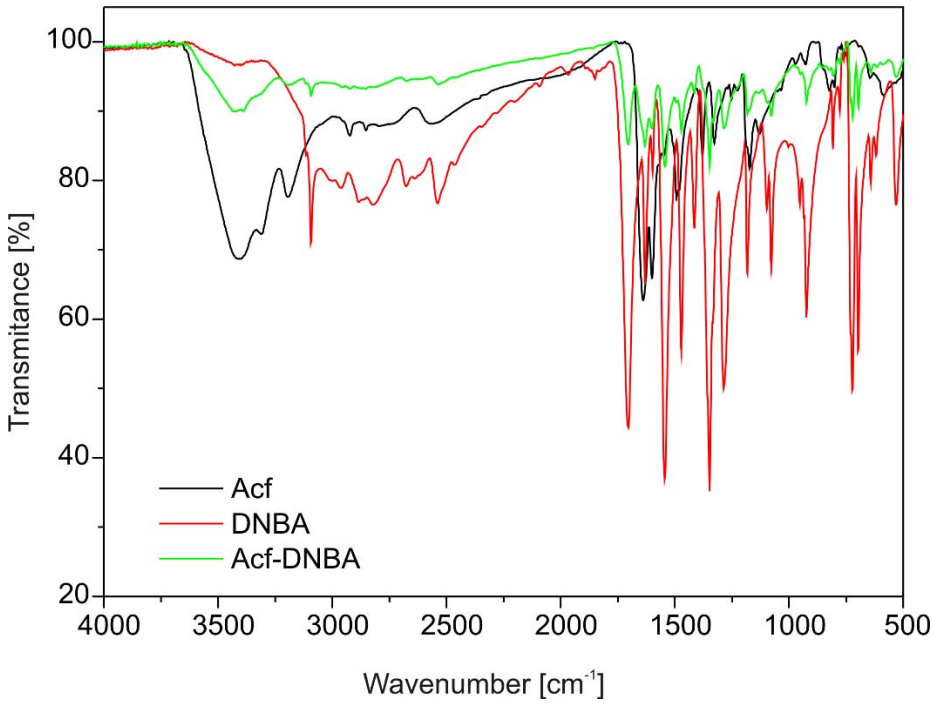


Figure S2 The FTIR spectra of acriflavine (Acf), 3,5-dinitrobenzoic acid (DNBA) and of Acf-DNBA complex in KBr pellet

3. DSC measurements

Differential scanning calorimetry (DSC) measurements were performed for title compound on a Netzsch DSC 204 instrument (Faculty of Chemistry, University of Gdansk, Poland). Sample weighing 3.0 mg were placed in an aluminum crucible (covered with an aluminum lid with pinholes) and heated at 10.0 K min^{-1} in a dynamic Ar atmosphere (m.p.=246.4 °C) (Fig. S3).

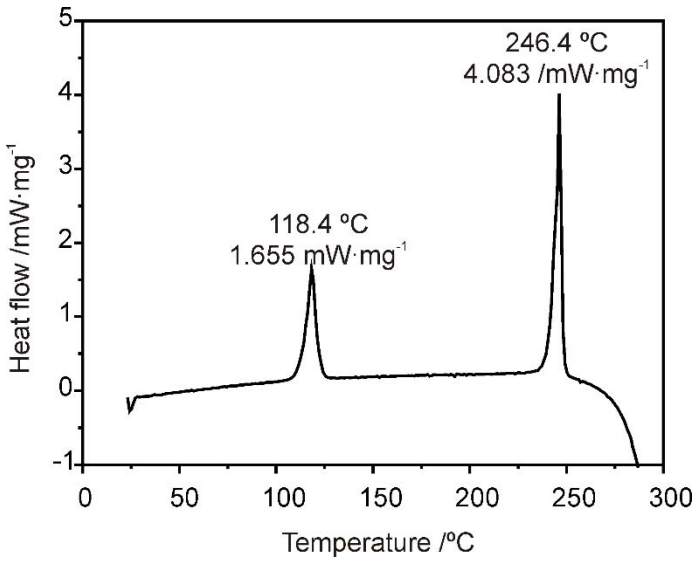


Figure S3 The DSC diagram of title compound.