

Structural revision of products resulting from the reaction of methylhydrazine with acridin-9-yl isothiocyanate due to unexpected acridinyl migration and further reactions

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>Summary of Data CCDC 632863

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>

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>

>Journal: ARKIVOC (1037)

>

>Compound: 2-(2-(9,10-dihydroacridin-9-yliden)-1-methylhydrazino)-4,5-

>dihydro-1,3-thiazol-4-one

>

>Formula: C17 H14 N4 O1 S1

>

>Unit cell parameters: a 5.1320(9) b 17.205(2) c 17.042(3) beta
90.183(15)

>

space group P21/c

>

>Summary of Data CCDC 632864

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>

>Authors:

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>

>Journal: ARKIVOC (1037)

>

>Compound: 1-(9,10-dihydroacridin-9-yliden)-2-methylthiosemicarbazide

>methanol solvate

>

>Formula: C16 H18 N4 O1 S1

>

>Unit cell parameters: a 13.0477(19) b 21.262(3) c 12.0046(19) beta
106.961(12)

>

space group C2/c

>

>

data_compound6

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_publ_contact_author_email 'us@chem.uni-potsdam.de'
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ARKIVOC

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on F, with F set to zero for negative F2. The threshold expression
of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc.
and is
not relevant to the choice of reflections for refinement. R-factors
based
on F2 are statistically about twice as large as those based on F,
and R-
factors based on ALL data will be even larger.
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P=(Fo2+2Fc2)/3'
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All hydrogen atoms were found from the difference Fourier map.
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C3 C 1.3033(7) 0.6515(2) -0.35867(18) 0.0356(9) Uani 1 1 d . . .
H3 H 1.132(7) 0.642(2) -0.3315(15) 0.043 Uiso 1 1 d . . .
C4 C 1.3887(8) 0.5928(2) -0.41058(18) 0.0405(10) Uani 1 1 d . . .
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C5 C 1.5969(7) 0.6085(2) -0.45904(18) 0.0350(9) Uani 1 1 d . . .
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C6 C 1.7246(6) 0.6802(2) -0.45622(15) 0.0272(8) Uani 1 1 d . . .
C7 C 2.0394(6) 0.7653(2) -0.51475(15) 0.0269(8) Uani 1 1 d . . .
C8 C 2.2293(7) 0.7778(2) -0.57308(16) 0.0344(10) Uani 1 1 d . . .
H8 H 2.276(6) 0.734(2) -0.6090(16) 0.041 Uiso 1 1 d . . .
C9 C 2.3406(8) 0.8500(2) -0.58182(17) 0.0433(11) Uani 1 1 d . . .
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C11 C 2.0906(7) 0.8992(2) -0.47344(17) 0.0349(9) Uani 1 1 d . . .
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C12 C 1.9776(7) 0.82648(19) -0.46236(16) 0.0256(8) Uani 1 1 d . . .
C13 C 1.8027(6) 0.8091(2) -0.39584(15) 0.0261(8) Uani 1 1 d . . .
C14 C 1.7841(8) 0.7818(2) -0.21849(19) 0.0343(9) Uani 1 1 d . . .
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C15 C 1.5059(7) 0.89364(19) -0.24293(15) 0.0264(8) Uani 1 1 d . . .
C16 C 1.1862(7) 1.0032(2) -0.22912(18) 0.0340(9) Uani 1 1 d . . .
H16A H 1.014(7) 1.008(2) -0.2556(14) 0.041 Uiso 1 1 d . . .
H16B H 1.228(7) 1.051(2) -0.2074(17) 0.041 Uiso 1 1 d . . .
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N2 N 1.8161(6) 0.86246(16) -0.33932(12) 0.0304(8) Uani 1 1 d . . .
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O O 1.0326(5) 0.94027(14) -0.11146(11) 0.0425(7) Uani 1 1 d . . .
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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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 C5 C6 N1 C7 172.6(3) ?
 C1 C6 N1 C7 -7.9(5) ?
 C1 C13 N2 N3 6.5(5) ?
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 S C15 N3 N2 4.7(4) ?
 N4 C15 N3 C14 -15.4(5) ?
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 S C15 N4 C17 2.7(4) ?
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Structural revision of products resulting from the reaction of methylhydrazine with acridin-9-ylisothiocyanate due to unexpected acridinyl migration and further reactions

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goodness of fit S are based on F2, conventional R-factors R are
based
on F, with F set to zero for negative F2. The threshold expression
of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc.
and is
not relevant to the choice of reflections for refinement. R-factors
based
on F2 are statistically about twice as large as those based on F,
and R-
factors based on ALL data will be even larger.
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P=(Fo2+2Fc2)/3'
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H2 H 0.458(2) -0.0527(12) -0.042(2) 0.041(7) Uiso 1 1 d . . .
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H14C H 0.393(4) -0.0357(19) 0.293(4) 0.106(14) Uiso 1 1 d . . .
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H41 H 0.195(2) -0.0408(12) -0.051(2) 0.041(7) Uiso 1 1 d . . .
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into account individually in the estimation of esds in distances,
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and torsion angles; correlations between esds in cell parameters are
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C8 C7 C12 C11 -2.0(3) ?
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S C15 N3 C14 -12.3(3) ?
C13 N2 N3 C15 -131.0(2) ?
C13 N2 N3 C14 75.0(3) ?

_diffn_measured_fraction_theta_max 0.999
_diffn_reflns_theta_full 24.99
_diffn_measured_fraction_theta_full 0.999
_refine_diff_density_max 0.506
_refine_diff_density_min -0.253
_refine_diff_density_rms 0.044