Crystal structure of 3-(*p*-chlorophenyl)-5-methyl-2-(8-quinolinyl)-4-thiazolidinone, C₁₉H₁₆ClN₂OS

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Abstract

C₁₉H₁₆ClN₂OS, orthorhombic, *Pca*2₁ (No. 29), *a* = 8.1248(1) Å, *b* = 19.1264(2) Å, *c* = 21.7702(2) Å, *V* = 3383.0 Å³, *Z* = 8, *R*_{gt}(*F*) = 0.069, *wR*_{ref}(*F*²) = 0.188, *T* = 293 K.

Source of material

Quinoline-8-[*N*-(*p*-chlorophenyl)formimidolyl] (0.01 mole) with thiolactic acid (0.015 mole) in dry benzene was refluxed on a water-bath for 15 hours, cooled and poured into water. The upper organic layer was washed with NaHCO₃ solution (15 ml, 10%) and then with water, dried (CaCl₂) and benzene distilled off. The residue on crystallisation from petroluem ether (313 K – 333 K) / EtOH (1:1) gave the thiazolidinones obtained high yields.

Discussion

4-Thiazolidinones are the derivatives of thiazolidine which belong to an important group of heterocyclic compounds. Diverse biological activities such as bactericidal, pesticidal, fungicidal, insecticidal, anticonvulsant, tuberculostatic, antiinflammatory, antihyroidal etc. have found to be associated with thiazolidinone derivatives [1–3]. The biological significance of that kind of compounds urged us to study the synthesis of some 4-thiazolidinones for their possible activities [4]. However, no examples substituted by the quinoline ring at 2-positions have been recorded. In order to elucidate the stereochemistry of the title compound, we carried out the crystal structure determination.

There are two independent molecules in the asymmetric unit. The quinolinyl ring is planar and thiazolidinone ring adopts envelope conformation. In molecule A, the folding angle between the least-squares planes of the quinolinyl and the phenyl ring is 87.3(2)° and in molecule B the corresponding value is 88.2(1)°. The quinolinyl and phenyl rings are planar in each case, with the largest deviations from the least-squares plane due to atoms C1A [0.039(1) Å] and C9B [0.010(5) Å] in molecule A and B respectively. The mean N—C distance in the quinolinyl ring is 1.333(8) Å and the mean C—C distance in the phenyl ring is 1.376(2) Å in the normal range [5]. In the both of the molecule, the angles C3—C4—C5 is greater than 120° [122.8(6)° in molecule A and 124.4(7)° in molecule B] and the angles N1—C9—C8 is smaller than 120° in molecule B [117.4(4)°] whilst 120.3(5)° in molecule A [6]. The dihedral angle between the plane of the quinolinyl and that of the phenyl ring is 87.3(2)°, that between the thiazolidinone and the quinolinyl rings is 73.1(2)° and that between the phenyl and thiazolidinone rings is 55.9(2)°. In molecule B, these angles are 88.2(1)°, 69.2(2)° and 57.9(3)°, respectively. The five-membered ring of the thiazolidinone moiety has an envelope conformation with the C18 atom out-of-plane in the molecule A and B [−0.121(1) Å, 0.197(1) Å, respectively] and the asymmetry parameters defined by Nardelli [7] are *q*₂ = 0.120(1), *φ*₂ = −141.0(3)° for molecule A and *q*₂ = 0.210(1), *φ*₂ = −151.0(2)° for molecule B.

Table 1. Data collection and handling.

Crystal:	light yellow, block, size 0.36 × 0.48 × 0.62 mm
Wavelength:	Mo K _α radiation (0.71073 Å)
μ:	3.6 cm ^{−1}
Diffraction, scan mode:	Siemens SMART CCD, ω
2θ _{max} :	50°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	13761, 5876
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 5023
<i>N</i> (<i>param</i>) _{refined} :	434
Programs:	PARST [7], SADABS [8], PLATON [9], SHELXTL [10]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1AA)	4a	0.4104	0.1520	0.5204	0.066
H(1AB)	4a	0.2889	0.0923	0.5890	0.070
H(2AA)	4a	0.0840	0.0128	0.5633	0.097
H(3AA)	4a	0.0140	−0.0016	0.4639	0.087
H(5AA)	4a	0.0795	0.0224	0.3520	0.080
H(6AA)	4a	0.2327	0.0881	0.2791	0.085
H(7AA)	4a	0.4247	0.1619	0.3107	0.063
H(10A)	4a	0.4994	0.2176	0.4639	0.076
H(12A)	4a	0.3703	0.3247	0.4560	0.086
H(13A)	4a	0.1933	0.4093	0.4337	0.100
H(15A)	4a	0.2683	0.3936	0.2566	0.097
H(16A)	4a	0.4769	0.3098	0.2751	0.097
H(18B)	4a	0.8437	0.1848	0.3581	0.126
H(19A)	4a	1.0019	0.2712	0.3660	0.166
H(19B)	4a	1.0581	0.1940	0.3783	0.166
H(19C)	4a	1.0290	0.2452	0.4335	0.166

Table 2. Continued.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1BA)	4a	−0.0791	0.3432	0.0107	0.059
H(1BB)	4a	−0.2162	0.4015	−0.0633	0.080
H(2BA)	4a	−0.4144	0.4822	−0.0394	0.080
H(3BA)	4a	−0.4742	0.5058	0.0637	0.093
H(5BA)	4a	−0.4203	0.4757	0.1759	0.109
H(6BA)	4a	−0.2752	0.4175	0.2453	0.093
H(7BA)	4a	−0.0694	0.3326	0.2129	0.085
H(10B)	4a	−0.0011	0.2767	0.0638	0.071
H(12B)	4a	−0.1167	0.1718	0.0750	0.091
H(13B)	4a	−0.3328	0.0927	0.0951	0.083
H(15B)	4a	−0.2202	0.1100	0.2747	0.120
H(16B)	4a	−0.0324	0.1956	0.2519	0.103
H(18A)	4a	0.4234	0.3017	0.1552	0.145
H(19D)	4a	0.5294	0.2210	0.0930	0.197
H(19E)	4a	0.5157	0.2943	0.0613	0.197
H(19F)	4a	0.3885	0.2354	0.0455	0.197

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cl(1A)	4a	0.0621(3)	0.4720(1)	0.3267(1)	0.114(2)	0.092(1)	0.112(2)	0.021(1)	0.002(2)	0.025(1)
S(1A)	4a	0.7261(3)	0.1497(2)	0.4315(1)	0.056(1)	0.159(2)	0.154(2)	−0.030(1)	−0.036(1)	0.102(2)
O(1A)	4a	0.7788(7)	0.3135(3)	0.3329(3)	0.113(4)	0.093(3)	0.090(4)	0.013(3)	0.053(3)	0.047(3)
N(1A)	4a	0.3378(6)	0.1221(2)	0.5085(2)	0.063(3)	0.045(2)	0.057(3)	0.004(2)	−0.001(2)	0.013(2)
N(2A)	4a	0.5701(6)	0.2586(2)	0.3820(2)	0.057(3)	0.058(3)	0.051(3)	−0.021(2)	−0.009(2)	0.025(2)
C(1A)	4a	0.2618(9)	0.0865(3)	0.5479(3)	0.075(4)	0.043(3)	0.058(4)	0.000(3)	0.017(3)	0.004(3)
C(2A)	4a	0.138(1)	0.0380(3)	0.5327(5)	0.075(5)	0.054(4)	0.114(7)	−0.014(3)	0.028(5)	0.008(4)
C(3A)	4a	0.0984(9)	0.0291(3)	0.4744(4)	0.072(4)	0.065(4)	0.081(5)	−0.030(3)	−0.002(4)	0.012(4)
C(4A)	4a	0.1854(8)	0.0664(3)	0.4266(4)	0.060(3)	0.034(2)	0.083(5)	0.001(2)	0.000(3)	0.008(3)
C(5A)	4a	0.1576(8)	0.0549(3)	0.3649(4)	0.065(4)	0.043(3)	0.092(5)	−0.022(3)	−0.026(4)	0.013(3)
C(6A)	4a	0.251(1)	0.0939(3)	0.3210(3)	0.095(5)	0.062(3)	0.055(4)	−0.002(4)	−0.010(4)	0.002(3)
C(7A)	4a	0.3640(8)	0.1380(3)	0.3402(2)	0.071(4)	0.051(3)	0.035(3)	0.008(3)	−0.005(3)	0.006(2)
C(8A)	4a	0.3994(6)	0.1517(3)	0.4031(3)	0.038(3)	0.055(3)	0.046(3)	0.002(2)	−0.009(2)	0.002(2)
C(9A)	4a	0.3067(7)	0.1141(3)	0.4468(3)	0.045(3)	0.048(3)	0.049(3)	0.014(2)	−0.003(2)	0.007(2)
C(10A)	4a	0.5297(8)	0.1988(3)	0.4235(3)	0.070(4)	0.077(4)	0.044(3)	−0.022(3)	−0.012(3)	0.025(3)
C(11A)	4a	0.4470(8)	0.3076(3)	0.3687(3)	0.073(4)	0.054(3)	0.045(3)	−0.029(3)	−0.006(3)	0.003(3)
C(12A)	4a	0.3554(9)	0.3384(4)	0.4154(3)	0.059(4)	0.109(5)	0.046(4)	−0.004(4)	0.001(3)	0.008(3)
C(13A)	4a	0.247(1)	0.3872(4)	0.4015(4)	0.089(5)	0.088(5)	0.072(5)	−0.012(4)	−0.006(4)	0.009(4)
C(14A)	4a	0.2092(9)	0.4074(3)	0.3435(4)	0.075(5)	0.062(4)	0.078(5)	−0.013(3)	−0.014(4)	0.015(4)
C(15A)	4a	0.292(1)	0.3797(4)	0.2965(3)	0.111(7)	0.085(5)	0.048(4)	0.013(5)	−0.013(4)	0.021(4)
C(16A)	4a	0.417(1)	0.3287(4)	0.3074(3)	0.128(7)	0.070(4)	0.043(4)	0.020(4)	0.009(4)	0.002(3)
C(17A)	4a	0.729(1)	0.2657(3)	0.3670(3)	0.086(5)	0.074(4)	0.060(4)	−0.016(4)	0.002(4)	0.003(3)
C(18A)	4a	0.8354(9)	0.2120(5)	0.3961(4)	0.085(5)	0.112(6)	0.118(7)	−0.003(5)	0.048(5)	0.017(5)
C(19A)	4a	0.9920(8)	0.2320(4)	0.3933(4)	0.067(4)	0.120(6)	0.145(7)	−0.014(4)	−0.031(4)	0.066(5)
Cl(1B)	4a	−0.4396(3)	0.0285(1)	0.2016(1)	0.096(1)	0.083(1)	0.098(2)	−0.005(1)	−0.011(1)	0.018(1)
S(1B)	4a	0.2236(3)	0.3433(2)	0.0924(2)	0.060(1)	0.163(2)	0.170(3)	0.021(1)	0.029(2)	0.120(2)
O(1B)	4a	0.2779(6)	0.1823(3)	0.1912(3)	0.079(4)	0.106(3)	0.121(5)	0.050(3)	0.000(3)	0.034(4)
N(1B)	4a	−0.1531(6)	0.3732(2)	0.0208(2)	0.047(3)	0.045(2)	0.057(3)	0.011(2)	−0.010(2)	−0.003(2)
N(2B)	4a	0.0678(7)	0.2447(3)	0.1479(2)	0.071(3)	0.069(3)	0.049(3)	0.027(2)	0.002(3)	0.004(2)
C(1B)	4a	−0.2392(9)	0.4099(3)	−0.0221(4)	0.068(4)	0.060(3)	0.071(4)	−0.002(3)	−0.017(4)	0.017(3)
C(2B)	4a	−0.3587(9)	0.4588(3)	−0.0082(4)	0.071(4)	0.061(4)	0.067(4)	−0.008(3)	−0.028(4)	0.017(3)
C(3B)	4a	−0.3949(9)	0.4728(3)	0.0533(5)	0.057(4)	0.045(3)	0.131(8)	0.006(3)	−0.025(4)	0.006(4)
C(4B)	4a	−0.3112(7)	0.4367(3)	0.0983(3)	0.045(3)	0.056(3)	0.069(4)	0.011(2)	−0.001(3)	0.000(3)
C(5B)	4a	−0.339(1)	0.4447(4)	0.1628(4)	0.092(6)	0.094(5)	0.086(6)	0.020(5)	0.011(5)	−0.038(5)
C(6B)	4a	−0.256(1)	0.4100(4)	0.2037(4)	0.087(5)	0.083(4)	0.064(4)	0.035(4)	0.023(4)	−0.012(4)
C(7B)	4a	−0.1280(9)	0.3580(3)	0.1837(4)	0.071(4)	0.069(4)	0.073(5)	0.030(3)	0.005(3)	−0.001(3)
C(8B)	4a	−0.1000(7)	0.3488(3)	0.1260(3)	0.056(3)	0.039(3)	0.055(3)	0.006(2)	−0.001(3)	0.009(2)
C(9B)	4a	−0.1903(6)	0.3865(2)	0.0795(3)	0.043(3)	0.029(2)	0.058(3)	0.005(2)	−0.005(3)	0.001(2)
C(10B)	4a	0.0336(7)	0.2982(3)	0.1025(3)	0.055(3)	0.068(4)	0.056(4)	0.031(3)	0.009(3)	0.013(3)
C(11B)	4a	−0.0590(7)	0.1918(3)	0.1623(3)	0.055(3)	0.064(4)	0.049(3)	0.011(3)	0.005(3)	0.009(3)
C(12B)	4a	−0.143(1)	0.1604(4)	0.1154(3)	0.093(5)	0.088(5)	0.046(4)	0.018(4)	0.010(4)	0.007(3)
C(13B)	4a	−0.2692(8)	0.1111(4)	0.1267(3)	0.055(3)	0.100(5)	0.053(4)	0.003(3)	−0.010(3)	−0.007(4)
C(14B)	4a	−0.2933(8)	0.0913(3)	0.1878(3)	0.074(5)	0.062(3)	0.060(4)	0.011(3)	−0.011(3)	0.004(3)
C(15B)	4a	−0.203(1)	0.1230(4)	0.2341(4)	0.146(9)	0.086(5)	0.068(5)	−0.029(6)	−0.018(5)	0.014(4)
C(16B)	4a	−0.089(1)	0.1737(5)	0.2203(4)	0.103(6)	0.098(6)	0.057(5)	−0.004(4)	0.002(4)	0.018(4)
C(17B)	4a	0.2300(8)	0.2288(3)	0.1608(3)	0.064(4)	0.076(4)	0.073(5)	0.021(3)	−0.016(3)	0.023(4)
C(18B)	4a	0.3533(9)	0.2786(5)	0.1247(5)	0.066(4)	0.150(7)	0.148(8)	0.058(5)	0.037(5)	0.095(6)
C(19B)	4a	0.455(1)	0.2556(4)	0.0775(5)	0.097(5)	0.097(5)	0.20(1)	0.022(4)	0.090(6)	0.013(6)

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