Crystal structure of 4-methyl-5-(5-{[5-(4-methyl-2-phenyl-1,3-thiazol-5-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl]disulfanyl}-4-phenyl-4*H*-1,2,4-triazol-3-yl)-2-phenyl-1,3-thiazol acetonitrile, (C₃₆H₂₆N₈S₄)(C₂H₃N)

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Abstract

C₃₈H₂₉N₉S₄, monoclinic, *P*12₁/*n*1 (No. 14), *a* = 13.099(7) Å, *b* = 19.66(1) Å, *c* = 13.914(7) Å, β = 94.97(1)°, *V* = 3569.8 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.056, *wR*_{ref}(*F*²) = 0.116, *T* = 140 K.

Source of material

The title compound was synthesized in accordance with published procedure [1,2]. The solution of title compound (0.25 g) in acetonitrile-benzene-methanol (1:1:1, 50 ml) left in room temperature for two weeks. The yellow crystals were filtered off, washed with cold acetonitrile-benzene-methanol (1:1:1, 8 ml) and dried in vacuum over P₄O₁₀ (mp 462 K; yield 60%). Elemental analyses were consistent with the stoichiometry C₃₆H₂₆N₈S₄ · C₂H₃N (found: C, 61.70%; H, 4.04%; N, 17.12%; calc.: C, 61.68%; H, 3.95%; N, 17.04%). Melting points were measured on an Electrothermal 9100 apparatus and are uncorrected. Elemental analyses were performed using a Heraeus CHN-O-Rapid analyzer.

Discussion

Thiazolo-1,2,4-triazole derivatives exhibit antibacterial and antifungal activity [1,2]. In the recent years there has been increasing interest in the determination of crystal structures of biologically active compounds [3–14].

In the crystal structure of title compound, the covalent bonds are found to be normal. Relevant bond lengths: *d*(S3–C3) = 1.720(2) Å, *d*(S3–C5) = 1.716(4) Å, *d*(S1–C1) = 1.731(4) Å, *d*(C2–C3) = 1.466(5) Å, *d*(S1–S2) = 2.074(2) Å, *d*(N1–C13) = 1.424(6) Å, *d*(C5–C6) = 1.461(6) Å, *d*(C4–C12) = 1.498(6) Å. The angles at the S atoms [102.3(2)° at S1, 100.8(2)° at S2 and 89.9(2)° at S3] are almost the same as in the previous reports [13–15]. The torsion angles ∠N4–C5–C6–C11, ∠N2–C2–C3–C4 and ∠C1–N1–C13–C18 (19.8(7)°, 14.1(7)° and 78.8(6)°, respectively)

show clearly that the four rings do not share a common plane, and probably it is the result of electrostatic repulsive and steric interactions [13–15]. The torsion angle ∠C1–S1–S2–C19 is 68.7(2)°, indicating that the conformation in along the S1–S2 bond is approximately *gauche* (*synclinal*) [15]. It seems that in this conformation electrostatic repulsive and steric interactions are in minimum limit in the presence of acetonitrile molecule in the crystal packing. Intermolecular ring stacking is observed within the crystals, probably is as a result of the presence of parallel aromatic rings in the crystal network. Intermolecular electrostatic attractive interactions between N6 and S2 atoms are observed within the crystals, probably is as a result of the presence of electron-poor (N6) and electron-rich (S2) atoms in suitable positions in the crystal network. These intermolecular interactions appears to be a plausible factors in the stabilization of the crystal packing.

Table 1. Data collection and handling.

Crystal:	yellow prism, size 0.1 × 0.15 × 0.2 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.09 cm ⁻¹
Diffractionmeter, scan mode:	Bruker SMART 1000 CCD, ϕ/ω
2 θ _{max} :	54.06°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	23605, 7788
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 2198
<i>N</i> (<i>param</i>) _{refined} :	463
Programs:	SHELXTL [16], SADABS [17]

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(7)	4e	0.0890	–0.1189	–0.6735	0.062
H(8)	4e	–0.0606	–0.1549	–0.7592	0.063
H(9)	4e	–0.0891	–0.2715	–0.7838	0.056
H(10)	4e	0.0279	–0.3495	–0.7177	0.054
H(11)	4e	0.1791	–0.3134	–0.6316	0.052
H(12A)	4e	0.4923	–0.2704	–0.4749	0.077
H(12B)	4e	0.5412	–0.1982	–0.4440	0.077
H(12C)	4e	0.5400	–0.2233	–0.5535	0.077
H(14)	4e	0.2677	–0.0669	–0.2841	0.092
H(15)	4e	0.0910	–0.0428	–0.2954	0.135
H(16)	4e	0.0201	0.0381	–0.3994	0.141
H(17)	4e	0.1235	0.0990	–0.4936	0.129
H(18)	4e	0.2986	0.0734	–0.4935	0.082
H(25)	4e	0.9996	0.1436	0.1408	0.056
H(26)	4e	1.1460	0.1845	0.2294	0.064
H(27)	4e	1.2698	0.1090	0.2956	0.064

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Table 2. Continued.

Atom	Site	x	y	z	<i>U</i> _{iso}
H(28)	4e	1.2485	−0.0063	0.2706	0.057
H(29)	4e	1.1036	−0.0492	0.1841	0.054
H(30A)	4e	0.7136	−0.1349	0.0391	0.082
H(30B)	4e	0.8033	−0.1552	0.1194	0.082
H(30C)	4e	0.8225	−0.1590	0.0074	0.082
H(32)	4e	0.7221	0.1270	−0.1891	0.043
H(33)	4e	0.7825	0.2388	−0.1674	0.052

Table 2. Continued.

Atom	Site	x	y	z	<i>U</i> _{iso}
H(34)	4e	0.7559	0.2978	−0.0279	0.060
H(35)	4e	0.6624	0.2497	0.0884	0.053
H(36)	4e	0.6005	0.1385	0.0705	0.050
H(38A)	4e	0.4506	0.3144	−0.0607	0.131
H(38B)	4e	0.5128	0.2734	−0.1361	0.131
H(38C)	4e	0.4427	0.2333	−0.0663	0.131

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

Atom	Site	x	y	z	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
S(1)	4e	0.4955(1)	0.09472(5)	−0.30463(8)	0.060(1)	0.0480(7)	0.0428(7)	−0.0117(7)	0.0006(6)	0.0025(6)
S(2)	4e	0.4375(1)	0.07778(5)	−0.17270(8)	0.0378(9)	0.0484(7)	0.0461(7)	−0.0011(6)	−0.0001(6)	0.0015(6)
S(3)	4e	0.2498(1)	−0.10921(5)	−0.53592(8)	0.0453(9)	0.0414(6)	0.0492(8)	0.0015(6)	0.0008(6)	−0.0050(6)
S(4)	4e	0.8481(1)	0.06554(5)	0.04760(8)	0.0348(9)	0.0417(6)	0.0572(8)	−0.0034(6)	0.0004(6)	0.0079(6)
N(1)	4e	0.4013(3)	−0.0185(2)	−0.3937(2)	0.049(3)	0.042(2)	0.039(2)	−0.007(2)	0.003(2)	−0.004(2)
N(2)	4e	0.5381(3)	−0.0788(2)	−0.4229(2)	0.031(3)	0.048(2)	0.051(2)	−0.003(2)	0.000(2)	0.006(2)
N(3)	4e	0.5695(3)	−0.0209(2)	−0.3728(3)	0.043(3)	0.044(2)	0.048(2)	−0.007(2)	−0.007(2)	0.006(2)
N(4)	4e	0.3275(3)	−0.2245(2)	−0.5736(2)	0.044(3)	0.040(2)	0.039(2)	−0.005(2)	0.003(2)	0.002(2)
N(5)	4e	0.6246(3)	0.0529(1)	−0.0697(2)	0.034(3)	0.035(2)	0.032(2)	−0.002(2)	0.006(2)	−0.004(2)
N(6)	4e	0.6164(3)	−0.0587(2)	−0.0521(2)	0.043(3)	0.039(2)	0.043(2)	0.000(2)	0.004(2)	−0.001(2)
N(7)	4e	0.5288(3)	−0.0368(2)	−0.1051(2)	0.041(3)	0.037(2)	0.035(2)	−0.000(2)	0.007(2)	−0.000(2)
N(8)	4e	0.9184(3)	−0.0498(2)	0.1062(2)	0.042(3)	0.048(2)	0.038(2)	0.007(2)	0.004(2)	−0.003(2)
N(9)	4e	0.2979(6)	0.2837(4)	−0.2287(5)	0.098(7)	0.247(7)	0.150(6)	−0.056(6)	−0.052(5)	0.052(5)
C(1)	4e	0.4896(4)	0.0145(2)	−0.3560(3)	0.044(4)	0.045(3)	0.038(3)	−0.005(3)	−0.002(3)	0.005(2)
C(2)	4e	0.4380(4)	−0.0761(2)	−0.4352(3)	0.044(4)	0.039(3)	0.033(3)	−0.002(3)	0.007(2)	0.006(2)
C(3)	4e	0.3728(4)	−0.1264(2)	−0.4887(3)	0.042(4)	0.041(2)	0.035(3)	0.000(2)	0.006(2)	0.004(2)
C(4)	4e	0.3999(4)	−0.1903(2)	−0.5183(3)	0.045(4)	0.041(3)	0.038(3)	−0.003(3)	0.007(2)	0.010(2)
C(5)	4e	0.2434(4)	−0.1879(2)	−0.5894(3)	0.039(4)	0.041(2)	0.036(3)	−0.001(2)	0.003(2)	0.005(2)
C(6)	4e	0.1498(4)	−0.2122(2)	−0.6433(3)	0.045(4)	0.037(3)	0.038(3)	0.005(2)	0.005(2)	−0.001(2)
C(7)	4e	0.0770(4)	−0.1662(2)	−0.6824(3)	0.061(4)	0.048(3)	0.045(3)	−0.001(3)	−0.003(3)	−0.008(2)
C(8)	4e	−0.0116(4)	−0.1872(2)	−0.7336(3)	0.039(4)	0.063(3)	0.054(3)	0.005(3)	−0.002(3)	−0.006(3)
C(9)	4e	−0.0287(4)	−0.2563(2)	−0.7475(3)	0.039(4)	0.055(3)	0.043(3)	−0.002(3)	−0.005(2)	−0.001(2)
C(10)	4e	0.0408(4)	−0.3022(2)	−0.7091(3)	0.046(4)	0.042(3)	0.047(3)	−0.009(3)	0.012(3)	−0.003(2)
C(11)	4e	0.1306(4)	−0.2808(2)	−0.6574(3)	0.039(4)	0.048(3)	0.042(3)	0.008(2)	0.005(2)	0.002(2)
C(12)	4e	0.5022(4)	−0.2234(2)	−0.4957(3)	0.051(4)	0.044(2)	0.059(3)	0.001(3)	0.008(3)	0.000(2)
C(13)	4e	0.2974(4)	0.0018(2)	−0.3905(4)	0.047(4)	0.049(3)	0.063(4)	−0.005(3)	0.010(3)	−0.024(3)
C(14)	4e	0.2384(5)	−0.0340(3)	−0.3283(4)	0.059(5)	0.114(5)	0.059(4)	−0.033(4)	0.021(3)	−0.018(3)
C(15)	4e	0.1340(7)	−0.0187(4)	−0.3352(5)	0.076(8)	0.181(9)	0.087(6)	−0.053(6)	0.040(5)	−0.075(5)
C(16)	4e	0.0915(6)	0.0292(4)	−0.3962(7)	0.041(6)	0.110(6)	0.21(1)	−0.013(5)	0.048(6)	−0.085(6)
C(17)	4e	0.1524(6)	0.0641(3)	−0.4526(6)	0.041(5)	0.053(4)	0.227(8)	0.003(3)	0.010(5)	−0.031(4)
C(18)	4e	0.2569(4)	0.0498(2)	−0.4518(4)	0.025(4)	0.042(3)	0.141(5)	−0.004(3)	0.023(3)	−0.005(3)
C(19)	4e	0.5351(4)	0.0288(2)	−0.1150(3)	0.041(4)	0.036(2)	0.035(3)	−0.006(2)	0.002(2)	−0.007(2)
C(20)	4e	0.6738(4)	−0.0039(2)	−0.0309(3)	0.044(4)	0.031(2)	0.032(3)	−0.002(2)	0.013(2)	−0.001(2)
C(21)	4e	0.7733(4)	−0.0054(2)	0.0229(3)	0.037(3)	0.035(2)	0.034(3)	0.001(2)	0.006(2)	0.001(2)
C(22)	4e	0.8243(4)	−0.0618(2)	0.0597(3)	0.035(3)	0.043(3)	0.041(3)	−0.003(2)	0.003(2)	−0.002(2)
C(23)	4e	0.9407(3)	0.0154(2)	0.1052(3)	0.033(3)	0.041(2)	0.038(3)	0.002(2)	0.013(2)	0.007(2)
C(24)	4e	1.0361(4)	0.0432(2)	0.1545(3)	0.042(4)	0.046(3)	0.032(3)	−0.004(2)	0.005(2)	0.006(2)
C(25)	4e	1.0500(4)	0.1127(2)	0.1678(3)	0.034(4)	0.056(3)	0.048(3)	−0.005(2)	−0.002(2)	0.013(2)
C(26)	4e	1.1369(4)	0.1370(2)	0.2202(3)	0.049(4)	0.046(3)	0.063(4)	−0.008(3)	−0.001(3)	0.007(3)
C(27)	4e	1.2104(4)	0.0924(2)	0.2590(3)	0.049(4)	0.053(3)	0.057(3)	−0.012(3)	0.000(3)	0.010(3)
C(28)	4e	1.1971(4)	0.0242(2)	0.2445(3)	0.032(4)	0.057(3)	0.054(3)	0.004(3)	0.003(3)	0.012(3)
C(29)	4e	1.1115(4)	−0.0015(2)	0.1932(3)	0.038(4)	0.050(3)	0.047(3)	0.004(3)	0.006(2)	0.003(2)
C(30)	4e	0.7878(4)	−0.1340(2)	0.0561(3)	0.048(4)	0.040(3)	0.074(4)	0.009(2)	−0.006(3)	0.004(2)
C(31)	4e	0.6572(4)	0.1229(2)	−0.0599(3)	0.039(3)	0.026(2)	0.038(3)	0.001(2)	0.000(2)	0.001(2)
C(32)	4e	0.7106(3)	0.1518(2)	−0.1324(3)	0.034(3)	0.036(2)	0.038(3)	0.000(2)	0.005(2)	0.005(2)
C(33)	4e	0.7462(4)	0.2178(2)	−0.1191(3)	0.038(4)	0.041(3)	0.051(3)	−0.004(2)	0.008(2)	0.008(2)
C(34)	4e	0.7295(4)	0.2530(2)	−0.0369(4)	0.049(4)	0.037(3)	0.064(4)	−0.002(3)	0.000(3)	−0.009(3)
C(35)	4e	0.6749(4)	0.2242(2)	0.0327(3)	0.041(4)	0.041(3)	0.051(3)	−0.002(2)	0.009(2)	−0.011(2)
C(36)	4e	0.6380(3)	0.1586(2)	0.0224(3)	0.046(4)	0.036(2)	0.044(3)	−0.003(2)	0.012(2)	−0.008(2)
C(37)	4e	0.3647(6)	0.2806(3)	−0.1739(5)	0.058(6)	0.099(4)	0.104(6)	−0.024(4)	−0.016(4)	0.013(4)
C(38)	4e	0.4492(5)	0.2750(3)	−0.1039(4)	0.064(5)	0.103(4)	0.094(5)	0.000(4)	0.005(4)	−0.010(4)

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