Crystal structure of [S-(R*,R*)]-1-[3-(2,2-dimethyl-4-phenyloxazolidine-3-yl)-1-methyl-2-[methylidene-3-oxopropyl]-4-phenyl-1,2,4-triazolidine-3,5-dione, C₁₁H₁₄NO(C₅H₆O)C₈H₆N₃O₂

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Abstract

C₂₄H₂₆N₄O₄, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 9.729(1) Å, *b* = 14.524(1) Å, *c* = 16.498(1) Å, *V* = 2331.2 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.052, *R*_w(*F*) = 0.045, *T* = 293 K.

Source of material

The title compound was prepared according to [1].

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.4 x 0.45 x 0.5 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ:	0.90 cm ⁻¹
Diffractometer, scan mode:	Siemens P4, ω
2θ _{max} :	55°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	7042, 5361
Criterion for <i>F</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>F</i> _{obs} > 3 σ(<i>F</i> _{obs}), 3820
<i>N</i> (<i>param</i>) _{refined} :	299
Program:	SHELXTL-plus [2]

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(2)	4a	0.628(3)	0.721(2)	0.428(2)	0.08
H(6)	4a	0.9084(2)	0.8669(2)	0.4954(1)	0.08
H(12A)	4a	0.8763(3)	1.1484(2)	0.6441(2)	0.08
H(12B)	4a	0.9027(3)	1.0487(2)	0.6771(2)	0.08
H(13)	4a	0.8942(2)	1.0132(2)	0.5415(1)	0.08
H(15)	4a	0.6121(3)	1.1635(2)	0.5236(2)	0.08
H(16)	4a	0.6000(4)	1.2770(2)	0.4258(2)	0.08
H(17)	4a	0.7865(6)	1.3047(2)	0.3404(2)	0.08
H(18)	4a	0.9872(4)	1.2180(3)	0.3559(2)	0.08
H(19)	4a	0.9969(3)	1.1021(2)	0.4528(2)	0.08
H(20A)	4a	0.9609(3)	0.8798(2)	0.3629(2)	0.08
H(20B)	4a	0.8687(3)	0.7942(2)	0.3428(2)	0.08
H(20C)	4a	1.0013(3)	0.7822(2)	0.3958(2)	0.08
H(21A)	4a	0.731(3)	0.926(2)	0.331(2)	0.08
H(21B)	4a	0.609(3)	0.991(2)	0.381(2)	0.08
H(22A)	4a	0.4369(3)	0.9754(3)	0.6457(2)	0.08
H(22B)	4a	0.4700(3)	1.0786(3)	0.6258(2)	0.08
H(22C)	4a	0.4639(3)	1.0455(3)	0.7162(2)	0.08
H(23A)	4a	0.6284(4)	0.8705(2)	0.6922(2)	0.08
H(23B)	4a	0.6534(4)	0.9359(2)	0.7663(2)	0.08
H(23C)	4a	0.7747(4)	0.9124(2)	0.7073(2)	0.08
H(42)	4a	0.8157(3)	0.4448(2)	0.5156(2)	0.08
H(43)	4a	0.8518(4)	0.3227(3)	0.6045(3)	0.08
H(44)	4a	0.8674(4)	0.3484(3)	0.7429(3)	0.08
H(45)	4a	0.8464(3)	0.4961(3)	0.7943(2)	0.08
H(46)	4a	0.8054(3)	0.6217(2)	0.7059(2)	0.08

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

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(1)	4a	0.7859(2)	0.7550(1)	0.4933(1)	0.047(1)	0.040(1)	0.050(1)	−0.002(1)	−0.0053(9)	0.0001(9)
N(2)	4a	0.7036(2)	0.6980(1)	0.4445(1)	0.043(1)	0.048(1)	0.059(1)	0.001(1)	−0.010(1)	−0.001(1)
C(3)	4a	0.6939(2)	0.6141(2)	0.4828(1)	0.035(1)	0.050(1)	0.063(1)	0.002(1)	−0.000(1)	−0.003(1)
O(3)	4a	0.6229(2)	0.5502(1)	0.4616(1)	0.051(1)	0.054(1)	0.096(1)	−0.010(1)	−0.011(1)	−0.002(1)
N(4)	4a	0.7820(2)	0.6186(1)	0.5493(1)	0.039(1)	0.043(1)	0.056(1)	−0.000(1)	0.003(1)	0.003(1)
C(5)	4a	0.8427(2)	0.7061(2)	0.5537(1)	0.041(1)	0.044(1)	0.046(1)	0.005(1)	0.008(1)	−0.005(1)
O(5)	4a	0.9284(2)	0.7322(1)	0.60262(9)	0.0497(9)	0.060(1)	0.0470(9)	−0.0019(9)	−0.0013(8)	−0.0014(8)
C(6)	4a	0.8425(2)	0.8400(2)	0.4592(1)	0.043(1)	0.042(1)	0.051(1)	−0.002(1)	0.004(1)	0.001(1)
C(7)	4a	0.7253(2)	0.9085(1)	0.4495(1)	0.042(1)	0.039(1)	0.042(1)	−0.004(1)	0.000(1)	−0.001(1)
C(8)	4a	0.6464(2)	0.9262(2)	0.5266(1)	0.039(1)	0.046(1)	0.044(1)	−0.000(1)	0.000(1)	0.004(1)
O(8)	4a	0.5466(2)	0.8790(1)	0.5439(1)	0.055(1)	0.070(1)	0.0560(9)	−0.021(1)	0.0067(9)	−0.0052(9)
N(9)	4a	0.6938(2)	0.9935(1)	0.57563(9)	0.045(1)	0.041(1)	0.0431(9)	−0.004(1)	0.0022(8)	−0.0009(9)
C(10)	4a	0.6403(3)	1.0060(2)	0.6592(1)	0.074(2)	0.059(2)	0.045(1)	−0.009(2)	0.000(1)	−0.007(1)
O(11)	4a	0.7103(3)	1.0873(1)	0.6840(1)	0.105(2)	0.071(1)	0.057(1)	−0.012(1)	−0.003(1)	−0.0163(9)
C(12)	4a	0.8403(3)	1.0869(2)	0.6471(2)	0.071(2)	0.070(2)	0.073(2)	−0.015(2)	−0.019(2)	0.000(2)
C(13)	4a	0.8184(2)	1.0482(2)	0.5624(1)	0.045(1)	0.041(1)	0.062(1)	−0.003(1)	−0.004(1)	−0.000(1)
C(14)	4a	0.8046(3)	1.1217(2)	0.4977(1)	0.054(1)	0.042(1)	0.057(1)	−0.008(1)	−0.001(1)	−0.006(1)
C(15)	4a	0.6895(3)	1.1740(2)	0.4888(2)	0.068(2)	0.069(2)	0.095(2)	0.008(2)	0.003(2)	0.027(2)
C(16)	4a	0.6823(4)	1.2411(2)	0.4312(2)	0.095(3)	0.082(2)	0.138(3)	0.011(2)	−0.020(3)	0.037(2)
C(17)	4a	0.7919(6)	1.2577(2)	0.3811(2)	0.144(4)	0.078(2)	0.084(2)	−0.037(3)	−0.027(3)	0.029(2)
C(18)	4a	0.9092(4)	1.2064(3)	0.3900(2)	0.111(3)	0.086(3)	0.077(2)	−0.036(2)	0.015(2)	0.012(2)
C(19)	4a	0.9150(3)	1.1385(2)	0.4474(2)	0.072(2)	0.064(2)	0.081(2)	−0.015(2)	0.012(2)	−0.004(2)
C(20)	4a	0.9260(3)	0.8224(2)	0.3832(2)	0.060(2)	0.069(2)	0.071(2)	0.014(2)	0.016(1)	0.003(2)
C(21)	4a	0.6864(3)	0.9452(2)	0.3811(2)	0.058(2)	0.062(2)	0.051(1)	0.006(2)	0.005(1)	0.003(1)
C(22)	4a	0.4891(3)	1.0284(3)	0.6620(2)	0.086(2)	0.114(3)	0.079(2)	0.004(2)	0.029(2)	−0.023(2)
C(23)	4a	0.6776(4)	0.9236(2)	0.7110(2)	0.126(3)	0.082(2)	0.057(2)	−0.024(2)	−0.007(2)	0.013(2)
C(41)	4a	0.8073(2)	0.5438(2)	0.6035(2)	0.036(1)	0.056(2)	0.072(2)	−0.002(1)	0.009(1)	0.017(1)
C(42)	4a	0.8212(3)	0.4557(2)	0.5729(2)	0.075(2)	0.052(2)	0.100(2)	0.001(2)	0.000(2)	0.014(2)
C(43)	4a	0.8429(4)	0.3841(3)	0.6253(3)	0.115(3)	0.060(2)	0.159(4)	−0.001(2)	−0.005(3)	0.037(3)
C(44)	4a	0.8518(4)	0.3991(3)	0.7069(3)	0.093(3)	0.106(3)	0.151(4)	−0.010(3)	−0.009(3)	0.081(3)
C(45)	4a	0.8393(3)	0.4859(3)	0.7370(2)	0.072(2)	0.127(3)	0.088(2)	−0.014(2)	0.008(2)	0.046(3)
C(46)	4a	0.8156(3)	0.5604(2)	0.6849(2)	0.059(2)	0.084(2)	0.067(2)	0.000(2)	0.010(1)	0.018(2)

References

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