Crystal structure of 2,4-dimethyl-5-4'-methoxyphenyl-7-thioxoimidazo-[1,5-*b*]pyridazine, C₆H₂N₃S(CH₃)₂C₆H₄OCH₃

K. Peters, E.-M. Peters

Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70506 Stuttgart, Germany

B. Schoknecht and A. Hetzheim

Universität Greifswald, Institut für Organische Chemie, Soldmannstraße 16, D-17487 Greifswald, Germany

Received May 8, 1998, CSD-No. 409311

Source of material: The title compound was prepared by reaction of 1-amino-2-thioxo-4-4'-methoxyphenylimidazoline with acetylacetone (see ref. 1).

Two parallel intermolecular hydrogen bridges (N1–H1–S1'; H1–S1' = 236 pm) build up a dimer of the title compound. The center of this dimer is coincident with one center of symmetry of the current space group.

C₁₅H₁₅N₃OS, monoclinic, *P*₂₁/*n* (No. 14), *a* = 10.534(1) Å, *b* = 10.602(1) Å, *c* = 13.073(1) Å, β = 101.94(1)°, *V* = 1428.4 Å³, *Z* = 4, *R*(*F*) = 0.056, *R*_w(*F*) = 0.062.

Table 1. Parameters used for the X-ray data collection

Crystal:	orange prism, size 0.55 x 0.75 x 0.8 mm
Wavelength:	Mo K _α radiation (0.71073 Å)
μ:	2.30 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
T _{measurement} :	293 K
2θ _{max} :	55°
N(<i>hkl</i>) _{unique} :	3276
Criterion for <i>F</i> _o :	<i>F</i> _o > 3 σ(<i>F</i> _o)
N(<i>param</i>) _{refined} :	186
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	0.119(4)	0.479(4)	0.589(3)	0.15(2)
H(5)	4e	0.6435(2)	0.2807(3)	0.4872(2)	0.08
H(10)	4e	0.2041(3)	0.5767(3)	0.7382(2)	0.08
H(11)	4e	0.1977(3)	0.5856(3)	0.9159(2)	0.08
H(13)	4e	0.4252(3)	0.2737(3)	0.9670(2)	0.08
H(14)	4e	0.4280(2)	0.2637(2)	0.7891(2)	0.08
H(15A)	4e	0.5651(2)	0.3528(3)	0.7326(2)	0.08
H(15B)	4e	0.6794(2)	0.3897(3)	0.6784(2)	0.08
H(15C)	4e	0.6461(2)	0.2473(3)	0.6916(2)	0.08
H(16A)	4e	0.6021(3)	0.2459(3)	0.3052(2)	0.08
H(16B)	4e	0.5071(3)	0.3446(3)	0.2407(2)	0.08
H(16C)	4e	0.4596(3)	0.2066(3)	0.2541(2)	0.08
H(17A)	4e	0.2270(4)	0.4897(4)	1.1733(3)	0.08
H(17B)	4e	0.1323(4)	0.4856(4)	1.0637(3)	0.08
H(17C)	4e	0.2405(4)	0.5893(4)	1.0875(3)	0.08

Table 3. Final 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
S(1)	4e	0.07503(6)	0.46911(7)	0.35769(5)	0.0354(3)	0.0696(5)	0.0438(3)	0.0071(3)	0.0059(3)	−0.0003(3)
N(1)	4e	0.1896(2)	0.4468(2)	0.5648(2)	0.035(1)	0.056(1)	0.044(1)	0.0055(9)	0.0069(8)	−0.0017(9)
C(1)	4e	0.1915(2)	0.4330(2)	0.4620(2)	0.032(1)	0.049(1)	0.046(1)	0.0013(9)	0.0090(9)	−0.001(1)
N(2)	4e	0.3120(2)	0.3846(2)	0.4632(2)	0.0335(9)	0.046(1)	0.045(1)	0.0031(8)	0.0095(8)	−0.0003(8)
N(3)	4e	0.3495(2)	0.3532(2)	0.3709(2)	0.041(1)	0.051(1)	0.049(1)	−0.0014(9)	0.0140(9)	−0.0037(9)
C(4)	4e	0.4687(2)	0.3134(2)	0.3853(2)	0.041(1)	0.046(1)	0.062(2)	0.001(1)	0.019(1)	−0.002(1)
C(5)	4e	0.5554(2)	0.3061(3)	0.4845(2)	0.037(1)	0.056(1)	0.063(2)	0.006(1)	0.015(1)	0.002(1)
C(6)	4e	0.5180(2)	0.3335(2)	0.5750(2)	0.034(1)	0.046(1)	0.058(1)	0.0012(9)	0.008(1)	0.006(1)
C(7)	4e	0.3845(2)	0.3714(2)	0.5658(2)	0.034(1)	0.043(1)	0.047(1)	−0.0010(9)	0.0058(9)	0.001(1)
C(8)	4e	0.3048(2)	0.4101(2)	0.6306(2)	0.035(1)	0.047(1)	0.045(1)	0.001(1)	0.0058(9)	0.001(1)
C(9)	4e	0.3144(2)	0.4176(2)	0.7449(2)	0.039(1)	0.050(1)	0.043(1)	−0.003(1)	0.007(1)	−0.001(1)

Table 3. (Continued)

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
C(10)	4e	0.2483(3)	0.5133(3)	0.7847(2)	0.047(1)	0.052(1)	0.048(1)	0.005(1)	0.005(1)	0.001(1)
C(11)	4e	0.2446(3)	0.5191(3)	0.8903(2)	0.056(2)	0.062(2)	0.049(1)	0.005(1)	0.008(1)	−0.008(1)
C(12)	4e	0.3086(3)	0.4297(3)	0.9576(2)	0.049(1)	0.063(2)	0.046(1)	−0.007(1)	0.005(1)	−0.004(1)
O(12)	4e	0.3067(2)	0.4228(2)	1.0619(1)	0.079(1)	0.087(2)	0.045(1)	0.004(1)	0.012(1)	−0.002(1)
C(13)	4e	0.3785(3)	0.3352(3)	0.9198(2)	0.051(1)	0.060(2)	0.050(1)	0.003(1)	0.004(1)	0.009(1)
C(14)	4e	0.3802(2)	0.3296(2)	0.8145(2)	0.041(1)	0.049(1)	0.054(1)	0.002(1)	0.011(1)	0.001(1)
C(15)	4e	0.6105(2)	0.3305(3)	0.6787(2)	0.035(1)	0.080(2)	0.065(2)	0.003(1)	0.005(1)	0.012(2)
C(16)	4e	0.5136(3)	0.2740(3)	0.2875(2)	0.051(1)	0.078(2)	0.069(2)	0.006(1)	0.024(1)	−0.011(2)
C(17)	4e	0.2196(4)	0.5032(4)	1.0997(3)	0.093(3)	0.103(3)	0.056(2)	−0.003(2)	0.022(2)	−0.019(2)

References

1. Hetzheim, A.; Schoknecht, B.: Syntheses of new anellated imidazoles. *J. Heterocycl. Chem.* In preparation.
2. Sheldrick, G. M.: Program Package SHELXTL-plus. Release 4.1. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.