Crystal structure of 1,2-*N,N*-phenylen-bis-chlorobenzo[2,1-*b*]-thienyl-carboxamide, C₂₄H₁₄Cl₂N₂O₂S₂

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Source of material: Synthesis starting from 3-chlorobenzo[2,1-*b*]-thiophen-2-carbonylchloride as intermediate which was condensed with 1,2-diaminobenzene.

C₂₄H₁₄Cl₂N₂O₂S₂, triclinic, *P* $\bar{1}$ (No. 2), *a* = 8.821(3) Å, *b* = 10.548(3) Å, *c* = 12.238(4) Å, α = 81.86(2)°, β = 77.86(2)°, γ = 81.18(2)°, *V* = 1093.0 Å³, *Z* = 2, *R*(*F*) = 0.031, *R*_w(*F*) = 0.031.

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

Crystal:	colorless, prismatic, size 0.14 x 0.17 x 0.30 mm
Wavelength:	Mo <i>K</i> α radiation (0.71073 Å)
μ :	5.05 cm ⁻¹
Diffractometer:	Philips PW1100 updated by Stoe
Scan mode:	ω/θ
<i>T</i> _{measurement} :	293 K
$2\theta_{\text{max}}$:	54°
<i>N</i> (<i>hkl</i>) _{unique} :	4786
Criterion for <i>F</i> _o :	<i>F</i> _o > 2.5 σ (<i>F</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	292
Program:	SHELX-76

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(N1)	2i	0.0173	0.3647	0.7138	0.071(5)
H(2)	2i	-0.0957(5)	0.8354(4)	1.0678(4)	0.071(5)
H(3)	2i	-0.3102(6)	0.7820(5)	1.2224(4)	0.071(5)
H(4)	2i	-0.4639(5)	0.6085(5)	1.2156(4)	0.071(5)
H(5)	2i	-0.3942(5)	0.4736(4)	1.0603(3)	0.071(5)
H(11)	2i	0.3492(5)	0.5036(4)	0.5327(3)	0.071(5)
H(12)	2i	0.4858(5)	0.4265(4)	0.3525(3)	0.071(5)
H(N2)	2i	-0.1245	0.2574	0.5185	0.071(5)
H(13)	2i	0.3798(5)	0.2692(4)	0.2699(3)	0.071(5)
H(14)	2i	0.1388(5)	0.1817(4)	0.3702(3)	0.071(5)
H(18)	2i	-0.4467(5)	-0.1463(4)	0.9786(3)	0.071(5)
H(19)	2i	-0.6954(5)	-0.1904(4)	0.9379(4)	0.071(5)
H(20)	2i	-0.7784(5)	-0.0986(4)	0.7622(4)	0.071(5)
H(21)	2i	-0.6147(5)	0.0360(4)	0.6192(4)	0.071(5)

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)	2i	0.0280(1)	0.6982(1)	0.8592(1)	0.0529(7)	0.0422(6)	0.0528(6)	-0.0185(5)	-0.0065(5)	-0.0089(5)
Cl(1)	2i	-0.2165(1)	0.3837(1)	0.8514(1)	0.0568(7)	0.0634(7)	0.0562(7)	-0.0346(6)	0.0058(5)	-0.0166(6)
O(1)	2i	0.1714(3)	0.6209(3)	0.6475(2)	0.068(2)	0.052(2)	0.050(2)	-0.031(2)	0.010(2)	-0.002(1)
N(1)	2i	0.0777(4)	0.4297(3)	0.6559(3)	0.048(2)	0.049(2)	0.038(2)	-0.024(2)	0.003(2)	-0.008(2)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(1)	2i	-0.1209(5)	0.6819(4)	0.9753(3)	0.047(2)	0.044(3)	0.044(2)	-0.004(2)	-0.011(2)	-0.006(2)
C(2)	2i	-0.1597(5)	0.7566(4)	1.0658(4)	0.060(3)	0.056(3)	0.062(3)	-0.000(2)	-0.018(2)	-0.022(2)
C(3)	2i	-0.2804(6)	0.7270(5)	1.1512(4)	0.068(3)	0.072(3)	0.052(3)	0.009(3)	-0.012(3)	-0.026(3)
C(4)	2i	-0.3663(5)	0.6269(5)	1.1482(4)	0.050(3)	0.079(4)	0.049(3)	-0.003(3)	-0.003(2)	-0.011(3)
C(5)	2i	-0.3286(5)	0.5518(4)	1.0612(3)	0.046(3)	0.063(3)	0.047(3)	-0.009(2)	-0.005(2)	-0.009(2)
C(6)	2i	-0.2026(5)	0.5785(4)	0.9728(3)	0.046(3)	0.045(2)	0.036(2)	-0.008(2)	-0.010(2)	-0.002(2)
C(7)	2i	-0.1371(4)	0.5144(3)	0.8756(3)	0.041(2)	0.038(2)	0.041(2)	-0.012(2)	-0.009(2)	-0.005(2)
C(8)	2i	-0.0147(4)	0.5662(3)	0.8063(3)	0.041(2)	0.037(2)	0.038(2)	-0.013(2)	-0.008(2)	-0.002(2)
C(9)	2i	0.0873(4)	0.5403(4)	0.6960(3)	0.043(2)	0.044(2)	0.036(2)	-0.013(2)	-0.007(2)	0.000(2)
C(10)	2i	0.1628(4)	0.3872(4)	0.5533(3)	0.040(2)	0.052(3)	0.035(2)	-0.015(2)	-0.002(2)	-0.004(2)
C(11)	2i	0.3017(5)	0.4339(4)	0.4972(3)	0.047(3)	0.061(3)	0.048(3)	-0.023(2)	0.001(2)	-0.009(2)
C(12)	2i	0.3785(5)	0.3901(4)	0.3958(3)	0.041(3)	0.067(3)	0.052(3)	-0.013(2)	0.005(2)	-0.004(2)
S(2)	2i	-0.2145(1)	0.0195(1)	0.8292(1)	0.0563(7)	0.0556(7)	0.0402(6)	-0.0228(6)	-0.0147(5)	0.0060(5)
Cl(2)	2i	-0.3532(2)	0.1732(1)	0.5209(1)	0.100(1)	0.115(1)	0.0747(9)	-0.0725(9)	-0.0552(8)	0.0508(8)
O(2)	2i	0.0455(3)	0.1492(3)	0.7163(2)	0.051(2)	0.062(2)	0.062(2)	-0.023(2)	-0.027(2)	0.015(2)
N(2)	2i	-0.0388(3)	0.2465(3)	0.5593(2)	0.041(2)	0.044(2)	0.039(2)	-0.016(2)	-0.009(2)	0.001(2)
C(13)	2i	0.3199(5)	0.3012(4)	0.3496(3)	0.052(3)	0.061(3)	0.042(2)	-0.005(2)	0.005(2)	-0.013(2)
C(14)	2i	0.1839(5)	0.2529(4)	0.4056(3)	0.055(3)	0.049(3)	0.046(3)	-0.010(2)	-0.004(2)	-0.010(2)
C(15)	2i	0.1052(4)	0.2952(4)	0.5068(3)	0.039(2)	0.046(2)	0.037(2)	-0.013(2)	-0.009(2)	0.000(2)
C(16)	2i	-0.0531(5)	0.1683(3)	0.6577(3)	0.042(2)	0.033(2)	0.042(2)	-0.008(2)	-0.006(2)	-0.004(2)
C(17)	2i	-0.3925(4)	-0.0264(3)	0.8204(3)	0.045(2)	0.038(2)	0.040(2)	-0.010(2)	-0.001(2)	-0.009(2)
C(18)	2i	-0.4834(5)	-0.1056(4)	0.9009(3)	0.066(3)	0.050(3)	0.041(2)	-0.020(2)	0.002(2)	-0.003(2)
C(19)	2i	-0.6221(5)	-0.1300(4)	0.8772(4)	0.058(3)	0.057(3)	0.058(3)	-0.025(2)	0.012(2)	-0.005(2)
C(20)	2i	-0.6687(5)	-0.0786(4)	0.7775(4)	0.041(3)	0.058(3)	0.082(3)	-0.020(2)	-0.007(2)	0.001(3)
C(21)	2i	-0.5782(5)	-0.0025(4)	0.6975(4)	0.048(3)	0.051(3)	0.068(3)	-0.015(2)	-0.018(2)	0.003(2)
C(22)	2i	-0.4377(4)	0.0242(3)	0.7196(3)	0.042(2)	0.034(2)	0.047(2)	-0.009(2)	-0.006(2)	-0.000(2)
C(23)	2i	-0.3249(5)	0.1006(4)	0.6507(3)	0.047(3)	0.039(2)	0.043(2)	-0.013(2)	-0.010(2)	0.005(2)
C(24)	2i	-0.2002(4)	0.1070(3)	0.6964(3)	0.041(2)	0.036(2)	0.036(2)	-0.009(2)	-0.010(2)	-0.000(2)

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