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(Z)-N-tert-butyl-1-(2-(3,5-dichlorobenzamido)phenyl) methanimine oxide, C₁₈H₁₈Cl₂N₂O₂ **Table 1:** Data collection and handling.

Crystal:	Prism, colorless
Size:	0.16 × 0.15 × 0.1 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	3.34 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, φ and ω -scans
$\theta_{\max}$, completeness:	67.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7211, 3226, 0.030
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2616
$N(\text{param})_{\text{refined}}$:	262
Programs:	CrysAlis ^{PRO} [1], OLEX2 [2], SHELX [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O1	0.7343(2)	0.37127(11)	−0.14162(16)	0.0616(5)
O2	0.91319(18)	0.54987(11)	0.15085(15)	0.0567(4)
H14	0.567(3)	0.6076(18)	0.142(3)	0.064(8)*
N1	0.7921(2)	0.46754(11)	−0.01806(17)	0.0473(4)
H1	0.853(3)	0.4831(17)	0.042(3)	0.056(8)*
N2	0.7816(2)	0.57343(11)	0.18308(17)	0.0472(4)
Cl1	1.19920(11)	0.17705(6)	−0.02130(8)	0.0984(4)
Cl2	1.08811(12)	0.32755(5)	0.34982(6)	0.0871(3)
C1	0.8065(3)	0.39704(14)	−0.05467(19)	0.0470(5)
C2	0.9191(2)	0.34926(13)	0.02263(19)	0.0457(5)
C3	0.9938(3)	0.29141(14)	−0.0262(2)	0.0504(5)
H3	0.978(3)	0.2827(18)	−0.100(3)	0.061*
C4	1.1005(3)	0.24796(15)	0.0409(2)	0.0542(6)
C5	1.1327(3)	0.25780(15)	0.1568(2)	0.0541(6)
H5	1.206(3)	0.2270(19)	0.199(3)	0.065*
C6	1.0540(3)	0.31410(15)	0.2032(2)	0.0537(6)
C7	0.9486(3)	0.36066(14)	0.1387(2)	0.0530(5)
H7	0.896(3)	0.3992(19)	0.170(3)	0.064*
C8	0.7006(2)	0.52458(13)	−0.0750(2)	0.0468(5)
C9	0.6745(3)	0.52720(17)	−0.1931(2)	0.0598(6)
H9	0.718(4)	0.491(2)	−0.229(3)	0.072*
C10	0.5779(4)	0.58187(18)	−0.2471(2)	0.0674(7)
H10	0.561(4)	0.582(2)	−0.324(3)	0.081*
C11	0.5075(4)	0.63395(17)	−0.1861(3)	0.0674(7)
H11	0.442(4)	0.672(2)	−0.216(3)	0.081*
C12	0.5362(3)	0.63345(15)	−0.0692(3)	0.0591(6)
H12	0.485(4)	0.6685(19)	−0.023(3)	0.071*
C13	0.6359(2)	0.57980(13)	−0.0111(2)	0.0476(5)
C14	0.6548(3)	0.58641(14)	0.1120(2)	0.0516(5)
C15	0.7921(3)	0.58908(16)	0.3093(2)	0.0589(6)
C16 ^a	0.6376(12)	0.6159(7)	0.3427(13)	0.103(3)

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Abstract

C₁₈H₁₈Cl₂N₂O₂, monoclinic, *P*₂/n (no. 14), *a* = 8.5266(3) Å, *b* = 17.9521(7) Å, *c* = 11.8709(4) Å, β = 97.288(3)°, *V* = 1802.41(10) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0515, *wR*_{ref}(*F*²) = 0.1497, *T* = 293(2) K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title compound was prepared by the reaction of aryl-nitrone (0.2 mmol) and dioxazolones (0.22 mmol) with [IrCp*Cl₂]/AgNTf₂ (2 mol%/8 mol%) as catalyst, and 1,2-dichloroethane (1 mL) as solvent. The reaction mixture was stirred at room temperature for 0.5 h under a natural atmosphere. The solvents were removed under reduced pressure.

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Table 2 (continued)

Atom	x	y	z	U _{iso} ^a /U _{eq}
H16A ^a	0.5558	0.5808	0.3175	0.155*
H16B ^a	0.6119	0.6635	0.3082	0.155*
H16C ^a	0.6465	0.6207	0.4239	0.155*
C16A ^b	0.635(5)	0.593(3)	0.355(5)	0.103(3)
H16D ^b	0.6522	0.6025	0.4356	0.155*
H16E ^b	0.5804	0.5461	0.3421	0.155*
H16F ^b	0.5718	0.6320	0.3180	0.155*
C17 ^a	0.8336(9)	0.5139(4)	0.3677(4)	0.0891(17)
H17A ^a	0.8349	0.5193	0.4483	0.134*
H17B ^a	0.9360	0.4981	0.3516	0.134*
H17C ^a	0.7560	0.4775	0.3398	0.134*
C17A ^b	0.913(3)	0.5425(14)	0.3776(16)	0.0891(17)
H17D ^b	1.0130	0.5677	0.3854	0.134*
H17E ^b	0.9224	0.4956	0.3400	0.134*
H17F ^b	0.8817	0.5339	0.4514	0.134*
C18 ^a	0.9270(9)	0.6441(5)	0.3340(5)	0.108(3)
H18A ^a	0.8970	0.6910	0.2989	0.162*
H18B ^a	1.0187	0.6253	0.3042	0.162*
H18C ^a	0.9508	0.6508	0.4146	0.162*
C18A ^b	0.836(3)	0.6744(17)	0.327(2)	0.108(3)
H18D ^b	0.7669	0.7038	0.2740	0.162*
H18E ^b	0.9434	0.6822	0.3138	0.162*
H18F ^b	0.8232	0.6889	0.4029	0.162*

Occupancies: ^a = 0.785(10), ^b = 0.215(10)

and the residue was purified by chromatography to give the target title product. The compound was crystallized by slow evaporation from a mixture solution of CH₂Cl₂ and hexane at room temperature.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Nitrones are important and useful intermediates in chemical synthesis and can be easily converted into various heterocycles *via* diverse transformation [4–8]. Nitrones also are known to behave as efficient radical traps, and have been used in the synthesis of nitroxyl species [9]. *N*-arylamides are a key structural fragment in agrochemicals and pharmaceutical substances such as Boscalid, and Fluxapyroxad [10]. Herein we report a new compound containing amides and nitronone scaffolds.

The single-crystal structure of the title compound was determined and is shown in the figure. The torsion angle of C13–C14–N2–O2 is –1.8(4)° which shows the planarity of the C=N moiety with respect to *N*-phenyl ring. The torsion angle of C2–C1–N1–C8 is 177.4(2)° also indicates the planarity of this moiety. In the crystal structure, there is one intramolecular N(1)–H···O(2) hydrogen bond, a well known motif [11].

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