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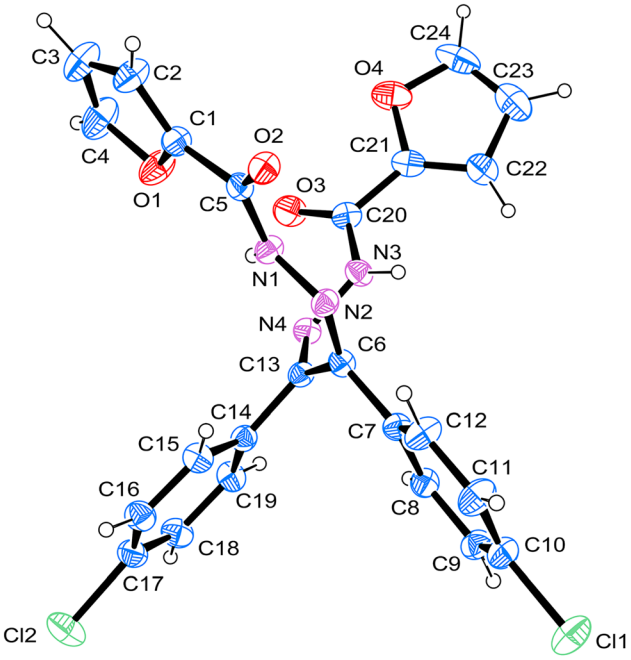
The crystal structure of N′,N″-[1,2-bis(4-chlorophenyl)ethane-1,2-diylidene]bis(furan-2-carbohydrazide), $C_{24}H_{16}Cl_2N_4O_4$



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Abstract

$C_{24}H_{16}Cl_2N_4O_4$, monoclinic, $P2_1/n$ (no. 14), a = 10.2264(4) Å, b = 16.1772(6) Å, c = 13.8429(6) Å, β = 102.463(5)°, V = 2236.13(16) Å^3, Z = 4, $R_{gt}(F)$ = 0.0574, $wR_{ref}(F^2)$ = 0.1588, T = 220(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	clear light yellow block
Size	0.14 × 0.12 × 0.11 mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ:	2.96 mm^{-1}
Diffractometer, scan mode:	Rigaku SuperNova, φ and ω scans
θ_{max}, completeness:	68.2°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8,922, 4,093, 0.041
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,842
$N(param)_{refined}$:	307
Programs:	Rigaku,[1] SHELX[2,3], WinGX and ORTEP[4]

1 Source of material

All chemicals were purchased from commercial sources and used as received without further purification. The 4,4′-dichloro benzil (1 mmol, 0.279 g), furan-2-carbohydrazide (2 mmol, 0.252 g) and diphenyltin dichloride (0.1 mmol, 0.034 g) were dissolved in MeOH (30 mL). The mixture was refluxed for 2 h. Finally, the title crystal was precipitated by controlling slowly at room temperature.

2 Experimental details

All H-atoms bonded to C atoms were placed geometrically and refined using a riding model with common isotropic displacement factors U_{iso}(H) = 1.2 or 1.5 U_{eq}(parent C-atom).

3 Comment

Salen-like ligands are important organic ligands that are widely used because of their good coordination ability. This type of ligand can provide multiple coordination sites in the molecule and can form stable complexes with many metal ions, such as Th(IV),[5] Cu(II),[6] Zn(II),[7] and Ln(III),[8] etc. In addition, salen-like ligands also have excellent electronic and spatial effects, which can effectively regulate the activity and

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.38084 (12)	0.87448 (6)	0.62069 (9)	0.0675 (3)
Cl2	0.73401 (11)	0.42855 (7)	0.97656 (7)	0.0680 (3)
O1	0.0556 (3)	0.25394 (15)	0.6202 (2)	0.0581 (7)
O2	−0.1401 (2)	0.43382 (14)	0.62561 (18)	0.0419 (5)
O3	0.2594 (3)	0.26742 (15)	0.4151 (2)	0.0583 (7)
O4	0.0631 (3)	0.27878 (18)	0.2408 (2)	0.0619 (8)
N1	0.0729 (3)	0.41528 (15)	0.6032 (2)	0.0368 (6)
H1	0.132757	0.379458	0.594477	0.044*
N2	0.0999 (3)	0.49795 (15)	0.60094 (19)	0.0360 (6)
N3	0.2367 (3)	0.40537 (17)	0.4415 (2)	0.0395 (6)
H3A	0.193187	0.450932	0.423258	0.047*
N4	0.3323 (3)	0.40051 (16)	0.52807 (19)	0.0362 (6)
C1	−0.0545 (3)	0.2986 (2)	0.6280 (3)	0.0406 (7)
C2	−0.1515 (4)	0.2480 (2)	0.6438 (3)	0.0545 (10)
H2	−0.236980	0.263718	0.651862	0.065*
C3	−0.1009 (5)	0.1670 (2)	0.6462 (4)	0.0674 (12)
H3	−0.145861	0.118044	0.655707	0.081*
C4	0.0235 (5)	0.1736 (2)	0.6321 (4)	0.0707 (13)
H4	0.081358	0.128726	0.630659	0.085*
C5	−0.0469 (3)	0.3886 (2)	0.6191 (2)	0.0364 (7)
C6	0.2207 (3)	0.51796 (19)	0.5955 (2)	0.0350 (7)
C7	0.2588 (3)	0.60564 (19)	0.6004 (2)	0.0358 (7)
C8	0.3797 (3)	0.6308 (2)	0.5798 (2)	0.0396 (7)
H8	0.437031	0.591321	0.561144	0.048*
C9	0.4172 (3)	0.7135 (2)	0.5863 (3)	0.0446 (8)
H9	0.499578	0.729743	0.572515	0.053*
C10	0.3334 (4)	0.7710 (2)	0.6128 (3)	0.0482 (9)
C11	0.2119 (4)	0.7482 (2)	0.6336 (3)	0.0549 (10)
H11	0.155160	0.788235	0.651770	0.066*
C12	0.1750 (4)	0.6658 (2)	0.6274 (3)	0.0476 (9)
H12	0.092698	0.649967	0.641529	0.057*
C13	0.3284 (3)	0.45395 (18)	0.5958 (2)	0.0337 (7)
C14	0.4317 (3)	0.44784 (18)	0.6889 (2)	0.0362 (7)
C15	0.3946 (3)	0.4628 (2)	0.7782 (2)	0.0403 (7)
H15	0.306246	0.478908	0.778217	0.048*
C16	0.4862 (3)	0.4544 (2)	0.8670 (3)	0.0458 (8)
H16	0.460111	0.463138	0.927291	0.055*
C17	0.6161 (4)	0.4330 (2)	0.8660 (3)	0.0459 (8)
C18	0.6549 (3)	0.4171 (2)	0.7786 (3)	0.0479 (9)
H18	0.743608	0.401601	0.779145	0.057*
C19	0.5623 (3)	0.4242 (2)	0.6901 (3)	0.0435 (8)
H19	0.588106	0.412937	0.630259	0.052*
C20	0.2133 (3)	0.3344 (2)	0.3851 (3)	0.0418 (8)
C21	0.1278 (3)	0.3470 (2)	0.2867 (3)	0.0450 (8)
C22	0.1033 (4)	0.4128 (3)	0.2277 (3)	0.0559 (10)
H22	0.134916	0.466908	0.242567	0.067*
C23	0.0207 (5)	0.3854 (4)	0.1386 (3)	0.0772 (14)
H23	−0.010631	0.417448	0.081717	0.093*
C24	−0.0050 (4)	0.3059 (4)	0.1496 (3)	0.0738 (14)
H24	−0.061279	0.273012	0.102126	0.089*

selectivity of reactions. Recent studies have found that organotin(IV) complexes based on salen-like ligands can kill cancer cells through multiple mechanisms of action.[9] Therefore, the synthesis and crystal structure of the title compound are important significance for the study of the application.

The asymmetric unit of the title compound is one N′,N″-[1,2-bis(4-chlorophenyl)ethane-1,2-diylidene]bis(furan-2-carbohydrazide) molecule. The ORTEP diagram is presented in Figure. Bond lengths and angles are all in the expected ranges.[10] The bond length of N2=C6 and N4=C13 are 1.294(4) Å and 1.282(4) Å, respectively. Which is similar to those reported in the literature.[11,12] The bond length of C6–C13 is 1.511(4) Å, shorter than normal C–C single bonds, which is similar to those reported in the literature.[13]

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