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Crystal structure of (*E*)-2,3-dibromo-4-((2,6-diisopropylphenyl-imino)methyl)-6-methoxyphenol, $C_{20}H_{23}Br_2NO_2$

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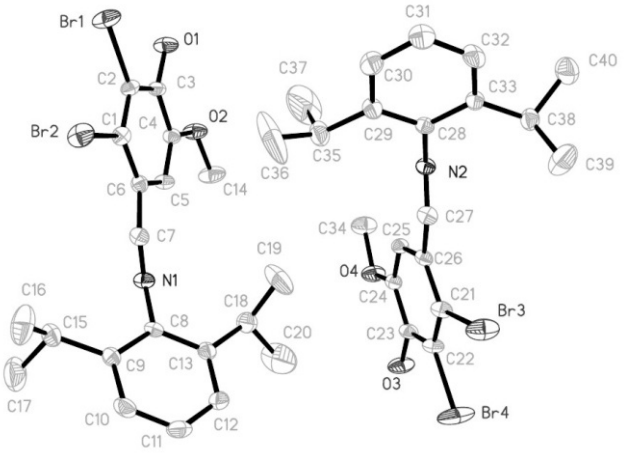

Abstract

$C_{20}H_{23}Br_2NO_2$, $P\bar{1}$ (No. 2), a = 12.629(8) Å, b = 12.653(8) Å, c = 14.032(9) Å, α = 71.268(6)°, β = 81.172(7)°, γ = 76.448(6)°, V = 2056.9Å^3, Z = 4, $R_{gt}(F)$ = 0.0410, $wR_{ref}(F^2)$ = 0.0965, T = 296 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.24×0.2×0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	39.53 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, ω and φ
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14894, 7518
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4307
$N(param)_{refined}$:	463
Programs:	SHELX [9]

Source of material

2,3-Dibromo-4-hydroxy-5-methoxybenzaldehyde (0.310g, 1mmol) and 2,6-diisopropylaniline (0.1780g, 1mmol) were mixed in methanol (20 mL). The mixture was stirred at room temperature for 10-12 hours to give a yellow solution. Yellow block-shaped single crystals were obtained by slow evaporation of the solution containing the compound in air.

Experimental details

All H atoms were positioned geometrically (C–H = 0.93-0.96 Å) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Discussion

Schiff bases have acted as important precursors for compounds reported to possess a variety of biological activities, such as antibacterial [1], antifungal [2] properties. Meanwhile, Schiff bases have also been found to be useful ligands to form stable complexes with a variety of transition metal ions [3-4]. As an extension of our work on the structural characterization of Schiff base compounds [5-7], in this paper we present a new structure of a Schiff base compound. In the title compound, all the bond lengths are within normal ranges [9]. There are two independent molecules in the asymmetric unit of the title compound (see the Figure) and each molecule of the compound exists in a *trans* configuration with respect to the C=N double bond. The dihedral angle between the benzene ring with two bromide substituents and the benzene ring with two isopropyl substituents is 50.3(2)°. There are intramolecular O1–H1···N2 and O3–H3···N1 hydrogen bonds. Their symmetry code are (1-x, 1-y, 1-z) and (1-x,-y,1-z) respectively. In addition, the C14–H14B– π interaction with a 2.590Å distance of C14–Cg(1) exist in the compound. These hydrogen bonds and the C14–H14B–π interaction determines the molecule packing in the structure.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(5)	2*i*	0.5206	0.2713	0.2814	0.043
H(7)	2*i*	0.2778	0.3413	0.1672	0.042
H(10)	2*i*	0.1218	0.0518	0.1498	0.057
H(11)	2*i*	0.0658	–0.0209	0.3159	0.060
H(12)	2*i*	0.1531	–0.0018	0.4392	0.054
H(14A)	2*i*	0.6088	0.2601	0.4153	0.092
H(14B)	2*i*	0.7309	0.2685	0.4141	0.092
H(14C)	2*i*	0.6958	0.2271	0.3318	0.092
H(15)	2*i*	0.3334	0.2123	0.0554	0.065
H(16A)	2*i*	0.1345	0.2022	–0.0039	0.152
H(16B)	2*i*	0.2211	0.2687	–0.0750	0.152
H(16C)	2*i*	0.1586	0.3084	0.0170	0.152
H(17A)	2*i*	0.3909	0.0212	0.0617	0.145
H(17B)	2*i*	0.3663	0.0973	–0.0483	0.145
H(17C)	2*i*	0.2820	0.0249	0.0190	0.145
H(18)	2*i*	0.3892	0.1156	0.3955	0.069
H(19A)	2*i*	0.2583	0.2761	0.3944	0.143
H(19B)	2*i*	0.3152	0.2254	0.4956	0.143
H(19C)	2*i*	0.1977	0.2066	0.4921	0.143
H(20A)	2*i*	0.2675	–0.0017	0.5580	0.214
H(20B)	2*i*	0.3891	0.0103	0.5533	0.214
H(20C)	2*i*	0.3590	–0.0623	0.4933	0.214
H(25)	2*i*	0.3835	0.2647	0.6828	0.040
H(27)	2*i*	0.1035	0.3603	0.6677	0.044
H(30)	2*i*	0.1165	0.7258	0.4066	0.063
H(31)	2*i*	0.0085	0.8301	0.5032	0.067
H(32)	2*i*	–0.0056	0.7550	0.6753	0.060
H(34A)	2*i*	0.5664	0.1969	0.6364	0.092
H(34B)	2*i*	0.6525	0.1179	0.7115	0.092
H(34C)	2*i*	0.5523	0.1988	0.7488	0.092
H(35)	2*i*	0.2439	0.4369	0.4901	0.072
H(36A)	2*i*	0.1226	0.5349	0.3649	0.275

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Table 2. continued.

Atom	Site	x	y	z	U_{iso}
H(36B)	2*i*	0.2381	0.4803	0.3242	0.275
H(36C)	2*i*	0.2085	0.6114	0.3107	0.275
H(37A)	2*i*	0.3598	0.6091	0.3955	0.257
H(37B)	2*i*	0.4039	0.4776	0.4186	0.257
H(37C)	2*i*	0.3747	0.5325	0.5072	0.257
H(38)	2*i*	0.1445	0.4926	0.8159	0.052
H(39A)	2*i*	–0.0818	0.5739	0.8187	0.134
H(39B)	2*i*	–0.0220	0.4792	0.9073	0.134
H(39C)	2*i*	–0.0225	0.4559	0.8042	0.134
H(40A)	2*i*	0.1612	0.6675	0.8264	0.106
H(40B)	2*i*	0.0906	0.6070	0.9214	0.106
H(40C)	2*i*	0.0337	0.7067	0.8342	0.106
H(1)	2*i*	0.6496	0.5735	0.2432	0.073
H(3)	2*i*	0.4686	–0.1050	0.7877	0.085

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	2*i*	0.44347(4)	0.72474(4)	0.04927(4)	0.0685(4)	0.0341(3)	0.0707(4)	–0.0155(2)	–0.0217(3)	0.0088(2)
Br(2)	2*i*	0.29353(4)	0.55144(4)	0.03134(4)	0.0542(3)	0.0530(3)	0.0582(3)	–0.0120(2)	–0.0253(3)	–0.0001(3)
Br(3)	2*i*	0.02566(4)	0.16892(4)	0.79106(5)	0.0387(3)	0.0468(3)	0.1148(5)	–0.0085(2)	–0.0177(3)	–0.0149(3)
Br(4)	2*i*	0.16835(5)	–0.09609(4)	0.85154(6)	0.0594(4)	0.0342(3)	0.1632(7)	–0.0199(3)	–0.0081(4)	–0.0037(4)
C(1)	2*i*	0.4040(3)	0.4978(4)	0.1210(3)	0.027(2)	0.038(3)	0.038(3)	–0.005(2)	–0.002(2)	–0.010(2)
C(2)	2*i*	0.4673(3)	0.5713(3)	0.1267(3)	0.035(3)	0.025(2)	0.037(3)	–0.005(2)	–0.001(2)	–0.003(2)
C(3)	2*i*	0.5490(3)	0.5337(3)	0.1922(3)	0.036(3)	0.027(2)	0.039(3)	–0.012(2)	–0.002(2)	–0.010(2)
C(4)	2*i*	0.5692(3)	0.4195(3)	0.2483(3)	0.034(3)	0.027(2)	0.036(3)	–0.005(2)	–0.009(2)	–0.007(2)
C(5)	2*i*	0.5065(3)	0.3472(3)	0.2424(3)	0.038(3)	0.024(2)	0.046(3)	–0.006(2)	–0.008(2)	–0.007(2)
C(6)	2*i*	0.4225(3)	0.3853(3)	0.1795(3)	0.031(2)	0.031(3)	0.033(2)	–0.004(2)	–0.002(2)	–0.011(2)
C(7)	2*i*	0.3476(3)	0.3090(4)	0.1882(3)	0.032(2)	0.037(3)	0.040(3)	–0.005(2)	–0.009(2)	–0.013(2)
C(8)	2*i*	0.2871(3)	0.1401(3)	0.2453(3)	0.029(2)	0.024(2)	0.039(3)	–0.004(2)	–0.011(2)	–0.011(2)
C(9)	2*i*	0.2386(3)	0.1243(3)	0.1692(3)	0.038(3)	0.040(3)	0.034(3)	–0.010(2)	–0.007(2)	–0.013(2)
C(10)	2*i*	0.1560(4)	0.0630(4)	0.1989(4)	0.053(3)	0.050(3)	0.051(3)	–0.018(3)	–0.017(3)	–0.021(3)
C(11)	2*i*	0.1231(4)	0.0183(4)	0.2981(4)	0.046(3)	0.038(3)	0.069(4)	–0.020(2)	0.007(3)	–0.019(3)
C(12)	2*i*	0.1745(4)	0.0313(4)	0.3716(4)	0.057(3)	0.034(3)	0.043(3)	–0.014(2)	0.006(2)	–0.012(2)
C(13)	2*i*	0.2572(3)	0.0922(3)	0.3476(3)	0.047(3)	0.024(2)	0.036(3)	–0.002(2)	–0.007(2)	–0.008(2)
C(14)	2*i*	0.6734(4)	0.2777(4)	0.3729(4)	0.068(4)	0.038(3)	0.074(4)	–0.016(3)	–0.041(3)	0.010(3)
C(15)	2*i*	0.2784(4)	0.1673(4)	0.0594(3)	0.066(3)	0.067(4)	0.042(3)	–0.026(3)	–0.006(3)	–0.022(3)
C(16)	2*i*	0.1901(5)	0.2436(6)	–0.0066(4)	0.116(5)	0.122(6)	0.043(4)	–0.004(4)	–0.019(4)	–0.002(4)
C(17)	2*i*	0.3345(5)	0.0686(5)	0.0193(4)	0.123(6)	0.104(5)	0.060(4)	–0.010(4)	0.015(4)	–0.040(4)
C(18)	2*i*	0.3161(5)	0.1059(4)	0.4276(3)	0.087(4)	0.049(3)	0.038(3)	–0.022(3)	–0.015(3)	–0.007(2)
C(19)	2*i*	0.2675(5)	0.2131(5)	0.4549(5)	0.128(6)	0.090(5)	0.093(5)	–0.005(4)	–0.036(4)	–0.061(4)
C(20)	2*i*	0.3345(7)	0.0042(6)	0.5157(5)	0.26(1)	0.092(5)	0.085(5)	–0.039(6)	–0.102(6)	0.005(4)
C(21)	2*i*	0.1792(3)	0.1389(3)	0.7654(3)	0.039(3)	0.031(3)	0.046(3)	–0.005(2)	–0.016(2)	–0.010(2)
C(22)	2*i*	0.2371(4)	0.0284(3)	0.7934(3)	0.044(3)	0.023(2)	0.053(3)	–0.007(2)	–0.011(2)	–0.009(2)
C(23)	2*i*	0.3493(4)	0.0056(3)	0.7793(3)	0.047(3)	0.022(2)	0.041(3)	–0.003(2)	–0.012(2)	–0.007(2)
C(24)	2*i*	0.4044(3)	0.0957(3)	0.7395(3)	0.038(3)	0.028(3)	0.033(3)	–0.005(2)	–0.008(2)	–0.009(2)
C(25)	2*i*	0.3462(3)	0.2050(3)	0.7107(3)	0.042(3)	0.026(2)	0.031(2)	–0.008(2)	–0.005(2)	–0.005(2)
C(26)	2*i*	0.2330(3)	0.2288(3)	0.7222(3)	0.037(3)	0.025(2)	0.032(2)	–0.002(2)	–0.013(2)	–0.009(2)
C(27)	2*i*	0.1753(3)	0.3470(3)	0.6834(3)	0.032(3)	0.034(3)	0.042(3)	0.000(2)	–0.011(2)	–0.011(2)
C(28)	2*i*	0.1564(3)	0.5414(3)	0.6236(3)	0.031(2)	0.026(2)	0.035(3)	–0.002(2)	–0.008(2)	–0.008(2)
C(29)	2*i*	0.1675(3)	0.5845(4)	0.5182(3)	0.045(3)	0.036(3)	0.038(3)	0.003(2)	–0.011(2)	–0.010(2)
C(30)	2*i*	0.1105(4)	0.6942(4)	0.4764(4)	0.065(3)	0.044(3)	0.038(3)	0.002(3)	–0.015(3)	–0.001(2)
C(31)	2*i*	0.0464(4)	0.7572(4)	0.5335(4)	0.059(3)	0.036(3)	0.056(3)	0.018(2)	–0.019(3)	–0.002(3)
C(32)	2*i*	0.0384(4)	0.7119(4)	0.6362(4)	0.053(3)	0.037(3)	0.052(3)	0.015(2)	–0.009(2)	–0.016(2)
C(33)	2*i*	0.0934(3)	0.6048(3)	0.6835(3)	0.033(2)	0.032(3)	0.033(3)	–0.002(2)	–0.004(2)	–0.008(2)
C(34)	2*i*	0.5765(4)	0.1515(4)	0.7050(4)	0.036(3)	0.047(3)	0.101(4)	–0.010(2)	–0.001(3)	–0.021(3)
C(35)	2*i*	0.2416(4)	0.5175(4)	0.4534(3)	0.077(4)	0.049(3)	0.043(3)	0.008(3)	–0.002(3)	–0.017(3)
C(36)	2*i*	0.1989(8)	0.5379(7)	0.3545(5)	0.28(1)	0.158(8)	0.092(6)	0.119(8)	–0.094(7)	–0.090(6)
C(37)	2*i*	0.3549(6)	0.5358(8)	0.4427(7)	0.111(7)	0.21(1)	0.24(1)	–0.056(6)	0.100(7)	–0.156(9)
C(38)	2*i*	0.0835(4)	0.5573(4)	0.7974(3)	0.045(3)	0.042(3)	0.038(3)	0.000(2)	0.000(2)	–0.011(2)
C(39)	2*i*	–0.0200(5)	0.5126(5)	0.8353(4)	0.088(5)	0.114(5)	0.066(4)	–0.052(4)	0.004(3)	–0.010(4)
C(40)	2*i*	0.0931(4)	0.6425(5)	0.8497(4)	0.090(4)	0.075(4)	0.052(3)	–0.015(3)	–0.008(3)	–0.025(3)
N(1)	2*i*	0.3728(3)	0.2025(3)	0.2225(2)	0.037(2)	0.028(2)	0.045(2)	–0.007(2)	–0.013(2)	–0.006(2)
N(2)	2*i*	0.2183(3)	0.4308(3)	0.6706(2)	0.033(2)	0.026(2)	0.038(2)	–0.000(2)	–0.009(2)	–0.006(2)
O(1)	2*i*	0.6064(3)	0.6064(2)	0.1999(2)	0.054(2)	0.032(2)	0.064(2)	–0.015(2)	–0.025(2)	–0.005(2)
O(2)	2*i*	0.6510(2)	0.3913(2)	0.3100(2)	0.050(2)	0.031(2)	0.065(2)	–0.010(2)	–0.029(2)	–0.000(2)
O(3)	2*i*	0.4033(2)	–0.1028(2)	0.8051(3)	0.045(2)	0.022(2)	0.092(3)	–0.001(1)	–0.007(2)	–0.004(2)
O(4)	2*i*	0.5147(2)	0.0644(2)	0.7322(2)	0.035(2)	0.030(2)	0.081(2)	–0.003(1)	–0.004(2)	–0.013(2)

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