Crystal structure of *N*-(diphenylmethylene)diphenylmethanamine, $C_{26}H_{21}N$

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Abstract

$C_{26}H_{21}N$, monoclinic, $P12_1/c1$ (no. 14), $a = 27.861(2)$ Å, $b = 8.7867(5)$ Å, $c = 24.504(1)$ Å, $\beta = 94.624(1)^\circ$, $V = 5979.2$ Å³, $Z = 12$, $R_g(F) = 0.055$, $wR_{ref}(F^2) = 0.146$, $T = 292$ K.

Source of material

The title compound was synthesized from diphenylmethanamine according to the reported literature [1]. Colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol/acetone (3:1) solution of the title compound under ambient conditions.

Experimental details

All H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of $d(Csp^2-H) = 0.93$ Å with $U_{iso} = 1.2 U_{eq}(\text{parent atom})$, and $d(Csp^3-H) = 0.98$ Å with $U_{iso} = 1.5 U_{eq}(\text{parent atom})$.

Discussion

Compounds with the structure of $-C=N-$ (azomethine group) are known as Schiff bases, which are usually synthesized from the condensation of primary amines and active carbonyl groups. Schiff bases belong to a widely used group of organic intermediates important for production of specialty chemicals, e.g., pharmaceuticals or rubber additives [2], and as amino protective

groups in organic synthesis [3]. They also have applications as liquid crystals [4], and in analytical chemistry [5], and polymer chemistry [6].

The title crystal structure contains three molecules in the asymmetric unit with intermolecular $C-H\cdots\pi$ interactions and $d(H43\cdots Cg2(C8/C9/C10/C11/C12/C13)) = 2.73$ Å, $d(C43\cdots Cg2) = 3.690(3)$ Å. The double bond distances of $N1=C14$, $N2=C40$ and $N3=C66$ in these three molecules are 1.278(2), 1.269(3) and 1.272(3) Å, respectively. All these values are within normal ranges for Schiff bases. The molecules are packed mainly by intermolecular $C-H\cdots\pi$ interactions to form three-dimensional structure.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.20 × 0.20 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.67 cm ⁻¹
Diffractometer, scan mode:	Bruker SMART CCD, ϕ/ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	37179, 10533
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 5956
$N(param)_{refined}$:	730
Programs:	SHELXS-97 [7], SHELXL-97 [8], SHELXTL [9]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.0190	0.5436	0.1623	0.069
H(3)	4e	0.0161	0.3967	0.2417	0.093
H(4)	4e	0.0518	0.2654	0.3157	0.113
H(5)	4e	0.1338	0.2531	0.3299	0.118
H(6)	4e	0.1802	0.3708	0.2696	0.130
H(7)	4e	0.1455	0.5013	0.1958	0.104
H(9)	4e	0.0918	0.7047	0.0798	0.091
H(10)	4e	0.1140	0.9565	0.0757	0.109
H(11)	4e	0.1065	1.1142	0.1487	0.105
H(12)	4e	0.0779	1.0200	0.2269	0.104
H(13)	4e	0.0555	0.7687	0.2320	0.085
H(16)	4e	-0.0151	0.2109	0.0092	0.073
H(17)	4e	0.0104	0.0811	-0.0652	0.089
H(18)	4e	0.0905	0.0759	-0.0806	0.094
H(19)	4e	0.1454	0.2056	-0.0227	0.092
H(20)	4e	0.1205	0.3391	0.0504	0.077
H(22)	4e	-0.0046	0.1576	0.1439	0.073
H(23)	4e	-0.0815	0.1317	0.1709	0.085
H(24)	4e	-0.1394	0.3082	0.1453	0.094
H(25)	4e	-0.1212	0.5113	0.0919	0.104
H(26)	4e	-0.0446	0.5386	0.0645	0.083
H(27)	4e	0.3101	0.4947	0.4113	0.086
H(29)	4e	0.3155	0.6120	0.4964	0.120
H(30)	4e	0.2822	0.7468	0.5650	0.146
H(31)	4e	0.2010	0.7868	0.5610	0.142

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Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(32)	4e	0.1528	0.7004	0.4881	0.121
H(33)	4e	0.1846	0.5679	0.4191	0.097
H(35)	4e	0.2474	0.2864	0.4765	0.103
H(36)	4e	0.2289	0.0300	0.4665	0.123
H(37)	4e	0.2308	-0.0864	0.3828	0.132
H(38)	4e	0.2494	0.0542	0.3080	0.134
H(39)	4e	0.2688	0.3067	0.3177	0.109
H(42)	4e	0.2041	0.6877	0.2863	0.098
H(43)	4e	0.1748	0.8147	0.2088	0.120
H(44)	4e	0.2262	0.9329	0.1540	0.126
H(45)	4e	0.3076	0.9233	0.1761	0.113
H(46)	4e	0.3379	0.8008	0.2545	0.088
H(48)	4e	0.3435	0.8445	0.3928	0.083
H(49)	4e	0.4245	0.8654	0.4162	0.098
H(50)	4e	0.4769	0.6913	0.3846	0.111
H(51)	4e	0.4479	0.4961	0.3285	0.117
H(52)	4e	0.3661	0.4766	0.3045	0.097
H(53)	4e	0.3521	0.5088	0.0830	0.077
H(55)	4e	0.4115	0.6891	0.1708	0.112

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(56)	4e	0.4321	0.9425	0.1774	0.135
H(57)	4e	0.4355	1.0876	0.0998	0.121
H(58)	4e	0.4194	0.9765	0.0156	0.113
H(59)	4e	0.3986	0.7228	0.0086	0.096
H(61)	4e	0.3379	0.4105	-0.0053	0.106
H(62)	4e	0.3621	0.2797	-0.0794	0.137
H(63)	4e	0.4412	0.2170	-0.0839	0.132
H(64)	4e	0.4968	0.2874	-0.0148	0.114
H(65)	4e	0.4735	0.4208	0.0594	0.090
H(68)	4e	0.3272	0.1546	0.0970	0.091
H(69)	4e	0.2459	0.1329	0.0765	0.121
H(70)	4e	0.1944	0.3008	0.1134	0.148
H(71)	4e	0.2249	0.4868	0.1724	0.167
H(72)	4e	0.3063	0.5078	0.1929	0.122
H(74)	4e	0.3406	0.1822	0.2374	0.097
H(75)	4e	0.3774	0.0573	0.3121	0.124
H(76)	4e	0.4596	0.0577	0.3282	0.133
H(77)	4e	0.5056	0.1905	0.2706	0.125
H(78)	4e	0.4697	0.3211	0.1970	0.097

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(1)	4e	0.05406(7)	0.5441(2)	0.16052(9)	0.044(1)	0.070(2)	0.060(2)	-0.004(1)	0.011(1)	-0.016(1)
C(2)	4e	0.07699(8)	0.4622(2)	0.21026(9)	0.058(1)	0.055(1)	0.057(2)	-0.008(1)	0.011(1)	-0.011(1)
C(3)	4e	0.04953(9)	0.3917(3)	0.2469(1)	0.082(2)	0.085(2)	0.066(2)	-0.028(2)	0.017(1)	-0.011(2)
C(4)	4e	0.0710(1)	0.3132(3)	0.2915(1)	0.134(3)	0.082(2)	0.069(2)	-0.039(2)	0.021(2)	-0.002(2)
C(5)	4e	0.1195(1)	0.3056(3)	0.3000(1)	0.136(3)	0.077(2)	0.082(2)	0.004(2)	0.000(2)	0.013(2)
C(6)	4e	0.1468(1)	0.3756(4)	0.2641(1)	0.086(2)	0.124(3)	0.113(3)	0.019(2)	0.004(2)	0.035(2)
C(7)	4e	0.12599(9)	0.4536(3)	0.2198(1)	0.063(2)	0.108(2)	0.089(2)	0.006(2)	0.012(1)	0.031(2)
C(8)	4e	0.07093(7)	0.7085(2)	0.15618(9)	0.045(1)	0.059(1)	0.061(2)	0.003(1)	0.002(1)	-0.004(1)
C(9)	4e	0.08867(9)	0.7675(3)	0.1099(1)	0.090(2)	0.072(2)	0.065(2)	-0.001(1)	0.008(1)	-0.004(1)
C(10)	4e	0.1020(1)	0.9188(3)	0.1074(1)	0.107(2)	0.074(2)	0.093(2)	0.001(2)	0.017(2)	0.015(2)
C(11)	4e	0.09774(9)	1.0123(3)	0.1507(1)	0.088(2)	0.058(2)	0.116(3)	0.008(1)	0.005(2)	0.004(2)
C(12)	4e	0.0806(1)	0.9563(3)	0.1970(1)	0.097(2)	0.065(2)	0.099(2)	0.011(2)	0.013(2)	-0.021(2)
C(13)	4e	0.06721(8)	0.8055(3)	0.2001(1)	0.076(2)	0.066(2)	0.073(2)	0.007(1)	0.016(1)	-0.011(1)
C(14)	4e	0.03440(7)	0.3735(2)	0.08633(8)	0.055(1)	0.046(1)	0.052(1)	0.000(1)	0.002(1)	0.003(1)
C(15)	4e	0.04992(7)	0.2883(2)	0.03816(8)	0.062(1)	0.042(1)	0.049(1)	0.001(1)	0.005(1)	0.004(1)
C(16)	4e	0.01735(8)	0.2106(2)	0.00294(9)	0.073(2)	0.055(1)	0.056(2)	-0.009(1)	0.009(1)	-0.004(1)
C(17)	4e	0.0327(1)	0.1322(3)	-0.0416(1)	0.102(2)	0.062(2)	0.059(2)	-0.012(1)	0.011(1)	-0.008(1)
C(18)	4e	0.0803(1)	0.1297(3)	-0.0510(1)	0.109(2)	0.063(2)	0.065(2)	0.008(2)	0.022(2)	-0.006(1)
C(19)	4e	0.1129(1)	0.2069(3)	-0.0164(1)	0.078(2)	0.081(2)	0.073(2)	0.015(2)	0.019(2)	-0.000(2)
C(20)	4e	0.09801(8)	0.2862(3)	0.02756(9)	0.065(2)	0.065(2)	0.063(2)	0.007(1)	0.007(1)	-0.004(1)
C(21)	4e	-0.01609(7)	0.3525(2)	0.10185(8)	0.052(1)	0.044(1)	0.046(1)	-0.003(1)	0.000(1)	-0.001(1)
C(22)	4e	-0.02790(8)	0.2300(2)	0.13342(9)	0.070(2)	0.052(1)	0.060(2)	-0.001(1)	0.004(1)	0.007(1)
C(23)	4e	-0.07396(9)	0.2143(3)	0.14952(9)	0.085(2)	0.067(2)	0.061(2)	-0.020(2)	0.013(1)	0.008(1)
C(24)	4e	-0.10844(9)	0.3191(3)	0.1342(1)	0.059(2)	0.089(2)	0.089(2)	-0.013(2)	0.014(1)	-0.001(2)
C(25)	4e	-0.09762(8)	0.4400(3)	0.1025(1)	0.057(2)	0.082(2)	0.120(2)	0.006(1)	0.005(2)	0.018(2)
C(26)	4e	-0.05171(8)	0.4563(3)	0.0863(1)	0.059(2)	0.062(2)	0.086(2)	-0.001(1)	0.004(1)	0.023(1)
C(27)	4e	0.27503(8)	0.4917(3)	0.4041(1)	0.059(1)	0.074(2)	0.083(2)	0.001(1)	0.007(1)	0.031(2)
C(28)	4e	0.25348(9)	0.5745(3)	0.4497(1)	0.069(2)	0.067(2)	0.076(2)	-0.011(1)	0.009(1)	0.024(1)
C(29)	4e	0.2825(1)	0.6294(4)	0.4943(2)	0.086(2)	0.112(3)	0.099(2)	-0.026(2)	-0.006(2)	0.022(2)
C(30)	4e	0.2625(2)	0.7097(4)	0.5356(2)	0.156(4)	0.115(3)	0.093(3)	-0.047(3)	0.004(3)	-0.002(2)
C(31)	4e	0.2144(2)	0.7342(4)	0.5330(2)	0.157(4)	0.095(3)	0.107(3)	-0.016(3)	0.033(3)	0.007(2)
C(32)	4e	0.1857(1)	0.6822(4)	0.4898(2)	0.106(2)	0.098(2)	0.101(3)	0.005(2)	0.026(2)	0.014(2)
C(33)	4e	0.20487(9)	0.6030(3)	0.4484(1)	0.077(2)	0.086(2)	0.082(2)	-0.002(2)	0.015(2)	0.012(2)
C(34)	4e	0.25992(8)	0.3247(3)	0.3980(1)	0.052(1)	0.072(2)	0.086(2)	0.004(1)	0.006(1)	0.020(2)
C(35)	4e	0.24802(9)	0.2403(3)	0.4424(1)	0.082(2)	0.076(2)	0.101(2)	-0.001(2)	0.020(2)	0.027(2)
C(36)	4e	0.2370(1)	0.0860(4)	0.4363(2)	0.083(2)	0.079(2)	0.147(3)	-0.001(2)	0.020(2)	0.042(2)
C(37)	4e	0.2379(1)	0.0167(4)	0.3865(2)	0.084(2)	0.072(2)	0.173(4)	0.003(2)	0.002(2)	0.006(3)
C(38)	4e	0.2493(1)	0.1003(4)	0.3422(2)	0.114(3)	0.086(3)	0.133(3)	0.008(2)	0.002(2)	-0.004(2)
C(39)	4e	0.26056(9)	0.2518(4)	0.3481(1)	0.089(2)	0.081(2)	0.102(2)	0.009(2)	0.008(2)	0.016(2)
C(40)	4e	0.29310(8)	0.6495(3)	0.3299(1)	0.059(1)	0.054(1)	0.075(2)	-0.004(1)	0.014(1)	0.006(1)
C(41)	4e	0.27473(8)	0.7299(2)	0.2792(1)	0.068(2)	0.047(1)	0.070(2)	-0.005(1)	0.005(1)	0.004(1)
C(42)	4e	0.22533(9)	0.7356(3)	0.2645(1)	0.069(2)	0.081(2)	0.095(2)	-0.007(1)	0.003(2)	0.013(2)
C(43)	4e	0.2079(1)	0.8114(4)	0.2180(1)	0.087(2)	0.099(2)	0.108(2)	-0.003(2)	-0.024(2)	0.024(2)
C(44)	4e	0.2384(1)	0.8816(3)	0.1853(1)	0.116(3)	0.096(2)	0.097(2)	-0.015(2)	-0.025(2)	0.028(2)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(45)	4e	0.2867(1)	0.8765(3)	0.1986(1)	0.108(2)	0.093(2)	0.080(2)	-0.023(2)	-0.005(2)	0.026(2)
C(46)	4e	0.30485(9)	0.8021(3)	0.2455(1)	0.074(2)	0.070(2)	0.074(2)	-0.013(1)	-0.001(1)	0.010(1)
C(47)	4e	0.34603(8)	0.6587(3)	0.34633(9)	0.062(1)	0.052(1)	0.058(2)	0.002(1)	0.011(1)	0.007(1)
C(48)	4e	0.36441(9)	0.7734(3)	0.3795(1)	0.067(2)	0.075(2)	0.068(2)	0.003(1)	0.011(1)	0.001(1)
C(49)	4e	0.4129(1)	0.7861(3)	0.3937(1)	0.084(2)	0.089(2)	0.070(2)	-0.008(2)	0.001(2)	-0.004(2)
C(50)	4e	0.4440(1)	0.6830(4)	0.3748(1)	0.066(2)	0.110(3)	0.099(2)	0.001(2)	-0.002(2)	0.011(2)
C(51)	4e	0.4268(1)	0.5669(4)	0.3415(1)	0.073(2)	0.097(2)	0.126(3)	0.025(2)	0.025(2)	-0.001(2)
C(52)	4e	0.37773(9)	0.5553(3)	0.3273(1)	0.074(2)	0.072(2)	0.099(2)	0.006(1)	0.019(2)	-0.009(2)
C(53)	4e	0.38733(8)	0.5117(3)	0.0848(1)	0.052(1)	0.068(2)	0.073(2)	-0.001(1)	0.005(1)	0.020(1)
C(54)	4e	0.40302(7)	0.6779(3)	0.0889(1)	0.051(1)	0.067(2)	0.071(2)	0.003(1)	0.006(1)	0.009(1)
C(55)	4e	0.4130(1)	0.7463(3)	0.1391(1)	0.115(2)	0.081(2)	0.083(2)	-0.004(2)	-0.001(2)	0.005(2)
C(56)	4e	0.4253(1)	0.8986(4)	0.1431(2)	0.140(3)	0.078(2)	0.116(3)	-0.005(2)	-0.015(2)	-0.012(2)
C(57)	4e	0.4275(1)	0.9850(4)	0.0971(2)	0.083(2)	0.067(2)	0.152(3)	-0.001(2)	0.002(2)	0.001(2)
C(58)	4e	0.4178(1)	0.9188(3)	0.0472(2)	0.093(2)	0.069(2)	0.121(3)	0.003(2)	0.019(2)	0.026(2)
C(59)	4e	0.40539(9)	0.7660(3)	0.0430(1)	0.091(2)	0.069(2)	0.080(2)	0.001(1)	0.012(1)	0.015(2)
C(60)	4e	0.40307(8)	0.4294(3)	0.0354(1)	0.061(2)	0.057(1)	0.064(2)	-0.012(1)	0.004(1)	0.016(1)
C(61)	4e	0.3703(1)	0.3862(3)	-0.0068(1)	0.082(2)	0.105(2)	0.077(2)	-0.028(2)	-0.004(2)	0.012(2)
C(62)	4e	0.3847(2)	0.3076(4)	-0.0512(1)	0.139(3)	0.121(3)	0.081(2)	-0.053(3)	-0.009(2)	-0.001(2)
C(63)	4e	0.4316(2)	0.2708(4)	-0.0540(2)	0.160(3)	0.082(2)	0.090(3)	-0.029(2)	0.033(3)	-0.008(2)
C(64)	4e	0.4646(1)	0.3126(3)	-0.0129(1)	0.104(2)	0.082(2)	0.104(2)	0.004(2)	0.027(2)	0.000(2)
C(65)	4e	0.45060(9)	0.3921(3)	0.0316(1)	0.070(2)	0.076(2)	0.080(2)	0.000(1)	0.007(1)	0.001(2)
C(66)	4e	0.37840(8)	0.3470(2)	0.16036(9)	0.068(2)	0.051(1)	0.065(2)	-0.004(1)	0.017(1)	0.000(1)
C(67)	4e	0.32531(8)	0.3324(3)	0.14746(9)	0.068(2)	0.055(2)	0.066(2)	-0.007(1)	0.019(1)	0.004(1)
C(68)	4e	0.30656(9)	0.2222(3)	0.1126(1)	0.076(2)	0.077(2)	0.075(2)	-0.009(1)	0.010(1)	0.004(2)
C(69)	4e	0.2580(1)	0.2093(4)	0.1001(1)	0.101(2)	0.111(3)	0.088(2)	-0.032(2)	-0.004(2)	0.015(2)
C(70)	4e	0.2275(1)	0.3084(6)	0.1221(2)	0.067(2)	0.157(4)	0.146(4)	-0.013(2)	-0.001(2)	0.035(3)
C(71)	4e	0.2457(1)	0.4193(5)	0.1570(2)	0.077(2)	0.144(4)	0.201(4)	0.019(2)	0.051(3)	-0.012(3)
C(72)	4e	0.2943(1)	0.4314(3)	0.1694(1)	0.079(2)	0.098(2)	0.133(3)	0.000(2)	0.038(2)	-0.029(2)
C(73)	4e	0.40112(9)	0.2652(2)	0.2088(1)	0.083(2)	0.050(1)	0.061(2)	-0.002(1)	0.011(1)	-0.003(1)
C(74)	4e	0.3739(1)	0.1851(3)	0.2439(1)	0.107(2)	0.069(2)	0.067(2)	-0.010(2)	0.012(2)	0.008(1)
C(75)	4e	0.3961(2)	0.1095(4)	0.2885(1)	0.148(3)	0.089(2)	0.074(2)	-0.010(2)	0.011(2)	0.016(2)
C(76)	4e	0.4450(2)	0.1103(4)	0.2984(1)	0.162(4)	0.090(2)	0.076(2)	0.009(2)	-0.017(2)	0.009(2)
C(77)	4e	0.4722(1)	0.1893(4)	0.2640(1)	0.113(2)	0.103(2)	0.091(2)	0.009(2)	-0.022(2)	0.005(2)
C(78)	4e	0.4508(1)	0.2669(3)	0.2198(1)	0.086(2)	0.077(2)	0.079(2)	-0.005(2)	0.003(2)	0.000(2)
N(1)	4e	0.06574(6)	0.4591(2)	0.11192(7)	0.056(1)	0.067(1)	0.059(1)	-0.005(1)	0.0093(9)	-0.012(1)
N(2)	4e	0.26274(7)	0.5726(2)	0.35426(8)	0.082(1)	0.085(2)	0.072(1)	-0.027(1)	-0.004(1)	0.018(1)
N(3)	4e	0.40567(7)	0.4291(2)	0.13337(8)	0.075(1)	0.076(1)	0.066(1)	-0.015(1)	0.002(1)	0.012(1)

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References

- Orito, K.; Hatakeyama, T.; TaKeo, M.; Uchiito, S.; Tokuda, M.; Suginoe, H.: Dimerization of anilines and benzylamines with Mercury(II) oxide-iodine reagent. *Tetrahedron* **54** (1998) 8403-8410.
- Macho, V.; Kralik, M.; Hudec, J.; Cingelova, J.: One stage preparation of Schiff bases from nitroarenes, aldehydes and carbon monoxide at presence of water. *J. Mol. Catal. A: Chem.* **209** (2004) 69-73.
- Bezas, B.; Zervas, L.: On the peptides of L-Lysine. *J. Am. Chem. Soc.* **83** (1961) 719-723.
- Adams, J. P.: Imines, enamines and oximes. *J. Chem. Soc., Perkin Trans. I* (2000) 125-139.
- Abbaspour, A.; Esmailbeig, A. R.; Jarrahpour, A. A.; Khajeh, B.; Kia, R.: Aluminium(III)-selective electrode based on a newly synthesized tetradentate Schiff base. *Talanta* **58** (2002) 397-403.
- Higuchi, M.; Yamamoto, K.: Novel cyclic molecules: selective synthesis of cyclic phenylazomethines. *Org. Lett.* **1** (1999) 1881-1883.
- Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
- Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
- Sheldrick, G. M.: SHELXTL. Structure Determination Software Suite. Version 6.14. Bruker AXS, Madison, Wisconsin, USA 2000.