

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)
$$B_{eq} = (1/3) \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B _{eq}
N(1)	0.5465 (2)	0.1990 (6)	0.4560 (3)	4.70 (17)
C(2)	0.5855 (3)	0.2136 (8)	0.4033 (3)	3.95 (22)
C(3)	0.5574 (3)	0.3366 (8)	0.3384 (3)	4.90 (23)
N(4)	0.4891 (2)	0.4177 (7)	0.3340 (2)	3.94 (16)
C(5)	0.3764 (3)	0.4744 (9)	0.3788 (3)	4.56 (23)
C(6)	0.3412 (3)	0.4479 (8)	0.4340 (3)	3.83 (20)
C(7)	0.3724 (3)	0.3527 (9)	0.5025 (4)	5.93 (26)
C(8)	0.4440 (3)	0.2750 (9)	0.5086 (3)	5.40 (25)
C(9)	0.4791 (3)	0.2945 (9)	0.4543 (3)	4.64 (25)
C(10)	0.4482 (3)	0.3894 (9)	0.3873 (3)	4.31 (24)
C(11)	0.6481 (3)	0.0964 (8)	0.3995 (3)	3.89 (21)
C(12)	0.7036 (3)	0.0755 (9)	0.4720 (3)	4.00 (22)
C(13)	0.7651 (3)	-0.0379 (9)	0.4779 (4)	6.18 (26)
C(14)	0.7705 (3)	-0.1308 (10)	0.4149 (3)	5.99 (26)
C(15)	0.7157 (3)	-0.1190 (8)	0.3470 (3)	4.78 (24)
C(16)	0.6553 (3)	-0.0004 (9)	0.3405 (3)	4.49 (23)
C(17)	0.6007 (3)	0.3795 (8)	0.2849 (3)	3.67 (21)
C(18)	0.5662 (3)	0.4077 (9)	0.2045 (3)	4.76 (23)
C(19)	0.6116 (3)	0.4526 (9)	0.1565 (3)	5.51 (24)
C(20)	0.6909 (3)	0.4680 (9)	0.1786 (4)	5.99 (25)
C(21)	0.7247 (3)	0.4485 (9)	0.2575 (3)	5.38 (22)
C(22)	0.6787 (3)	0.4041 (9)	0.3127 (4)	5.79 (28)
C(231)	0.2255 (7)	0.5849 (14)	0.3747 (9)	7.53 (57)
C(232)	0.2207 (6)	0.5297 (19)	0.4633 (8)	7.39 (60)
N(5)	0.2643 (3)	0.5178 (8)	0.4330 (4)	8.39 (26)
C(24)	0.1457 (4)	0.6389 (11)	0.4134 (4)	7.66 (33)
C(25)	0.1073 (4)	0.7137 (11)	0.3543 (4)	8.39 (33)
O(1)	0.1248 (3)	0.7420 (12)	0.2906 (3)	16.79 (37)
O(2)	0.0289 (2)	0.7325 (7)	0.3454 (3)	8.64 (20)
C(26)	-0.0224 (4)	0.7977 (14)	0.2843 (4)	10.07 (37)
C(27)	-0.0975 (4)	0.7691 (14)	0.2762 (5)	11.47 (40)
C(28)	0.1297 (3)	0.6279 (10)	0.4857 (4)	8.42 (31)
O(3)	0.1618 (3)	0.5455 (8)	0.5431 (3)	11.04 (26)
O(4)	0.0668 (2)	0.7201 (7)	0.4961 (3)	9.32 (20)
C(29)	0.0449 (5)	0.7103 (13)	0.5744 (4)	11.30 (39)
C(30)	-0.0272 (5)	0.7981 (12)	0.5605 (4)	9.79 (38)

Table 2. Selected geometric parameters (Å, °)

N(1)—C(2)	1.304 (7)	C(7)—C(8)	1.380 (9)
C(2)—C(3)	1.482 (8)	C(8)—C(9)	1.285 (8)
C(3)—N(4)	1.342 (7)	C(9)—N(1)	1.390 (7)
N(4)—C(10)	1.348 (7)	C(9)—C(10)	1.397 (8)
C(10)—C(5)	1.400 (8)	C(2)—C(11)	1.434 (7)
C(5)—C(6)	1.308 (8)	C(3)—C(17)	1.404 (8)
C(6)—C(7)	1.419 (8)	C(6)—N(5)	1.457 (8)
N(5)—C(231)	1.219 (16)	C(231)—C(24)	1.767 (15)
N(5)—C(232)	1.051 (14)	C(232)—C(24)	1.638 (15)
C(2)—N(1)—C(9)	122.8 (5)	C(5)—C(10)—C(9)	119.2 (6)
N(1)—C(2)—C(3)	119.2 (5)	C(6)—C(5)—C(10)	115.7 (6)
N(1)—C(2)—C(11)	122.1 (5)	C(5)—C(6)—C(7)	125.4 (6)
C(3)—C(2)—C(11)	118.0 (5)	C(5)—C(6)—N(5)	123.3 (6)
C(2)—C(3)—N(4)	117.5 (5)	C(7)—C(6)—N(5)	111.3 (6)
C(2)—C(3)—C(17)	123.2 (5)	C(6)—C(7)—C(8)	116.4 (6)
N(4)—C(3)—C(17)	119.2 (5)	C(7)—C(8)—C(9)	119.6 (6)
C(3)—N(4)—C(10)	121.0 (5)	C(8)—C(9)—N(1)	119.6 (6)
N(4)—C(10)—C(5)	118.5 (6)	C(8)—C(9)—C(10)	123.6 (6)
N(4)—C(10)—C(9)	121.9 (6)	N(1)—C(9)—C(10)	116.3 (5)
C(6)—N(5)—C(231)	119.7 (8)	N(5)—C(231)—C(24)	95.6 (9)
C(6)—N(5)—C(232)	145.7 (9)	N(5)—C(232)—C(24)	111.1 (10)

There is a twofold disorder at the C(23) atom and occupancy factors were fixed at 0.50 for both sites, C(231) and C(232), based on relative heights in a difference Fourier map. Positions of the H atoms, except those attached to the disordered C atom and its neighbouring N atom, were calculated and included in the F_c calculation with B_{iso} set at 0.5 Å² higher than the B_{eq} value of the parent C atom. The structure was solved using MULTAN80 (Main, Fiske, Hull, Lessinger, Germain,

Declercq & Woolfson, 1980). All remaining calculations were performed with a local version of the NRC program system (Ahmed & Singh, 1973).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the IUCr (Reference: KA1063). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Ahmed, F. R. & Singh, P. (1973). *J. Appl. Cryst.* **6**, 309–346, accession Nos. 133–147.
- Goljer, I., Milata, V. & Ilavský, D. (1989). *Magn. Reson. Chem.* **27**, 138–144.
- Hurley, J. & Le Fevre, R. J. W. (1967). *J. Chem. Soc. B*, pp. 824–827.
- Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.
- Woźniak, K., Krygowski, T. M. & Filipek, S. (1991). *Acta Cryst. C* **47**, 1326–1328.

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4,4'-Methylenediiminobis(benzophenone)

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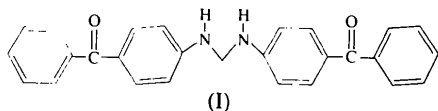
Abstract

The title compound [N,N'-bis(benzoylphenyl)methanediimine, C₂₇H₂₂N₂O₂] was prepared by condensation of 4-aminobenzophenone (ABP) and formaldehyde at room temperature. In the molecule, two ABP moieties are linked by a methylene group. The bond lengths and angles within the two ABP groups are very similar; however, the dihedral angles between the sets of ring planes are quite different [83.1 (5) and 57.5 (3)°].

Comment

Recently, crystals of 4-aminobenzophenone (ABP) were discovered to be a new and highly effective non-linear optical (NLO) material (Frazier & Cockerham, 1987). In an attempt to improve on this material, we carried out a condensation reaction

between ABP and formaldehyde (Yamamoto Katogi, Watanabe, Sato & Miyata, 1992). The structural studies reveal that the product is the title compound, ABPMDA. A drawing of the molecule with atom-numbering scheme is shown in Fig. 1. The large displacement parameters, found for O(1) and the C atoms of the phenyl ring C(11)–C(16), suggest dynamic disorder for these atoms; this is consistent with them occupying a large free space in the cell.



In the molecule, two ABP moieties are linked by a methylene group in an asymmetric fashion. Thus, although the bond lengths and angles within the two ABP groups are very similar, the dihedral angles between the sets of ring planes are quite different, having values of 83.1 (5) and 57.5 (3)°; the dihedral angle between the two ABP groups is 57.9 (5)°. This asymmetry may result from molecular-packing forces.

The title compound crystallizes in a centrosymmetric space group and therefore has no non-linear optical properties. This has been confirmed by second harmonic generation (SHG) efficiency measurements on a powder sample using the method of Kurtz & Perry (1968).

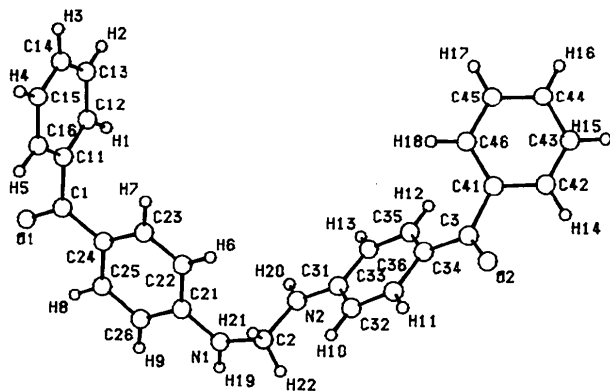


Fig. 1. Structure of an ABPMDA molecule.

Experimental

The title compound was prepared by condensation of 4-aminobenzophenone and formaldehyde. Crystals were grown from alcohol solution by evaporation at room temperature.

Crystal data

$C_{27}H_{22}N_2O_2$
 $M_r = 406.48$

Mo $K\alpha$ radiation
 $\lambda = 0.71069 \text{ \AA}$

Orthorhombic
Pbca
 $a = 10.003 (2) \text{ \AA}$
 $b = 14.636 (3) \text{ \AA}$
 $c = 28.724 (7) \text{ \AA}$
 $V = 4205 (3) \text{ \AA}^3$
 $Z = 8$
 $D_x = 1.28 \text{ Mg m}^{-3}$

Data collection

Enraf–Nonius CAD-4
diffractometer
 ω - 2θ scans [width (1.35 + 0.35tan θ)°]
Absorption correction:
empirical, based on
azimuthal scans
 $T_{\min} = 0.953$, $T_{\max} = 1.000$

Cell parameters from 25
reflections
 $\theta = 13\text{--}14^\circ$
 $\mu = 0.077 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
Transparent
 $0.4 \times 0.3 \times 0.3 \text{ mm}$
Yellow

Refinement

Refinement on F
 $R = 0.071$
 $wR = 0.082$
 $S = 1.63$
1502 reflections
280 parameters
H-atom parameters not
refined

$w = 1/\sigma^2(F)$
 $(\Delta/\sigma)_{\max} = 0.0001$
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$
Atomic scattering factors
from *International Tables*
for *X-ray Crystallography*
(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	B_{eq}
O(1)	−0.1916 (7)	0.0654 (7)	0.5683 (3)	17.3 (7)
O(2)	0.8979 (5)	0.5138 (3)	0.7046 (1)	5.5 (2)
N(1)	0.2479 (6)	0.1425 (4)	0.7205 (2)	5.0 (3)
N(2)	0.4660 (5)	0.1952 (3)	0.6979 (2)	4.3 (3)
C(1)	−0.0959 (9)	0.1143 (6)	0.5664 (3)	7.3 (5)
C(2)	0.3501 (7)	0.2115 (4)	0.7276 (2)	4.8 (4)
C(3)	0.8850 (6)	0.4506 (4)	0.6770 (2)	3.8 (3)
C(11)	−0.072 (1)	0.1627 (7)	0.5215 (3)	6.9 (5)
C(12)	0.019 (1)	0.132 (1)	0.4893 (5)	12.5 (9)
C(13)	0.036 (1)	0.176 (1)	0.4468 (5)	14 (1)
C(14)	−0.038 (1)	0.251 (1)	0.4376 (4)	11 (1)
C(15)	−0.124 (1)	0.282 (1)	0.4683 (5)	10.6 (9)
C(16)	−0.143 (1)	0.2364 (8)	0.5104 (3)	8.9 (7)
C(21)	0.1632 (7)	0.1410 (4)	0.6831 (2)	4.1 (3)
C(22)	0.1789 (6)	0.1977 (4)	0.6442 (2)	4.6 (3)
C(23)	0.0967 (7)	0.1885 (4)	0.6069 (2)	4.5 (4)
C(24)	−0.0065 (6)	0.1249 (5)	0.6056 (2)	4.3 (3)
C(25)	−0.0258 (7)	0.0702 (4)	0.6450 (3)	5.1 (4)
C(26)	0.0589 (7)	0.0780 (5)	0.6829 (2)	5.1 (4)
C(31)	0.5692 (6)	0.2565 (4)	0.6939 (2)	3.4 (3)
C(32)	0.5682 (6)	0.3404 (4)	0.7177 (2)	3.9 (3)
C(33)	0.6712 (6)	0.4011 (4)	0.7116 (2)	3.9 (3)
C(34)	0.7789 (6)	0.3832 (4)	0.6816 (2)	3.5 (3)
C(35)	0.7794 (6)	0.2987 (4)	0.6587 (2)	3.7 (3)
C(36)	0.6773 (6)	0.2366 (4)	0.6652 (2)	3.8 (3)
C(41)	0.9806 (7)	0.4445 (4)	0.6368 (2)	4.4 (4)
C(42)	1.1162 (8)	0.4561 (5)	0.6453 (3)	5.9 (4)
C(43)	1.2070 (8)	0.4544 (6)	0.6098 (4)	7.6 (5)
C(44)	1.165 (1)	0.4429 (6)	0.5649 (4)	7.5 (6)
C(45)	1.033 (1)	0.4314 (6)	0.5557 (3)	7.2 (5)
C(46)	0.9391 (7)	0.4320 (5)	0.5915 (2)	5.4 (4)

Table 2. Selected geometric parameters (Å, °)

O(1)—C(1)	1.196 (9)	C(21)—C(22)	1.400 (8)
O(2)—C(3)	1.224 (6)	C(22)—C(23)	1.356 (8)
N(1)—C(21)	1.369 (7)	C(23)—C(24)	1.391 (8)
N(1)—C(2)	1.451 (8)	C(24)—C(25)	1.398 (8)
N(2)—C(31)	1.372 (7)	C(25)—C(26)	1.385 (9)
N(2)—C(2)	1.459 (7)	C(31)—C(36)	1.390 (7)
C(1)—C(24)	1.45 (1)	C(31)—C(32)	1.406 (8)
C(1)—C(11)	1.49 (1)	C(32)—C(33)	1.370 (8)
C(3)—C(34)	1.454 (8)	C(33)—C(34)	1.404 (7)
C(3)—C(41)	1.503 (8)	C(34)—C(35)	1.401 (7)
C(11)—C(16)	1.33 (1)	C(35)—C(36)	1.380 (8)
C(11)—C(12)	1.37 (1)	C(41)—C(46)	1.378 (8)
C(12)—C(13)	1.39 (2)	C(41)—C(42)	1.389 (9)
C(13)—C(14)	1.35 (2)	C(42)—C(43)	1.37 (1)
C(14)—C(15)	1.31 (2)	C(43)—C(44)	1.37 (1)
C(15)—C(16)	1.40 (1)	C(44)—C(45)	1.35 (1)
C(21)—C(26)	1.392 (8)	C(45)—C(46)	1.39 (1)
C(21)—N(1)—C(2)	123.9 (5)	C(22)—C(23)—C(24)	122.5 (6)
C(31)—N(2)—C(2)	122.6 (5)	C(23)—C(24)—C(25)	117.7 (6)
O(1)—C(1)—C(24)	121.6 (9)	C(23)—C(24)—C(1)	123.4 (7)
O(1)—C(1)—C(11)	116.9 (8)	C(25)—C(24)—C(1)	118.9 (7)
C(24)—C(1)—C(11)	121.6 (7)	C(26)—C(25)—C(24)	120.3 (6)
N(1)—C(2)—N(2)	111.3 (5)	C(25)—C(26)—C(21)	121.0 (6)
O(2)—C(3)—C(34)	122.1 (6)	N(2)—C(31)—C(36)	119.9 (6)
O(2)—C(3)—C(41)	118.4 (6)	N(2)—C(31)—C(32)	121.7 (6)
C(34)—C(3)—C(41)	119.5 (6)	C(36)—C(31)—C(32)	118.5 (6)
C(16)—C(11)—C(12)	117 (1)	C(33)—C(32)—C(31)	119.9 (5)
C(16)—C(11)—C(1)	120 (1)	C(32)—C(33)—C(34)	122.3 (5)
C(12)—C(11)—C(1)	122 (1)	C(35)—C(34)—C(33)	117.1 (6)
C(11)—C(12)—C(13)	121 (1)	C(35)—C(34)—C(3)	123.6 (6)
C(14)—C(13)—C(12)	119 (1)	C(33)—C(34)—C(3)	119.3 (6)
C(15)—C(14)—C(13)	121 (1)	C(36)—C(35)—C(34)	121.0 (5)
C(14)—C(15)—C(16)	120 (1)	C(35)—C(36)—C(31)	121.2 (5)
C(11)—C(16)—C(15)	122 (1)	C(46)—C(41)—C(42)	118.5 (7)
N(1)—C(21)—C(26)	118.5 (6)	C(46)—C(41)—C(3)	122.8 (6)
N(1)—C(21)—C(22)	123.2 (6)	C(42)—C(41)—C(3)	118.6 (6)
C(26)—C(21)—C(22)	118.3 (6)	C(43)—C(42)—C(41)	121.0 (7)
C(23)—C(22)—C(21)	120.2 (6)		

The crystal was mounted in a random orientation on a glass fibre. Data were collected using *CONTROL* software (Molecular Structure Corporation, 1988). The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods using *MITHRIL* (Gilmore, 1983) and *DIRDIF* (Beurskens, 1984). The C, O and N atoms were located in an *E* map. H atoms were placed in geometrically calculated positions with C—H = 0.95 Å, but were not included in the refinement. Anomalous-dispersion corrections were not applied. All calculations were performed on a MicroVAX II computer using the *TEXSAN* (Molecular Structure Corporation, 1987) program package. Molecular graphics were produced using the *PLUTO* program (Motherwell & Clegg, 1976).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates, and a packing diagram of the unit cell have been deposited with the IUCr (Reference: LI1081). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Beurskens, P. T. (1984). *DIRDIF. Direct Methods for Difference Structures - an Automatic Procedure for the Phase Extension and Refinement of Difference Structure Factors*. Technical Report 1984/1. Crystallography Laboratory, Toernooiveld, 6525 ED Nijmegen, The Netherlands.
- Frazier, C. C. & Cockerham, M. P. (1987). *J. Opt. Soc. Am. B*, p. 1899.

- Gilmore, C. J. (1983). *MITHRIL. Computer Program for the Automatic Solution of Crystal Structures from X-ray Data*. Department of Chemistry, Univ. of Glasgow, Scotland.
- Kurtz, S. K. & Perry, T. T. (1968). *J. Appl. Phys.* **39**, 3798–3813.
- Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
- Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
- Motherwell, W. D. S. & Clegg, W. (1976). *Program for Plotting Molecular and Crystal Structures*. Univ. of Cambridge, England.
- Yamamoto, H., Katogi, S., Watanabe, T., Sato, H. & Miyata, S. (1992). *Appl. Phys. Lett.* **60**, 935–939.

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1-[4-(4-Bromobenzylideneamino)phenyl]-3-(4-bromophenyl)-2-propen-1-one

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Abstract

In the title compound, C₂₂H₁₅Br₂NO, the torsion angle O(1)—C(1)—C(2)—C(3) within the C₇H₇CO group is –21 (2)° and H atoms are in *trans* positions. The dihedral angles between the three phenyl rings are 46.2 (6), 168.2 (6) and 132.6 (6)°.

Comment

The chalcone derivatives are newly developed organic crystals with non-linear optical coefficients (Fichou, Watanabe, Takeda, Miyata, Goto & Nakayama, 1988). In order to explore the relationship between their structure and non-linear optical properties, we synthesized a series of substituted chalcones. The title compound, (I), is one of these, which happens to crystallize in a centrosymmetric space group and, therefore, has no non-linear optical properties. This has been confirmed by second harmonic generation (SHG) efficiency measurements on a powder sample using the method of Kurtz & Perry (1968).

