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4-Dimethylamino-4′-nitrobenzophenone

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.089
Data-to-parameter ratio = 12.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, $C_{15}H_{14}N_2O_3$, the two halves of the molecule, except for the central CO group, are nearly planar and the dihedral angle between the least-squares planes through the C atoms of the six-membered rings is 51.41 (6)°. The central O atom is displaced by −0.7389 (15) and 0.5439 (15) Å from these least-squares planes.

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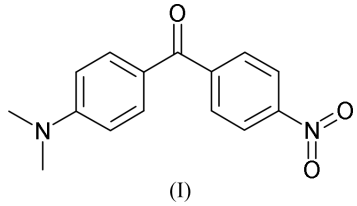
Comment

As part of our investigations on organic non-linear optical (NLO) materials, we have determined the crystal structure of the title compound, (I) (Fig. 1), which was first synthesized by Shah *et al.* (1932). It was suggested that (I) could be a good candidate for NLO and electro-optical applications.



(I)

Experimental

The title compound was synthesized according to Shah *et al.* (1932) in a two-step reaction, and the purity was confirmed by elemental analysis, IR, UV-vis and mass spectrometry. Crystals were grown from glacial acetic acid solution, by slow evaporation at room temperature, over a period of several weeks.

Crystal data

$C_{15}H_{14}N_2O_3$
M_r = 270.28
Monoclinic, $P2_1/n$
a = 6.1527 (3) Å
b = 28.9053 (15) Å
c = 7.4404 (4) Å
β = 92.036 (2)°
V = 1322.41 (12) Å^3
Z = 4
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8954 reflections
θ = 3.1–25.4°
μ = 0.10 mm^{-1}
T = 291 (1) K
Plate, yellow
0.50 × 0.20 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
375 frames *via* ω rotation ($\Delta\omega$ = 1°), with three sets at different κ angles and two × 70 s per frame
Absorption correction: none
8954 measured reflections
2365 independent reflections
1021 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°
$h = -7 \rightarrow 7$
$k = -34 \rightarrow 34$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.089
S = 0.93
2365 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

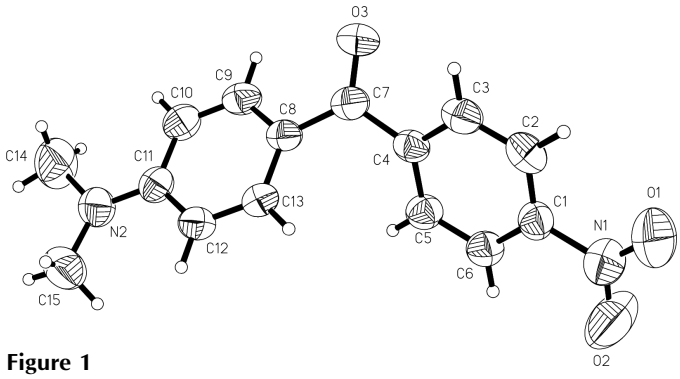


Figure 1
View of the title compound (*XP*; Sheldrick, 1991), showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 50% probability level. H atoms are drawn as circles of arbitrary radii.

H atoms were placed in calculated positions with U_{iso} constrained to be 1.5 times U_{eq} of the carrier atom for the methyl–H and 1.2 times U_{eq} for the remaining H atoms. The methyl groups were allowed to rotate but not to tip.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97, *PARST*95 (Nardelli, 1995) and *PLATON* (Spek, 2001).

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References

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Shah, R. C., Deshpande, R. K. & Chaubal, J. S. (1932). *J. Chem. Soc.* pp. 642–650.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus.* Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2001). *PLATON.* University of Utrecht, The Netherlands.