CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.
CURTIS, D. R., DUGGAN, A. W., FELIX, D. & JOHNSTON, G. A. R. (1971). *Brain Res.* **32**, 69–96.
DAHL, O. & LARSEN, S. (1979). *J. Chem. Res.* (*M*), pp. 4637–4645.
JOHNSON, C. K. (1971). *ORTEP* II. Report ORNL–3794, revised 1971, Oak Ridge National Laboratory, Tennessee.
JOHNSTON, G. A. R., CURTIS, D. R., DEGROAT, W. C. & DUGGAN, A. W. (1968). *Biochem. Pharmacol.* **17**, 2488–2489.
KROGSGAARD-LARSEN, P. (1978). *Amino Acids as Chemical Transmitters*, edited by F. FONNUM, pp. 305–321. New York: Plenum.
KROGSGAARD-LARSEN, P., HONORÉ, T. & THYSSEN, K. (1979). *GABA-Neurotransmitters. Pharmacochemical, Biochemical and Pharmacological Aspects*, edited by P. KROGSGAARD-LARSEN, J. SCHEEL-KRÜGER & H. KOFOD, pp. 201–216. Copenhagen: Munksgaard.
KROGSGAARD-LARSEN, P. & JOHNSTON, G. A. R. (1975). *J. Neurochem.* **25**, 797–802.
KROGSGAARD-LARSEN, P. & JOHNSTON, G. A. R. (1978). *J. Neurochem.* **30**, 1377–1382.
KROGSGAARD-LARSEN, P., JOHNSTON, G. A. R., CURTIS, D. R., GAME, C. J. A. & MCCULLOCH, R. M. (1975). *J. Neurochem.* **25**, 803–809.
KROGSGAARD-LARSEN, P., JOHNSTON, G. A. R., LODGE, D. & CURTIS, D. R. (1977). *Nature* (*London*), **268**, 53–55.
KROGSGAARD-LARSEN, P. & ROLDSKOV CHRISTIANSEN, T. (1979). *Eur. J. Med. Chem. Chim. Ther.* **14**, 157–164.
LA COUR, T. & RASMUSSEN, S. E. (1973). *Acta Chem. Scand.* **27**, 1845–1854.
LARSEN, F. K., LEHMANN, M. S., SØTOFTE, I. & RASMUSSEN, S. E. (1970). *Acta Chem. Scand.* **24**, 3248–3258.
MAIN, P., LESSINGER, L., WOOLFSON, M. M., GERMAIN, G. & DECLERCQ, J. P. (1977). *MULTAN* 77. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.
NYGAARD, L., CHRISTENSEN, D., NIELSEN, J. T., PEDERSEN, E. J., SNERLING, O., VESTERGAARD, E. & SØRENSEN, G. O. (1974). *J. Mol. Struct.* **22**, 401–413.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
XRAY system (1972). Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland.

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N-Nitrosodiphenylamine

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Abstract. $C_{12}H_{10}N_2O$, $M_r = 198{\cdot}08$, monoclinic, $C2/c$, $a = 16{\cdot}283$ (20), $b = 8{\cdot}827$ (10), $c = 16{\cdot}508$ (20) Å, $\beta = 117{\cdot}53$ (15)°, $V = 2104{\cdot}03$ Å^3, $D_m = 1{\cdot}25$, $D_c = 1{\cdot}251$ Mg m^{-3}, $Z = 8$, λ(Cu $K\alpha$) = 1·5418 Å, $F(000) = 832$, $R = 0{\cdot}067$ for 807 observed reflexions. The structure comprises discrete molecules with no intermolecular interactions other than van der Waals forces.

Introduction. *N*-Nitrosodiphenylamine is a brown crystalline solid readily obtainable by reacting diphenylamine with nitrous acid, and is used industrially as an anti-oxidant to slow the curing of rubber. Our sample was supplied by Imperial Chemical Industries Limited (trade name 'Vulcatard A') and the commerical material was purified by recrystallization from absolute ethanol. Unit-cell dimensions were obtained first from layer-line measurements on rotation photographs about several axes, but as the crystals were equi-dimensional with very similar a, c and [101]-axis lengths, their identification was difficult. No reflexions were observable in the high-angle region of Weissenberg photographs so the best values of the lattice parameters were calculated from the 2θ measurements of specific indexed reflexions.

Intensities were obtained from visual estimations of multiple-film Weissenberg photographs of layers $h0l$–$h5l$ and $hk0$ which was also used for inter-layer scaling. The data were corrected for Lp effects but not for absorption, which was small. The structure was determined with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1978) and refined using the NRC suite of programs (Ahmed, Hall, Pippy & Huber, 1973). There were 1067 reflexions within the region examined, of which 260 were $< 1{\cdot}0$ on the scale used.

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Table 1. *Final atomic coordinates and isotropic thermal parameters*

	x	*y*	*z*	B_{iso}(Å^2)
C(1)	0·2986 (3)	0·1977 (4)	0·3424 (2)	4·55 (18)
C(2)	0·2366 (3)	0·1377 (4)	0·3718 (3)	5·52 (22)
C(3)	0·1493 (3)	0·1037 (4)	0·3071 (4)	6·22 (25)
C(4)	0·1233 (3)	0·1121 (5)	0·2133 (3)	4·89 (20)
C(5)	0·1814 (3)	0·1754 (5)	0·1788 (4)	6·65 (25)
C(6)	0·2724 (3)	0·2114 (5)	0·2529 (3)	4·73 (20)
C(7)	0·4720 (3)	0·1769 (5)	0·4070 (3)	5·20 (22)
C(8)	0·5433 (3)	0·2725 (5)	0·4159 (3)	5·38 (22)
C(9)	0·6206 (3)	0·2028 (6)	0·4153 (3)	4·78 (20)
C(10)	0·6199 (3)	0·0573 (6)	0·3902 (4)	5·34 (22)
C(11)	0·5449 (4)	−0·0405 (6)	0·3742 (4)	6·77 (28)
C(12)	0·4665 (3)	0·0329 (6)	0·3774 (3)	7·05 (29)
N(1)	0·3920 (2)	0·2401 (3)	0·4108 (2)	4·51 (14)
N(2)	0·4110 (3)	0·3442 (4)	0·4765 (3)	5·96 (19)
O(1)	0·3441 (2)	0·3973 (3)	0·4793 (2)	8·18 (22)

The positions of the H atoms were calculated (C–H=1·08Å) and used in the structure-factor calculations with $B_{iso} = 8·0$ Å^2 but were not refined. After a number of cycles of least-squares calculations, using initially isotropic and finally anisotropic temperature factors, the shifts indicated were all less than $0·5\sigma$. The final positional and isotropic thermal parameters are listed in Table 1.*

Discussion. The numbering of the atoms is shown in Fig. 1, and a list of bond lengths and bond angles is in Table 2. The molecules in the crystal are discrete with no strong intermolecular bonds; the nearest approach of the O atom is to C(2) at 3·293 (7), and to C(3) at 3·477 (6) Å. The mean C–C distance in the benzene rings is 1·397 Å, and the N=O bond of the nitroso group is 1·206 Å. Pauling (1944) predicted the N=O bond length at 1·18 Å, but the majority of values which have been determined are greater than this, probably because of ionization or hybridization; *e.g.* 1·26 Å in *N*-nitrosodimethylamine (Krebs & Mandt, 1975) and 1·234 Å in 5-nitrososalicyclic acid (Talberg, 1977). The best agreement with our value is 1·199 Å in *S*-nitroso-*N*-acetyl-DL-penicillamine (Carnahan, Lenhert & Ravichandran, 1978).

The molecule lies in three planes defined by:

(*a*) C(1), C(2), C(3), C(4), C(5), C(6) $0·3743X - 0·9271Y - 0·0199Z = -0·8719$ from which the perpendicular distances of the atoms are, respectively, −0·003 (4), +0·017 (4), −0·033 (4), +0·035 (5), −0·020 (5), and +0·005 (5) Å.

(*b*) C(1), C(7), N(1), N(2), O(1) $0·3044X + 0·7335Y - 0·6077Z = -1·0887$ and the out-of-plane distances are, respectively, +0·007 (4), +0·007 (4), −0·023 (3), +0·008 (4) and −0·010 (3) Å.

(*c*) C(7), C(8), C(9), C(10), C(11), C(12) $0·0400X + 0·2463Y - 0·9684Z = -5·1355$ and the atom deviations are, respectively, −0·066 (4), +0·058 (5), −0·033 (5), +0·013 (6), −0·016 (5) and +0·045 (5) Å.

The angle between planes (*a*) and (*b*) is 123·64 (5), between (*b*) and (*c*) 38·62 (5), and between (*a*) and (*c*) 101·19 (5)°.

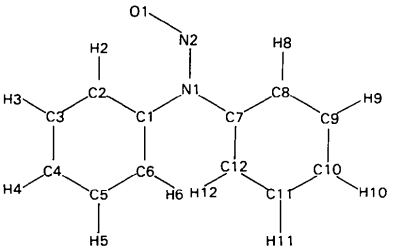

Fig. 1. Chemical formula showing numbering of atoms.

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)–C(2)	1·411 (7)	C(7)–C(8)	1·387 (7)
C(2)–C(3)	1·360 (7)	C(8)–C(9)	1·405 (8)
C(3)–C(4)	1·406 (7)	C(9)–C(10)	1·349 (7)
C(4)–C(5)	1·425 (8)	C(10)–C(11)	1·418 (8)
C(5)–C(6)	1·456 (7)	C(11)–C(12)	1·454 (8)
C(6)–C(1)	1·341 (5)	C(12)–C(7)	1·350 (7)
C(1)–N(1)	1·462 (6)	N(1)–N(2)	1·344 (5)
C(7)–N(1)	1·445 (6)	N(2)–O(1)	1·206 (7)

C(1)–C(2)–C(3)	117·8 (4)	C(7)–C(8)–C(9)	116·2 (5)
C(2)–C(3)–C(4)	121·8 (4)	C(8)–C(9)–C(10)	122·6 (5)
C(3)–C(4)–C(5)	122·9 (5)	C(9)–C(10)–C(11)	121·4 (5)
C(4)–C(5)–C(6)	110·9 (4)	C(10)–C(11)–C(12)	114·7 (5)
C(5)–C(6)–C(1)	126·0 (4)	C(11)–C(12)–C(7)	121·3 (5)
C(6)–C(1)–C(2)	120·0 (4)	C(12)–C(7)–C(8)	121·6 (5)
N(1)–C(1)–C(2)	118·9 (4)	C(1)–N(1)–C(7)	120·2 (3)
N(1)–C(1)–C(6)	121·1 (4)	C(1)–N(1)–N(2)	124·6 (3)
N(1)–C(7)–C(8)	119·2 (4)	C(7)–N(1)–N(2)	115·0 (3)
N(1)–C(7)–C(12)	117·9 (4)	N(1)–N(2)–O(1)	114·9 (4)

* Lists of structures factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36858 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

AHMED, F. R., HALL, S. R., PIPPY, M. E. & HUBER, C. P. (1973). NRC Crystallographic Programs for the IBM/360 System. National Research Council, Ottawa, Canada.

CARNAHAN, G. E., LENHERT, P. G. & RAVICHANDRAN, R. (1978). *Acta Cryst.* B**34**, 2645–2648.

KREBS, B. & MANDT, J. (1975). *Chem. Ber.* **108**, 1130–1137.

MAIN, P., LESSINGER, L., WOOLFSON, M. M., GERMAIN, G. & DECLERCQ, J. P. (1978). *MULTAN. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain-la-Neuve, Belgium.

PAULING, L. (1944). *The Nature of the Chemical Bond,* p. 267. Ithaca: Cornell Univ. Press.

TALBERG, H. J. (1977). *Acta Chem. Scand. Ser. A,* **31**, 485–491.