Table 7 (*cont.*)

Dihedral angles between planes (°)

$T\wedge B1$	73·9	$B1\wedge B2$	76·6	$B2\wedge B3$	56·6	$B3\wedge B4$	71·1	$B4\wedge P1$	39·0	$P1\wedge P2$	54·2
$T\wedge B2$	72·0	$B1\wedge B3$	76·6	$B2\wedge B4$	74·7	$B3\wedge P1$	86·3	$B4\wedge P2$	89·2		
$T\wedge B3$	16·1	$B1\wedge B4$	5·6	$B2\wedge P1$	66·4	$B3\wedge P2$	76·8				
$T\wedge B4$	68·4	$B1\wedge P1$	37·2	$B2\wedge P2$	22·1						
$T\wedge P1$	82·3	$B1\wedge P2$	89·5								
$T\wedge P2$	87·2										

the four benzene rings $B1$, $B2$, $B3$ and $B4$ are 1·38, 1·37, 1·38 and 1·37 Å respectively. The bond lengths in the two carbonyl groups, 1·22 and 1·21 Å are quite satisfactory.

The intramolecular distance O(1)–O(2) = 3·74 Å is much longer than the sum of the van der Waals radii of the corresponding atoms. Other distances are within expected values.

Fig. 2 is a clinographic projection of the structure showing the molecular packing of CBDT in the unit cell. The various intermolecular distances are normal. It is of interest to note that the shortest Cl–Cl intermolecular distance is 3·83 Å, slightly over two van der Waals radii.

Thanks are due to Professor N. E. Alexandrou and Dr E. D. Micromastoras, Laboratory of Organic Chemistry, Aristotle University of Thessaloniki, Greece, for providing the CBDT crystals. We also thank the University of Thessaloniki for the use of its UNIVAC 1106 computer.

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The Crystal Structure of *O*-(Phenyl-cyano-nitromethyl)-benzoyl-cyanoxime

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(*Received* 20 *March* 1975; *accepted* 23 *April* 1975)

The crystal structure of *O*-(phenyl-cyano-nitromethyl)-benzoyl-cyanoxime, $C_{16}H_{10}N_4O_3$, has been determined from three-dimensional intensities, measured with an automated Philips PW 1100 single-crystal diffractometer (3094 independent reflexions). The structure was solved by direct phase determination. The cell constants, obtained by least-squares calculations from direct θ-value measurements on the diffractometer, are $a = 13·0346$ (14), $b = 9·8186$ (7), $c = 12·0830$ (12) Å, $\beta = 101·60$ (1)°, $Z = 4$; the space group is $P2_1/n$. The positional and vibrational parameters, with anisotropic temperature factors for the non-hydrogen atoms, were refined by full-matrix least-squares calculations to a final $R = 0·078$. The molecule of the compound has the *O*-cyanoxime structure. All the atoms of the main chain lie on a plane, which forms a small angle with one of the benzene rings. An interesting peculiarity of the structure is the rather long C–NO_2 distance of 1·617 Å.

Introduction

The silver salt of phenylnitroacetonitrile, $[C_6H_5C(CN)(NO_2)]Ag$, reacts with CS_2 (Alexandrou, 1965) or with some alkylation reagents (Lianis, 1975) and yields a compound with the molecular formula $C_{16}H_{10}N_4O_3$. From chemical and spectroscopic data (Alexandrou & Lianis, 1975) it could not be decided whether it contained an open chain or a heterocyclic ring. This necessitated an X-ray structure analysis.

which clearly showed that the product is not heterocyclic.

The structure determination of *O*-(phenyl-cyano-nitromethyl)-benzoyl-cyanoxime (OPBC in the following) was undertaken as part of a systematic programme to elucidate the structures of interesting new compounds, prepared at the Laboratory of Organic Chemistry of the Aristotle University of Thessaloniki.

Table 1. *Crystal data for OPBC*

(Standard errors, given in parentheses, refer to last digit)

$C_{16}H_{10}N_4O_3$	F.W. 306·28
Monoclinic	$Z=4$
Space group $P2_1/n$	$F(000)=632$
$a=13·0346$ (14) Å	$\varrho_{\text{calc}}=1·343$ g cm^{-3}
$b=$ 9·8186 (7)	$\varrho_{\text{meas}}=1·330$ g cm^{-3}
$c=12·0830$ (12)	m.p. 122–123 °C
$\beta=101·60$ (1)°	$\mu=1·03$ cm^{-1}
$V=1514·83$ Å^3	λ(Mo $K\alpha$)$=0·71609$ Å

Experimental

Pure, colourless OPBC crystals were kindly provided by Professor N. E. Alexandrou and Mr P. S. Lianis of the Organic Chemistry Laboratory. The crystals are monoclinic plates. A well developed transparent single crystal, with dimensions 0·35 × 0·35 × 0·17 mm, was selected and centred on a computer-controlled Philips PW1100 four-circle single-crystal diffractometer. With Mo $K\alpha$ radiation ($\lambda=0·71609$ Å) the cell constants were determined first by using the PH (Peak Hunting) routine of the instrument. To achieve greater accuracy, the θ angles of strong reflexions with large θ values were directly measured on the diffractometer and subsequently processed with the least-squares programme *PARAM* [part of the X-RAY System of Crystallographic Programs (Stewart, Kruger, Ammon, Dickinson & Hall, 1972)]. The final values obtained are given in Table 1. Systematic absences led to the space group $P2_1/n$. The density of the crystals was measured by flotation in a potassium bromide solution.

Three-dimensional intensity data were collected with a scintillation counter on the PW1100 diffractometer in the ω-scan mode, using Mo $K\alpha$ radiation, monochromatized with a graphite monochromator. The intensities of 3094 independent reflexions up to $2\theta=60°$ (max. $h,k,l=\pm14,10,12$ respectively) were measured.

Integrated intensities were converted to $|F_o|$ values in the usual way, using a modified version of the special measurement treatment program by Hornstra & Stubbe (1972). No absorption correction was applied. For all subsequent computations, the programs of the X-RAY System were used.

Determination of the structure and refinement

The structure was solved by direct phase determination, with the program *PHASE* of the X-RAY System. The phases of 309 strong reflexions were determined and on the resulting E map it was possible to locate all the atoms of the asymmetric unit. A structure-factor calculation gave $R=0·39$.

Refinement of the structure was carried out by full-matrix least-squares calculations, using the program *CRYLSQ* of the X-RAY System. The atomic scattering factors for N, O and C were from Cromer & Waber

Table 2. *Atomic coordinates, anisotropic temperature coefficients* (× 10^4) *and equivalent isotropic temperature factors for the non-hydrogen atoms in OPBC, with standard deviations in parentheses*

Anisotropic temperature factor $T=\exp\left[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)\right]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	B
O(1)	0·9872 (4)	0·1020 (5)	0·8972 (4)	1103 (34)	1283 (40)	846 (29)	146 (30)	326 (25)	−148 (27)	8·51 Å^2
O(2)	0·1307 (4)	0·1966 (5)	0·9030 (4)	1301 (40)	1207 (40)	1147 (37)	−317 (33)	108 (30)	−590 (32)	9·62
O(3)	0·9684 (2)	0·0916 (3)	0·2352 (2)	466 (15)	453 (16)	528 (16)	−78 (12)	−58 (11)	47 (12)	3·81
N(1)	0·0662 (3)	0·1223 (4)	0·8690 (3)	483 (20)	557 (23)	591 (23)	9 (17)	57 (17)	74 (17)	4·29
N(2)	0·9093 (3)	0·1694 (4)	0·1444 (3)	554 (20)	515 (21)	513 (20)	−10 (16)	37 (15)	65 (16)	4·17
N(3)	0·2796 (3)	0·0082 (5)	0·7685 (4)	496 (25)	1055 (38)	1001 (35)	19 (24)	108 (22)	116 (29)	6·72
N(4)	0·3393 (4)	0·0619 (5)	0·4846 (4)	1094 (37)	801 (33)	720 (29)	−211 (28)	32 (26)	−256 (25)	6·88
C(1)	0·0794 (3)	0·0333 (4)	0·7601 (3)	438 (20)	386 (20)	433 (21)	−76 (15)	74 (15)	−59 (15)	3·31
C(2)	0·0265 (3)	0·1095 (4)	0·6555 (3)	478 (21)	352 (20)	457 (21)	44 (15)	76 (15)	−16 (15)	3·39
C(3)	0·9227 (3)	0·0798 (4)	0·6054 (3)	520 (23)	493 (24)	495 (23)	3 (18)	56 (17)	−22 (18)	3·97
C(4)	0·8750 (4)	0·1529 (5)	0·5116 (4)	763 (31)	578 (28)	479 (25)	129 (23)	−83 (21)	−76 (20)	4·79
C(5)	0·4279 (4)	0·2467 (5)	0·9682 (4)	944 (38)	590 (30)	509 (27)	235 (27)	135 (25)	107 (22)	5·38
C(6)	0·5296 (4)	0·2162 (5)	0·0181 (5)	922 (39)	650 (33)	712 (34)	109 (28)	371 (29)	235 (26)	6·01
C(7)	0·0800 (3)	0·2118 (5)	0·6115 (4)	558 (25)	500 (25)	708 (30)	−96 (20)	159 (21)	43 (21)	4·65
C(8)	0·1946 (3)	0·0198 (5)	0·7685 (4)	487 (25)	554 (26)	545 (25)	−42 (19)	−1 (18)	27 (19)	4·18
C(9)	0·4506 (3)	0·2126 (4)	0·6393 (3)	506 (22)	419 (22)	474 (22)	−30 (17)	165 (17)	−37 (16)	3·68
C(10)	0·5448 (3)	0·1504 (4)	0·7089 (3)	494 (21)	325 (19)	491 (22)	62 (15)	199 (16)	−22 (15)	3·45
C(11)	0·5429 (4)	0·0147 (5)	0·7381 (4)	636 (28)	483 (26)	790 (33)	47 (21)	274 (24)	34 (22)	5·02
C(12)	0·3700 (5)	0·0449 (5)	0·1949 (5)	854 (38)	592 (31)	864 (37)	220 (27)	362 (30)	231 (27)	6·08
C(13)	0·7192 (4)	0·0302 (7)	0·8401 (5)	743 (36)	931 (44)	701 (34)	367 (32)	92 (26)	−20 (30)	6·25
C(14)	0·7242 (4)	0·1633 (6)	0·8085 (5)	480 (27)	763 (37)	1040 (42)	116 (24)	49 (25)	−236 (31)	6·01
C(15)	0·6372 (3)	0·2248 (4)	0·7427 (4)	553 (26)	431 (24)	874 (34)	1 (19)	236 (23)	−53 (22)	4·89
C(16)	0·3872 (4)	0·1293 (5)	0·5510 (4)	670 (28)	542 (27)	574 (27)	−11 (22)	90 (21)	−52 (21)	4·70

(1965), and for H from Stewart, Davidson & Simpson (1965). A single scale factor was used for the whole set of reflexion data.

With isotropic temperature factors and unit weights, refinement reduced R to 0·156 in nine cycles. Two further cycles with anisotropic temperature coefficients reduced R to 0·117. The H atoms were then located on a difference Fourier synthesis and included in further refinement cycles with isotropic temperature factors assigned to them, equal to those of the corresponding C atoms to which they are bonded. At this stage the weighting function $w=1/(A+B|F_o|+C|F_o|^2)$ (Cruickshank, Pilling, Bujosa, Lovell & Truter, 1961) was introduced and a systematic weight analysis was carried out with the programs *WTANAL* and *WTLSSQ* of the X-RAY System. This led to the values $A=2{\cdot}72$, $B=0{\cdot}015$ and $C=0{\cdot}0002$. Convergence was reached at $R=0{\cdot}078$.

The final positional parameters and anisotropic temperature coefficients for the non-hydrogen atoms are given in Table 2. The final coordinates and isotropic temperature factors for the hydrogen atoms are shown in Table 3. Comparison between $|F_o|$ and $|F_c|$ values, obtained with the parameters in Tables 2 and 3, is made in Table 4. Interatomic distances and bond angles are given in Tables 5 and 6.

Table 3. *Atomic coordinates and isotropic temperature factors for the hydrogen atoms in OPBC*

	x	y	z	B
H(C3)	0·886 (3)	0·021 (5)	0·640 (4)	5·2Å^2
H(C4)	0·805 (3)	0·130 (5)	0·474 (4)	5·3
H(C5)	0·391 (4)	0·197 (5)	0·901 (4)	6·6
H(C6)	0·572 (4)	0·151 (5)	0·987 (4)	7·1
H(C7)	0·152 (3)	0·233 (5)	0·648 (4)	5·1
H(C11)	0·523 (4)	0·030 (6)	0·284 (4)	7·3
H(C12)	0·375 (4)	0·139 (6)	0·174 (4)	7·1
H(C13)	0·221 (4)	0·006 (6)	0·115 (4)	7·1
H(C14)	0·782 (4)	0·220 (6)	0·831 (5)	7·4
H(C15)	0·141 (3)	0·181 (4)	0·220 (3)	3·7

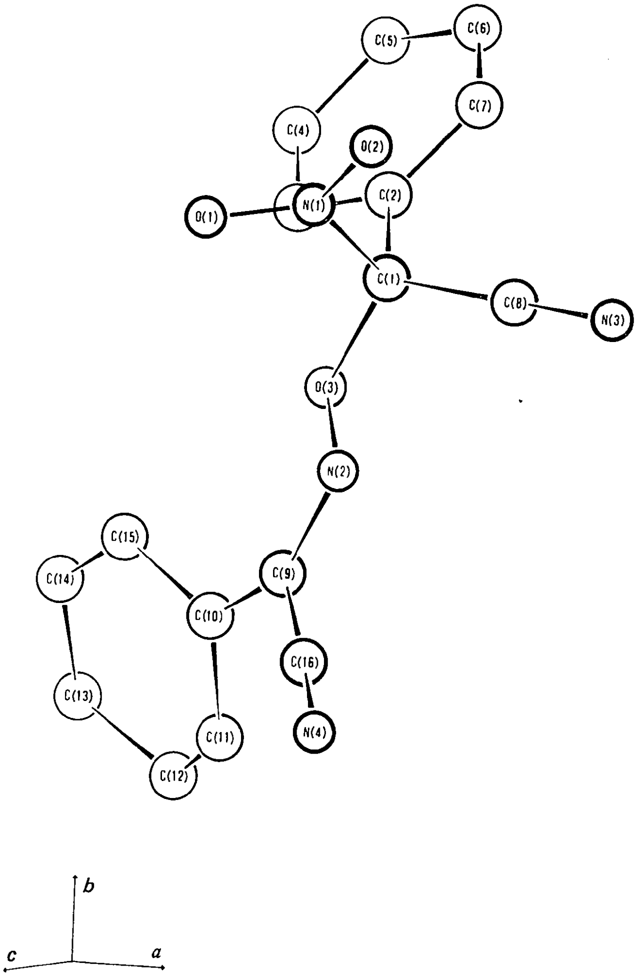

Fig. 1. Clinographic projection of the OPBC molecule, showing its conformation.

Description of the structure and discussion

The structural and conformational features of the OPBC molecule are shown in the clinographic projection of Fig. 1. Obviously it is not a heterocyclic compound but an oxime ether. The carbon atom C(1) at the beginning of the main chain C(1)–O(3)–N(2)–C(9) is tetrahedrally connected to one benzene ring $B1$, one CN group, one NO_2 group and O(3), with all angles around it approximating the normal tetrahedral angle (see Table 6). The carbon atom C(9) at the end of the chain is linked to the second benzene ring, $B2$, and the second CN group.

The two benzene rings of the molecule are planar to a good approximation. In Table 7 are listed the various least-squares planes of the OPBC molecule, together with the dihedral angles between them. The atoms of the main chain form a plane, $P2$, at an angle of 22° with the benzene ring $B1$. The atoms of the second CN group are very near this plane. The plane $P1$ of the nitro group is almost perpendicular to $P2$ (83·1°) and to a lesser degree to $B1$ (74·7°).

The geometrical features of the benzene rings are in very good agreement with the usually accepted values (see Tables 5 and 6). Mean bond lengths in these are 1·381 and 1·380 Å respectively. The bond length between the first benzene ring, $B1$, and the atom C(1) of the main chain is normal, 1·510 Å, whereas that between the second benzene ring, $B2$, and the atom C(9) is shortened to 1·474 Å, because of the adjacent double bond to N(2). This is in good agreement with the value 1·47–1·48 Å suggested by Lide (1962) for such a bond length. The C–CN groups are practically linear.

It is of interest to note that, while all the other bond lengths are normal, the distance C(1)–N(1), *i.e.* the bond distance to the nitro group, is rather too long,

Table 4. *Observed and calculated structure factors for OPBC*

H	K	L	F(O)	F(C)
0	2	1	40.4	41.7
		2	41.0	40.4
		3	63.0	63.2
		4	46.5	47.1
		5	16.5	15.8
		6	25.3	24.8
		7	12.8	12.6
		8	3.4	2.4
		9	4.7	4.1
		10	4.6	4.1
		11	2.6	4.2
		12	8.3	7.9
	3	1	5.1	5.3
		2	7.4	7.4
		3	5.3	4.4
		5	29.0	27.7
		6	21.5	21.4
		7	12.7	12.7
		8	3.9	4.8
		10	3.6	3.4
		11	5.2	4.4
		12	.5	.5
	4	0	4.0	3.9
		1	17.7	16.0
		2	32.4	31.4
		3	6.7	6.9
		4	36.5	35.7
		5	14.2	13.6
		6	11.1	11.1
		7	.5	3.5
		8	9.5	10.1
		9	6.2	5.8
		10	4.8	3.4
		11	6.5	8.0
		12	.5	3.3
	5	1	19.1	19.3
		2	.4	1.7
		3	4.0	5.7
		4	3.6	3.3
		5	13.6	13.0
		6	15.0	17.0
		8	12.4	12.1
		9	8.1	7.3
		10	.5	5.7
		11	.4	2.6
		12	.5	2.8
	6	0	4.6	5.9
		1	18.1	16.7
		2	19.0	19.0
		3	18.3	18.7
		4	6.1	5.8
		5	7.0	9.0
		6	.4	3.7
		7	23.6	24.9
		8	5.0	5.0
		9	.4	4.8
		10	.4	.0
		11	5.9	5.5
		12	.5	.3
	7	1	.4	3.2
		2	3.5	2.0
		3	17.2	16.9
		4	4.2	4.6
		5	19.7	16.0
		6	5.8	6.0
		7	10.6	9.7
		8	7.3	7.2
		9	.4	.1
		10	.7	1.9
		11	4.4	1.8
		12	5.0	4.5
	8	0	8.1	9.0
		1	5.0	4.7
		2	5.3	4.2
		3	24.8	24.8
		4	7.0	5.8
		5	24.4	24.3
		6	.5	.9
		7	4.3	3.2
		9	.4	1.1
		10	6.0	6.2
		11	.7	.0
		12	.5	1.3
	9	1	.5	.7
		2	7.1	7.0
		3	13.7	14.0
		5	4.4	4.5
		6	4.7	4.7
		7	.6	.0
		9	6.7	7.0
		10	.4	4.2
		11	5.3	3.0
		12	4.6	2.4
	10	0	1.6	1.5
		1	17.8	18.6
		2	3.0	4.9
		3	5.8	5.0
		4	5.8	7.6
		5	.6	2.6
		6	4.2	5.5
		7	4.8	4.7
		8	.8	3.9
		9	10.8	10.0
		10	4.5	3.9
		11	.4	3.2
	0	3	42.1	41.1
		5	3.1	2.7
		7	43.8	44.8
		9	24.3	25.2
		11	23.6	23.5
	1	1	14.0	13.2
		2	13.0	12.7
		3	39.8	40.5
		4	35.6	33.8
		5	17.7	16.7
		6	13.7	13.9
		7	5.4	4.6
		8	11.2	10.2
		9	16.3	16.2
		10	9.6	10.7
		11	4.7	4.0
		12	.6	2.5
	2	0	3.3	1.9
		1	39.3	36.3
		2	.4	.9
		3	22.8	22.5
		4	19.6	19.1
		5	60.4	59.7
		6	15.8	14.9
		7	18.8	19.0
		8	7.1	7.7
		9	11.0	11.0
		10	3.7	2.6
		11	5.9	5.6
		12	2.2	2.4
	3	0	39.1	38.3
		1	43.9	44.0
		2	19.1	19.9
		3	54.2	53.2
		4	23.2	22.4
		5	17.7	15.9
		6	10.8	11.0
		7	5.6	4.4
		8	19.3	20.1
		9	2.3	1.1
		10	4.0	2.6
		11	4.0	1.8
		12	4.6	6.6
	4	0	25.7	24.9
		1	23.1	22.4
		2	4.9	5.2
		3	19.0	19.3
		4	37.2	39.0
		5	15.8	16.9
		6	18.2	17.9
		7	.6	.0
		8	1.7	1.2
		9	.6	.7
		10	.4	2.9
		11	4.0	8.8
		12	.4	.8
	5	0	49.2	47.2
		1	20.7	19.9
		2	18.7	17.9
		3	11.3	11.7
		4	1.7	.8
		5	1.9	1.2
		6	7.4	7.1
		7	11.2	10.7
		8	16.1	16.8
		9	3.8	4.3
		10	.4	5.2
1	5	11	6.2	6.9
		12	5.4	5.1
	6	0	14.0	13.5
		1	16.2	16.9
		2	1.6	.8
		3	4.9	4.8
		4	15.5	16.3
		5	6.8	7.3
		6	7.7	6.5
		7	8.7	8.6
		8	.8	1.5
		9	4.0	1.1
		10	6.1	5.0
		11	.6	3.2
		12	1.0	3.5
	7	0	4.6	3.8
		1	.8	.5
		2	12.6	12.9
		3	16.1	14.6
		4	5.5	5.2
		5	21.7	23.0
		6	14.7	14.7
		7	8.0	7.9
		8	.4	2.5
		9	.5	2.0
		11	.5	.9
		12	.4	1.6
	8	0	2.1	.9
		1	4.8	4.4
		2	10.1	10.1
		3	6.3	4.5
		4	17.2	17.5
		5	.3	.8
		6	17.8	18.6
		7	2.6	4.3
		8	4.0	10.0
		9	7.2	5.8
		10	.4	2.3
		11	.5	.6
		12	.9	2.3
	9	1	.4	.8
		2	5.6	6.5
		3	9.6	8.9
		4	9.0	10.6
		5	9.0	9.1
		6	.6	3.8
		7	4.1	2.1
		8	4.9	6.3
		10	.4	2.5
		11	.4	1.5
		12	.7	1.1
	10	0	7.3	7.4
		1	.5	5.2
		2	10.3	9.9
		3	.7	1.2
		4	.4	1.8
		5	.6	.2
		6	.5	.7
		7	.5	.6
		8	.6	2.4
		10	5.5	4.8
		11	.5	.5
2	0	0	121.5	125.7
		2	85.9	85.1
		4	39.3	38.1
		6	28.8	29.8
		8	21.6	20.8
		10	2.6	2.3
		12	4.3	4.1
	1	0	.4	1.0
		1	80.5	79.9
		2	5.7	5.8
		3	4.1	2.5
		4	44.8	44.1
		5	15.3	15.9
		6	15.7	16.5
		7	.7	1.1
		8	4.7	3.6
		9	13.2	13.6
		10	8.6	8.4
		11	4.7	4.2
		12	4.4	2.4
	2	0	48.8	46.9
		1	40.9	40.6
		2	15.6	16.3
		3	3.7	4.1
		4	9.9	10.2
		5	14.3	13.7
		6	6.6	4.9
		7	11.6	11.4
		8	11.5	11.2
		9	4.0	3.6
		10	4.7	5.0
		11	.5	2.3
		12	2.9	3.3
	3	0	50.0	49.6
		1	26.5	26.1
		2	14.3	14.4
		3	25.7	24.3
		4	24.2	23.2
		5	28.0	27.2
		6	31.8	31.7
		7	7.2	7.4
		8	.5	2.5
		9	.4	.9
		10	8.0	8.0
		11	.5	2.8
		12	.4	3.2
	4	0	44.3	43.2
		1	8.6	7.7
		2	15.9	16.6
		3	22.8	22.8
		4	7.2	7.4
		6	1.3	3.5
		7	4.0	3.6
		8	9.1	10.4
		9	4.6	3.2
		11	6.6	3.4
		12	.4	2.5
	5	1	9.5	8.8
		2	4.6	4.9
		3	26.3	26.5
		4	10.8	10.3
		5	6.7	6.6
		6	15.9	15.8
		7	2.5	2.9
		8	6.0	7.5
		9	13.3	13.6
		10	5.0	5.2
		11	4.2	4.5
		12	.4	3.7
	6	0	29.3	28.3
		1	3.9	4.5
		2	17.5	17.3
		3	4.9	4.7
		4	4.6	3.9
		5	4.4	4.1
		6	8.8	8.4
		7	8.4	8.1
		8	7.0	7.4
		9	.5	2.8
		12	.7	2.3
	7	0	5.2	4.7
		2	7.2	7.2
		3	2.8	4.2
		4	11.5	11.2
		5	28.5	29.6
		6	14.8	15.4
		7	7.7	7.5
		8	.5	1.8
		9	.7	3.6
		10	.5	.2
		11	1.3	.4
		12	.4	1.2
	8	0	5.2	6.0
		1	2.3	2.4
		2	3.8	.6
		3	23.2	24.2
		4	5.6	4.4
		5	10.3	10.8
		6	.4	4.4
		7	.4	1.1
		8	3.0	2.6
		9	.5	3.0
		10	5.3	.7
		11	.4	.3
		12	.5	.6
	9	0	4.8	5.2
		2	17.4	17.5
		3	.4	2.5
		4	.4	2.8
		5	5.1	4.0
2	9	6	4.0	3.0
		7	4.8	4.3
		8	4.4	3.2
		9	5.0	3.7
		10	4.8	4.5
		11	3.5	1.5
		12	.4	.4
	10	0	7.2	6.2
		1	4.7	5.7
		2	2.2	1.8
		3	.5	1.6
		4	.5	1.5
		5	.5	2.8
		6	.9	1.8
		7	.5	2.5
		9	.7	3.5
3	0	1	39.3	41.4
		3	12.2	13.3
		5	26.6	28.0
		7	.5	1.9
		9	27.3	27.3
		11	8.3	8.5
	1	0	63.4	59.3
		1	3.2	4.3
		2	34.0	31.9
		3	2.0	.8
		4	18.0	17.1
		5	19.0	14.6
		6	4.7	4.4
		7	11.7	12.0
		8	2.1	.9
		9	4.6	4.2
		10	4.7	4.1
		11	6.6	8.5
		12	.9	1.9
	2	0	13.6	13.0
		1	33.9	32.7
		2	6.0	6.2
		3	44.5	44.2
		4	29.1	28.1
		6	7.5	17.1
		7	5.1	5.4
		8	13.9	11.3
		9	.8	2.8
		10	13.4	13.2
		11	6.7	7.0
		12	7.4	7.5
	3	0	16.5	16.5
		1	17.4	16.7
		2	8.7	8.4
		3	74.2	73.7
		4	17.7	17.7
		5	22.0	21.8
		6	4.1	4.4
		7	10.4	9.9
		9	8.7	9.5
		10	.4	3.1
		11	5.2	4.5
		12	1.0	1.4
	4	0	7.3	7.6
		1	33.0	32.4
		2	2.1	.6
		3	9.8	10.4
		4	5.9	5.7
		5	9.0	4.5
		6	25.2	25.7
		7	4.4	7.5
		8	.4	2.1
		9	16.9	17.0
		10	.4	2.4
		11	5.0	6.4
		12	.6	.9
	5	0	52.1	51.4
		1	16.6	16.5
		2	3.6	2.7
		3	.4	1.0
		4	.4	2.9
		5	8.4	7.6
		6	12.6	13.5
		7	2.4	3.1
		8	.4	2.1
		9	3.8	3.1
		10	3.1	1.1
		11	.5	3.9
	6	0	4.5	4.0
		1	2.0	4.0
		2	6.9	6.2
		3	17.7	17.7
		4	2.3	3.0
		5	.6	1.9
		6	.4	1.3
		7	5.2	5.3
		8	5.5	5.7
		9	3.9	5.7
		10	5.6	4.6
		11	.8	1.7
		12	.4	3.9
	7	0	4.7	10.4
		1	7.6	7.4
		2	17.8	19.6
		3	2.4	1.9
		4	25.6	26.3
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		6	2.2	2.2
		7	7.7	7.8
		8	.4	1.5
		10	.4	.1
		11	.4	1.5
		12	.6	2.3
	8	0	.4	2.8
		2	5.8	6.4
		3	13.3	12.7
		4	15.7	15.6
		5	.8	2.7
		6	8.1	4.5
		7	5.9	4.9
		8	.4	.5
		9	.4	3.1
		10	.4	1.9
		11	5.4	3.6
		12	4.8	3.3
	9	0	.5	3.4
		1	4.9	4.9
		2	13.2	13.5
		3	7.3	7.4
		5	7.1	4.6
		6	.6	.3
		7	2.7	3.2
		8	.4	2.5
		10	6.0	7.3
		11	.4	1.2
	10	0	11.4	12.0
		1	.4	1.6
		2	4.3	2.4
		3	.5	2.9
		4	8.7	4.0
		5	4.9	5.0
		6	4.9	3.9
		7	1.0	.7
		8	4.8	5.2
		9	.5	.4
		10	.5	2.1
4	0	0	12.7	13.1
		2	41.4	41.7
		4	5.9	5.7
		6	22.4	22.7
		10	5.1	3.1
		12	3.9	3.6
	1	0	14.0	15.3
		1	68.8	67.8
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		3	17.5	17.9
		4	9.1	8.6
		5	9.6	10.2
		6	1.9	2.1
		7	12.7	13.1
		8	2.6	2.0
		9	14.1	14.7
		10	6.4	6.9
		11	4.9	4.4
		12	.5	1.6
	2	0	45.2	45.3
		1	27.1	26.6
		2	23.4	22.9
		3	15.8	15.3
		4	16.6	15.9
		5	10.2	10.8
		6	5.1	4.3
		7	.4	7.6
		8	4.3	2.5
		9	.5	2.7
		10	.4	.2
4	2	11	.7	1.3
		12	7.8	8.1
	3	0	14.2	13.5
		1	14.2	12.6
		2	16.2	15.6
		3	34.6	33.3
		4	9.8	9.4
		5	9.1	8.5
		6	19.8	20.4
		7	.5	3.2
		8	.5	1.6
		9	.4	2.1
		10	.4	4.7
		11	4.4	3.9
		12	6.3	6.0
	4	0	7.4	6.6
		1	4.2	4.9
		2	4.4	7.9
		3	31.5	31.6
		4	2.1	2.9
		5	15.9	15.1
		6	6.1	5.7
		7	6.2	7.5
		8	4.9	3.9
		9	4.9	3.4
		10	7.2	7.4
		11	.4	.6
	5	0	6.2	6.6
		1	17.1	17.2
		2	.4	2.7
		3	8.6	8.8
		4	15.5	15.9
		5	16.7	17.1
		6	.4	3.0
		7	2.6	1.9
		8	6.1	7.9
		9	7.3	8.5
		10	5.3	3.7
		11	5.2	4.4
		12	.5	4.5
	6	0	6.7	5.7
		2	14.5	15.1
		4	13.0	10.6
		5	2.3	2.9
		6	7.8	9.0
		7	4.8	10.8
		8	5.9	5.7
		9	.8	2.3
		10	.4	.4
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		12	4.5	3.4
	7	0	3.5	3.7
		1	13.8	13.2
		2	8.7	9.0
		3	5.4	5.4
		4	29.4	30.8
		5	4.2	2.9
		6	13.4	10.8
		8	4.2	3.6
		9	.5	1.4
		10	.4	.6
		11	5.9	4.7
	8	0	5.6	7.4
		1	19.4	19.9
		2	7.5	7.5
		3	12.4	14.5
		5	.8	3.1
		6	7.5	2.4
		7	4.1	1.9
		9	1.4	.5
		10	.7	.5
		11	.6	.4
		12	.6	1.4
	9	0	9.2	9.9
		1	.4	1.5
		2	13.0	13.2
		3	.5	1.4
		4	.4	.1
		5	.5	1.4
		6	7.4	7.4
		7	7.1	6.2
		8	.6	1.7
		9	.5	.3
		11	.5	1.5
	10	0	9.4	8.7
		1	.4	3.1
		2	.4	.6
		3	.4	1.5
		4	2.5	2.8
		5	.4	4.3
		6	5.8	5.0
		7	.5	1.5
		8	4.2	1.8
		9	.6	1.2
		10	.5	1.1
5	0	1	45.3	38.5
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		5	1.7	2.7
		7	9.7	9.6
		9	38.4	39.5
		11	.7	3.0
	1	0	21.3	20.3
		1	17.8	17.2
		2	8.6	7.8
		3	8.6	9.4
		4	7.0	6.8
		6	1.9	.7
		7	16.1	16.2
		8	23.1	20.6
		9	8.6	9.3
		10	.5	4.5
		11	.4	3.1
		12	.6	4.3
	2	0	39.0	38.6
		1	4.6	4.7
		2	13.4	9.9
		3	19.8	20.6
		4	28.8	27.9
		5	.5	3.1
		6	24.6	25.7
		7	3.8	2.7
		8	8.2	9.1
		9	3.9	2.8
		10	6.8	6.7
		11	.6	1.1
		12	3.3	3.3
	3	0	13.0	9.7
		1	33.6	31.4
		2	14.3	14.5
		3	19.3	18.0
		4	13.6	11.3
		5	4.0	2.7
		6	7.9	7.3
		7	5.9	4.2
		8	.4	.0
		9	10.7	10.9
		10	.4	3.9
		11	.5	.8
		12	.5	1.1
	4	0	19.8	19.5
		1	9.0	9.1
		2	8.9	8.2
		3	6.3	5.0
		4	15.6	15.8
		5	8.0	8.1
		6	.4	1.3
		7	9.9	5.4
		8	.5	1.6
		9	11.4	12.1
		10	2.4	2.8
		11	.8	.8
		12	3.2	3.8
	5	0	34.2	34.1
		1	18.0	17.7
		2	7.9	7.7
		3	19.9	20.5
		4	.5	.5
		5	4.9	2.9
		6	10.2	9.3
		8	.5	4.9
		10	1.2	1.1
		11	.6	.8
		12	.7	.2
	6	0	5.0	4.9
		1	27.6	28.3
		2	14.7	15.7
		3	21.0	19.7
		4	.5	1.7
		5	7.6	7.8
		6	7.7	8.3
		8	2.7	3.1
		9	.4	3.0
5	6	10	3.1	3.6
		11	.5	2.5
		12	.5	.4
	7	0	.5	1.8
		1	2.7	1.8
		2	22.2	22.6
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		4	9.2	8.7
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		7	4.4	2.7
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		9	.5	2.1
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		12	.4	2.7
	8	0	9.7	10.9
		1	4.3	2.6
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		5	.7	3.0
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		7	.5	1.7
		8	2.6	.8
		9	.5	.0
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		5	3.1	2.3
		6	.4	4.9
		7	.6	.3
		9	.6	2.8
		10	1.7	1.8
	10	0	9.1	10.2
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		3	.8	3.3
		4	2.8	2.4
		5	4.8	5.5
		6	.5	4.1
		8	5.5	5.8
		9	.6	1.6
6	0	0	35.6	35.2
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		8	7.5	8.9
		10	6.2	5.9
		12	3.2	1.3
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		6	28.7	29.3
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		9	9.7	11.0
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		11	.5	1.6
		12	1.0	1.1
	2	0	14.6	14.9
		1	.4	1.0
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		3	11.2	12.6
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		10	.4	.4
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		5	.4	.3
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		11	.6	1.9
		12	.8	.4
	6	0	9.5	10.6
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		3	4.4	5.4
		4	.5	4.2
		5	6.7	8.5
		6	7.6	7.4
		7	.4	2.0
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		11	.7	2.7
		12	.6	.3
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		9	1.0	.7
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		11	.4	3.6
	8	0	2.6	1.2
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		5	.7	1.4
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		9	.4	2.5
		11	.6	3.0
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		7	2.9	.9
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		9	.5	.7
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		3	.5	.2
		5	.6	1.3
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		7	.5	.1
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7	0	1	27.8	28.4
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		9	5.7	6.5
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	1	0	5.0	3.9
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		4	.4	2.3
7	1	5	3.4	2.6
		6	14.3	20.3
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		9	.4	4.7
		10	.5	4.6
		11	.6	2.7
		12	.5	.5
	2	0	6.8	6.0
		1	5.2	5.8
		2	2.1	2.7
		3	2.4	.0
		5	2.7	3.7
		6	20.4	21.6
		7	6.3	6.1
		8	9.5	8.5
		9	4.1	4.3
		10	4.1	3.5
	3	0	5.8	5.9
		1	.6	.6
		2	4.1	2.9
		3	11.2	10.4
		4	14.9	15.2
		6	6.8	8.2
		7	.5	3.7
		8	5.6	5.2
		10	.4	3.6
		11	.5	.4
		12	6.0	3.5
	4	0	7.5	7.7
		1	.4	2.1
		2	15.1	15.4
		3	5.5	6.0
		4	.3	2.8
		5	2.8	1.8
		6	2.7	3.5
		7	12.6	13.3
		8	.5	3.7
		9	.6	2.6
		10	.4	5.2
		11	.5	1.1
		12	.5	2.8
	5	0	2.1	2.3
		2	2.7	.9
		3	2.3	2.2
		4	4.8	5.8
		5	.4	2.1
		6	.4	1.4
		7	.4	4.9
		8	.5	.1
		9	2.4	1.5
		10	.6	.1
		11	.5	1.0
		12	.5	.6
	6	0	.4	3.1
		1	23.6	24.7
		2	10.7	11.6
		3	5.9	5.7
		4	4.8	5.3
		5	.6	.1
		6	2.5	2.3
		7	.4	3.3
		9	6.6	6.7
		10	4.4	1.7
		11	.9	4.0
	7	0	4.5	4.2
		1	3.7	4.2
		2	.4	2.2
		3	12.1	12.0
		4	4.1	4.0
		5	7.0	8.3
		6	.4	2.2
		7	.6	.6
		8	.7	2.5
		9	5.3	2.8
		10	5.1	2.0
		11	4.6	3.2
	8	0	2.9	.2
		1	6.9	5.5
		2	.5	.7
		3	.4	4.5
		4	7.8	7.8
		5	.5	1.7
		7	.6	1.5
		9	.4	1.8
		10	5.7	3.9
	9	0	2.5	1.4
		1	.4	3.0
		2	.5	1.8
		3	5.2	4.7
		4	.8	3.0
		5	2.9	2.9
		6	.4	3.1
		7	5.1	5.6
		8	.9	.3
		9	.4	2.6
	10	0	.4	1.3
		1	.4	4.6
		2	.5	.0
		3	.7	2.6
		4	2.9	1.7
		5	.5	.8
		6	.4	2.6
		7	4.3	1.7
8	0	0	11.3	10.6
		2	13.5	11.0
		4	13.0	12.3
		6	4.5	4.7
		8	16.1	15.7
		10	4.8	3.9
		12	3.3	3.0
	1	0	8.3	7.3
		1	11.5	12.4
		2	.5	2.2
		4	.4	2.4
		5	4.6	8.4
		6	12.2	12.9
		7	3.9	6.3
		8	5.3	4.3
		9	.6	.4
		11	.4	4.6
	2	0	8.6	8.0
		1	4.6	4.0
		2	4.6	3.2
		3	7.2	6.4
		4	17.1	17.0
		5	11.1	12.2
		6	15.1	15.2
		7	1.0	1.3
		8	5.4	6.4
		9	.5	1.4
		11	.6	2.7
		12	.6	3.3
	3	0	12.5	12.7
		1	4.1	4.7
		2	11.5	13.1
		3	12.0	11.9
		4	21.9	22.6
		6	.4	.8
		7	5.8	6.3
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		9	2.3	.5
		10	.4	3.8
		11	4.8	3.5
		12	6.6	4.2
	4	0	8.5	8.2
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		4	8.4	8.8
		5	13.5	14.4
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		7	7.1	6.9
		8	.5	3.7
		9	4.0	1.2
		10	1.3	1.5
		11	.5	3.1
		12	.5	.3
	5	0	11.0	12.0
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		5	.4	1.7
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		7	.5	2.8
		8	5.6	5.5
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		10	.6	2.7
		11	1.0	.7
		12	.4	1.9
	6	0	.6	.7
		1	16.5	15.8
8	6	2	10.4	10.5
		3	4.8	3.8
		4	4.9	4.9
		5	.5	4.9
		6	4.4	1.7
		7	5.6	3.8
		8	2.9	1.5
		9	.5	2.5
		10	.5	.6
		11	.5	1.1
	7	0	3.0	4.3
		1	4.9	10.2
		2	4.4	4.9
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		7	.6	1.5
		8	.5	2.1
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		10	.5	.6
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		3	8.6	8.9
		5	.4	2.7
		6	3.2	.5
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	9	0	3.2	2.4
		1	5.9	5.3
		2	.5	4.3
		3	.4	1.8
		4	5.4	4.9
		5	4.6	3.0
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		7	.6	1.7
		8	.7	.3
	10	0	.5	1.7
		2	.6	.8
		3	1.0	1.7
		4	1.0	1.7
		5	4.9	2.2
		6	1.6	1.0
		7	.7	1.2
9	0	1	23.7	24.3
		3	22.3	23.4
		5	20.7	20.4
		7	.4	.9
		9	4.7	8.7
		11	.6	.8
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		2	2.6	2.3
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		4	4.7	6.5
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		6	8.1	8.4
		7	.4	.9
		8	.4	1.7
		9	.8	.3
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	2	0	8.1	8.4
		1	6.1	5.6
		2	14.7	15.9
		3	7.4	7.8
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		7	.4	1.9
		8	.4	3.3
		9	.6	.2
		10	.5	.8
		11	.5	2.3
	3	0	6.8	7.1
		2	5.5	5.1
		3	20.6	21.1
		4	.4	3.1
		5	4.3	3.1
		6	10.9	11.0
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		8	4.9	4.9
		9	3.5	1.2
		10	.5	3.1
		11	.7	2.7
		12	.5	1.9
	4	0	.4	2.9
		1	14.3	14.5
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	5	0	6.3	7.4
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		5	.7	2.1
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		11	.4	1.9
	6	0	5.0	5.2
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		4	.6	3.9
		5	4.2	4.0
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		7	6.7	6.8
		8	.8	.7
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		10	.4	1.9
	7	0	5.0	3.5
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		7	.4	3.7
		8	.6	.7
		9	.5	.7
		10	.4	.0
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		3	4.2	3.4
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		7	.6	1.8
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		1	.6	1.8
		2	.6	.8
		3	.6	.2
		4	.5	1.1
		5	.6	.7
		6	.5	.0
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		6	.4	1.3
10	0	0	7.4	6.6
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		6	7.9	7.1
		8	2.3	.2
		10	.4	2.0
		12	2.4	3.1
	1	0	4.9	4.8
		1	5.0	5.3
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	2	0	8.2	8.3
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		2	11.2	12.4
		3	8.7	9.7
		4	2.7	1.9
		5	4.7	5.9
10	2	6	.4	2.9
		7	.5	2.3
		8	4.8	4.8
		9	5.7	2.5
	3	0	11.5	11.6
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		2	8.3	8.8
		3	18.5	18.9
		4	4.1	11.1
		5	4.8	5.0
		6	.5	3.0
		7	.4	.0
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		9	3.4	3.7
		10	4.6	2.5
		11	.4	1.3
	4	1	23.1	23.4
		3	6.2	6.6
		4	3.1	2.7
		5	.4	2.0
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		7	.5	1.8
		8	5.6	4.8
		9	6.1	7.6
		11	.8	1.1
	5	0	2.5	.4
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		9	.4	1.2
		10	.4	.5
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		1	5.6	4.6
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	7	0	.5	1.8
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		9	.6	.1
	8	0	2.7	.4
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		3	.7	1.9
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		5	.4	1.0
		6	.5	.2
		7	.4	1.8
		8	1.0	.3
	9	0	3.2	1.8
		2	.6	3.0
		3	.4	3.1
		4	.4	3.0
		5	.5	.2
	10	0	.4	.3
		1	.6	.6
		2	.6	1.8
		3	.6	3.3
		4	.4	1.1
		5	.9	1.7
11	0	1	3.9	4.3
		3	6.5	6.8
		5	13.4	13.9
		7	.4	1.5
		9	.6	2.5
		11	.7	1.6
	1	0	19.7	21.1
		1	16.0	16.8
		2	22.3	22.2
		3	10.0	9.0
		4	.8	.2
		5	.4	2.9
		7	4.5	4.0
		8	5.7	2.4
		11	.4	1.7
	2	0	7.3	6.5
		1	7.4	7.7
		2	5.7	6.8
		3	.4	5.0
		4	4.4	3.4
		5	.4	3.1
		6	.7	3.5
		7	.7	3.2
		8	5.1	5.2
		9	.5	2.7
		10	.6	.3
		11	.5	.4
	3	0	4.1	.7
		1	8.2	9.0
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		3	11.3	12.4
		4	7.2	7.8
		5	.4	1.7
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		7	.8	1.8
		8	.4	2.3
		9	.4	1.3
		10	.4	.4
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		4	.4	2.4
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		10	.7	.2
	5	0	17.1	17.8
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		6	3.2	4.1
		7	.5	3.8
		8	4.6	5.0
		9	.5	5.2
	6	0	.4	3.0
		1	.6	.1
		3	.7	2.9
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		7	.6	1.9
		8	.5	1.9
		9	.8	.6
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		6	.6	.3
		7	.6	1.0
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	8	1	.4	.2
		5	.4	.7
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		5	.5	1.1
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		3	.4	.3
12	0	0	13.3	17.3
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		10	.4	3.0
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		5	5.0	3.2
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		7	.5	.9
		8	.7	1.8
		9	1.0	.1
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	2	1	3.9	4.8
		2	.4	2.6
12	2	3	10.7	10.6
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		8	.5	.4
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		5	.7	.2
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		5	.4	.0
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		5	3.1	3.5
		6	.4	1.7
		7	.6	4.5
	5	0	.5	.4
		1	.4	1.2
		2	4.1	1.8
		3	.4	2.8
		4	.6	3.3
		5	.4	1.2
	6	0	.5	.4
		1	.4	.8
		2	.4	.5
		3	.5	1.3
		4	.7	.4
	7	0	.8	.1
		1	1.0	.5
		2	.6	.5
		3	.5	1.4
		4	3.2	.6
	8	0	.4	.1
		1	.4	2.1
		2	.5	1.1

Table 4 (*cont.*)

H	K	L	F(O)	F(C)
-14	0	2	.5	1.8
		4	.4	.8
		6	7.5	6.3
		8	.5	6.2
		10	.9	2.2
	1	1	3.0	4.0
		2	6.2	6.5
		3	7.0	7.6
		4	5.6	4.1
		5	8.3	6.9
		6	7.8	6.8
		7	.4	3.5
		8	4.9	2.8
		9	.4	3.3
		10	.6	1.2
		12	.5	.7
		1	.4	1.3
		2	.4	.6
		4	3.2	4.3
		5	4.6	4.9
		6	5.2	6.6
		7	10.7	10.5
		8	3.3	2.1
		9	5.2	3.2
		10	1.3	.6
		11	.7	2.5
	3	1	6.4	3.3
		2	4.2	2.5
		3	.6	1.7
		5	.5	1.3
		6	.4	2.4
		8	5.5	4.9
		9	.4	3.6
		10	.8	.8
		11	.9	1.3
		12	3.2	1.3
	4	1	.9	5.2
		2	3.2	2.8
		3	4.8	2.6
		4	2.2	2.5
		5	.4	2.4
		6	.5	.9
		7	.6	2.3
		8	.6	2.4
		9	.5	.0
		10	1.2	.8
	5	1	.5	.6
		2	4.9	5.4
		3	6.9	5.8
		4	2.5	2.0
		5	4.9	6.0
		6	4.6	2.3
		7	.6	1.5
		10	.8	.1
		11	.6	2.1
	6	1	3.1	3.3
		2	5.7	4.5
		3	.4	.0
		4	2.7	3.4
		5	4.4	4.4
		6	.5	1.2
		7	.5	.2
		9	.4	.3
	7	1	6.3	6.0
		2	.6	.8
		3	5.7	4.2
		5	.4	.6
		6	.5	.6
		7	.5	3.0
		8	.8	1.4
		9	.6	3.6
	8	1	.8	1.3
		2	.6	2.4
		3	.4	3.0
		4	3.2	1.4
		5	3.0	2.1
		7	.4	1.4
-13	0	1	11.1	11.6
		3	14.8	13.3
		5	2.1	3.6
		7	4.3	5.0
		9	5.4	4.5
		11	2.9	4.5
	1	1	.4	1.7
		2	2.6	3.4
		3	5.3	4.3
		4	.4	2.3
		5	.6	1.6
		6	5.4	5.0
		7	5.7	6.8
		9	4.2	3.0
		10	.4	2.5
		11	.4	2.2
		12	.8	2.4
	2	1	2.3	2.9
		2	5.1	4.5
		3	4.4	3.5
		4	5.7	5.0
		6	.4	2.2
		8	.7	1.4
		10	.7	.1
		11	.9	.9
	3	2	.4	2.8
		3	.7	3.3
		4	1.9	3.8
		5	8.2	8.7
		6	.4	1.6
		7	4.3	4.6
		9	.4	1.7
		11	.7	2.9
		12	3.5	2.6
	4	2	5.9	6.5
		3	.5	2.4
		4	7.6	7.3
		5	.4	1.7
		6	5.9	4.8
		7	.4	2.2
		9	1.2	.4
		10	.5	1.4
	5	1	.5	2.8
		2	7.1	6.9
		3	2.8	2.2
		4	.5	2.4
		5	.4	3.8
		6	5.0	5.2
		7	.5	.3
		9	4.9	1.5
		10	.5	2.3
		11	.4	3.8
		12	.4	2.1
	6	1	.4	.9
		2	4.6	6.4
		3	.5	.6
		4	.4	2.1
		5	.5	1.5
		6	.5	.1
		7	.4	1.6
		8	.4	.7
		10	.9	2.2
	7	1	.4	.8
		2	.4	1.0
		3	.4	1.4
		4	.4	2.9
		5	.5	.8
		6	.5	.4
		7	.8	1.5
		8	4.9	2.0
		9	.4	.2
		10	.6	1.1
	8	2	.8	.2
		3	.6	2.5
		4	4.5	4.9
		5	3.0	3.1
		7	.7	1.8
		8	.5	1.2
		9	.4	.5
	9	1	.5	.2
		2	.6	4.7
		3	.5	2.6
		5	.6	1.1
		6	.6	.9
-12	0	2	27.1	21.9
		4	16.3	16.8
		6	11.0	11.6
		8	5.9	8.1
		12	5.0	3.2
	1	1	4.2	3.7
		2	6.2	7.5
		3	7.1	7.6
		4	3.8	3.1
		5	2.5	3.1
		6	13.9	13.5
-12	1	7	.5	4.4
		8	2.8	1.0
		9	.6	2.9
		10	.4	4.1
		11	.4	1.6
		12	.6	1.2
	2	1	7.7	7.8
		2	5.3	5.8
		3	12.6	12.3
		4	.5	1.7
		5	5.3	4.9
		6	.5	2.1
		7	11.8	12.8
		8	.4	3.4
		9	2.5	1.9
		10	6.1	1.9
		11	.4	1.8
		12	.6	1.4
	3	1	11.1	10.7
		3	8.0	8.9
		4	2.3	2.3
		5	10.8	10.6
		6	2.9	2.2
		8	4.1	4.5
		9	.6	1.8
		10	.8	1.3
	4	1	7.2	6.6
		3	4.9	4.7
		4	5.4	6.1
		5	.4	.0
		6	5.5	3.5
		7	3.4	2.0
		8	.5	3.0
		9	1.0	.5
		10	1.4	.0
		11	.9	.8
		12	.4	1.3
		1	.6	.0
		3	5.1	4.1
		4	.4	2.6
		5	.4	2.1
		6	4.0	3.2
		7	.5	.8
		8	.4	1.2
		9	1.3	.7
		10	3.1	1.9
		11	.8	2.5
		12	.9	3.9
	6	1	5.3	2.4
		2	6.5	3.3
		3	.4	1.7
		4	.5	1.6
		5	2.5	2.2
		6	.4	3.0
		7	4.3	3.4
		8	.7	.3
		9	.4	.8
		11	.5	2.6
		12	.9	2.1
	7	1	5.8	5.6
		2	4.3	2.8
		3	.4	3.1
		5	.4	1.4
		6	5.5	2.4
		7	1.0	1.1
		8	1.0	1.2
		9	5.1	3.7
		10	.9	.6
		11	.7	.7
	8	1	4.3	3.2
		2	4.4	3.1
		3	4.3	2.9
		4	.4	2.3
		6	.7	1.1
		8	.5	.2
		9	.6	2.0
		10	.8	.7
	9	1	4.9	2.7
		2	.5	.7
		3	.6	1.1
		4	2.8	3.6
		5	.7	.3
		6	.4	.7
		7	.4	1.6
		8	.5	2.7
	10	1	.6	.7
		2	4.7	2.3
		3	.6	.9
		5	.5	.6
-11	0	1	.4	.9
		3	5.1	4.5
		5	2.4	1.1
		7	2.2	1.0
		9	6.9	6.3
		11	6.2	5.7
	1	1	5.4	7.6
		2	6.5	5.3
		3	7.5	7.5
		4	6.8	6.4
		5	3.7	2.5
		6	10.1	11.1
		7	8.4	9.5
		8	7.9	7.5
		9	1.0	.6
		10	.4	1.9
		11	.5	3.3
		12	.6	.7
	2	2	.5	3.1
		3	7.1	8.4
		4	.4	3.3
		6	5.8	5.0
		7	2.0	.2
		8	7.7	6.4
		9	2.3	1.1
		10	4.8	4.3
		11	4.7	4.2
		12	.6	.7
	3	1	2.5	3.0
		2	7.3	6.7
		3	10.1	10.2
		4	12.2	12.6
		5	14.4	14.8
		6	6.9	7.1
		7	.8	2.4
		8	4.1	2.7
		9	.6	2.5
		10	.4	3.0
		12	4.1	7.2
	4	1	2.8	.8
		2	11.4	11.2
		3	.5	1.2
		4	7.3	7.8
		5	4.9	6.6
		6	.9	.5
		7	.6	4.3
		8	.6	.5
		9	.4	4.1
		10	4.5	6.9
		11	.4	3.0
		12	4.9	5.1
	5	1	7.2	6.6
		2	21.0	22.0
		3	.4	3.7
		4	6.9	5.0
		5	.4	1.2
		6	2.5	1.4
		7	5.6	6.4
		8	6.1	5.7
		9	7.6	6.9
		10	8.6	8.2
		11	6.6	6.8
		12	.4	.0
	6	1	7.3	6.6
		2	7.5	7.8
		3	4.9	3.8
		4	3.4	2.3
		6	.5	2.6
		7	.5	1.6
		8	.4	2.4
		9	.4	.9
		10	.7	2.0
		11	.4	2.7
		12	5.0	2.5
	7	1	7.4	8.3
		2	.6	3.0
		3	.7	4.6
		4	5.6	5.1
		5	.6	2.3
		6	.6	3.4
		7	.7	2.1
		8	.4	.6
		9	.7	.7
-11	7	10	5.1	1.8
		11	1.2	1.1
		12	1.3	1.4
	8	2	.6	2.1
		3	.6	2.6
		4	1.5	2.6
		5	3.1	4.5
		6	4.4	4.6
		7	.8	.6
		8	.5	2.4
		9	.6	.9
		10	.4	1.6
		11	.5	3.0
	9	1	.7	1.1
		2	.6	2.4
		3	5.2	5.6
		4	3.2	1.7
		5	.5	3.0
		6	4.5	4.4
		7	.8	1.6
		8	5.9	6.6
	10	1	.4	4.5
		2	.5	.7
		3	.4	3.6
		4	3.4	3.0
		5	.4	.1
		6	.5	.4
-10	0	2	11.4	11.4
		4	10.3	11.5
		6	13.5	12.4
		8	8.8	7.6
		10	4.5	5.4
		12	1.1	2.1
	1	1	.4	.6
		2	.5	.6
		3	.4	3.0
		4	.4	3.7
		5	14.4	14.3
		6	11.1	11.2
		7	8.4	4.1
		8	7.8	7.0
		9	11.6	11.6
		10	.4	1.7
		11	4.3	1.9
		12	.6	.3
	2	1	6.3	6.1
		2	.6	.6
		3	11.8	12.1
		4	6.3	6.3
		5	11.1	11.6
		6	4.1	4.2
		7	1.4	.7
		8	6.1	4.9
		9	7.1	8.0
		10	.5	1.8
		11	.4	1.9
		12	.5	1.2
	3	1	8.2	8.1
		2	2.4	3.7
		3	8.4	8.5
		4	19.1	19.9
		5	10.2	9.2
		6	11.7	11.7
		7	6.6	7.9
		8	9.2	10.2
		10	.5	1.7
		11	6.0	4.2
		12	.6	1.9
	4	1	2.4	3.0
		2	16.5	16.8
		3	2.3	4.5
		4	2.3	2.7
		5	2.4	3.8
		6	13.0	13.4
		8	6.0	5.9
		9	5.3	4.7
		10	.5	4.1
		11	.6	.0
		12	.4	3.0
	5	1	10.7	11.1
		2	14.4	14.8
		3	11.4	11.5
		5	.6	2.8
		7	.4	2.3
		8	5.2	5.7
		9	2.6	3.8
		11	6.5	6.0
		12	5.2	2.7
	6	1	4.1	4.2
		2	.5	4.2
		3	6.6	7.0
		5	6.8	6.9
		6	4.6	6.3
		7	8.2	8.7
		8	4.3	2.5
		9	4.8	3.0
		10	.4	.5
		11	.5	3.3
		12	.6	1.2
	7	1	5.9	4.0
		3	.6	4.4
		4	5.4	5.9
		5	6.0	7.9
		6	.9	3.6
		7	7.6	7.9
		8	.6	2.4
		9	4.8	5.1
		10	4.5	.4
		11	.9	1.1
		12	.5	2.2
	8	1	.4	3.2
		2	5.3	4.9
		3	.5	2.5
		4	5.6	4.9
		7	.7	2.9
		8	4.3	4.0
		9	.4	.1
		11	.4	1.9
	9	2	.5	.2
		4	3.0	3.4
		5	.4	2.3
		6	.4	3.6
		7	4.7	1.9
		8	4.6	4.1
		9	.4	3.0
	10	3	5.1	2.6
		5	.7	2.2
		6	.6	1.0
		7	.4	1.7
		8	1.0	1.7
-9	0	1	13.9	15.0
		3	7.6	7.4
		5	13.0	12.3
		7	10.1	10.5
		9	2.7	2.8
		11	6.4	6.5
	1	1	.4	3.8
		2	26.3	27.1
		3	6.0	7.6
		4	3.6	3.9
		5	2.6	1.7
		6	6.5	7.2
		7	6.7	6.9
		8	2.6	3.7
		9	3.8	1.9
		10	4.7	3.4
		11	4.9	3.8
		12	.4	.9
	2	1	5.3	3.6
		2	.6	2.0
		3	7.3	8.3
		4	3.3	1.9
		5	.5	.2
		6	14.8	14.4
		7	2.2	2.3
		8	9.3	9.4
		9	.5	.1
		10	6.1	5.5
		11	.5	.0
		12	.5	3.5
	3	1	11.8	11.8
		2	7.5	1.9
		3	6.0	5.9
		4	2.1	2.6
		5	15.8	15.6
		6	8.7	9.0
		8	12.1	12.3
		9	13.8	12.8
		10	.6	2.0
		11	4.5	3.5
	4	1	15.6	15.8
		2	17.9	17.3
-9	4	3	15.5	15.3
		4	6.0	6.1
		5	17.8	18.0
		6	8.3	7.5
		7	5.3	6.7
		8	5.2	4.3
		9	5.7	6.9
		10	9.6	10.6
		11	4.6	4.1
		12	.5	.9
	5	1	5.9	6.4
		2	8.7	8.3
		3	1.6	1.8
		4	10.8	10.7
		5	6.5	6.9
		6	8.5	9.6
		7	3.7	1.9
		8	.5	1.6
		9	3.1	2.1
		10	.5	3.4
		12	7.8	6.0
	6	1	10.1	10.1
		2	4.4	3.3
		3	.4	3.9
		4	6.5	6.9
		5	3.9	3.4
		6	4.2	5.6
		7	1.0	.2
		8	6.3	7.4
		10	4.1	4.6
		11	.5	1.7
		12	.4	.5
	7	1	6.3	6.0
		2	2.3	3.4
		3	3.9	4.8
		4	5.2	5.5
		5	.6	.0
		6	.4	4.0
		7	.6	3.5
		8	.7	.1
		9	.5	2.2
		10	5.9	6.7
		11	.5	1.6
		12	.6	.5
	8	1	2.5	3.7
		2	.6	2.5
		3	2.9	1.9
		4	.9	2.7
		5	7.4	7.7
		6	5.4	4.4
		7	4.6	3.8
		8	.4	4.4
		10	.5	.6
		11	.9	2.8
	9	1	.7	.3
		2	1.0	2.6
		3	4.9	4.6
		4	3.1	1.7
		5	5.3	5.3
		6	.4	.5
		8	.6	1.4
		10	.8	2.4
		11	.6	2.8
	10	1	4.4	4.6
		2	.5	1.5
		3	.5	.9
		4	.6	.8
		5	.6	2.6
		6	6.4	6.8
		7	.4	4.6
		8	5.3	4.9
-8	0	2	39.2	38.3
		4	5.3	5.7
		6	6.4	6.1
		8	6.0	6.1
		10	7.2	7.1
		12	6.3	3.8
	1	1	11.3	12.2
		2	16.7	17.1
		3	6.3	7.6
		4	.3	2.4
		5	21.6	21.4
		6	7.2	7.1
		7	.5	2.4
		8	12.2	11.9
		10	5.9	4.4
		11	5.0	5.9
		12	.5	.5
	2	1	16.2	15.3
		2	21.6	21.5
		3	25.4	25.2
		4	9.8	10.3
		5	2.0	.9
		6	3.5	4.0
		7	17.7	18.2
		8	7.3	7.1
		9	2.8	2.7
		10	.5	3.4
		11	.5	2.3
		12	7.3	6.9
	3	1	6.3	5.6
		2	5.7	6.0
		3	4.1	5.7
		4	14.8	16.1
		5	8.9	8.5
		6	5.8	5.6
		7	8.1	8.2
		8	9.0	9.8
		9	.7	9.1
		10	.4	1.1
		12	1.2	4.3
	4	1	22.2	21.7
		2	22.0	22.9
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		5	.4	.2
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		7	.9	2.2
		8	4.1	4.4
		9	2.7	2.4
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		12	4.0	2.5
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		10	.7	7.5
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		6	11.5	10.9
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		8	.4	.8
		9	.4	1.5
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		11	.4	.7
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	7	1	13.2	12.0
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		11	.6	1.3
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		8	.5	1.7
		9	.9	.5
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		12	.6	1.5
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		7	5.6	4.2
		8	.4	.0
		9	.6	1.0
		10	.6	1.6
		11	7.4	5.5
	10	1	5.8	4.3
		2	4.6	2.9
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		5	.8	.7
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-7	0	1	8.6	8.5
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		11	.5	1.7
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		11	.5	3.5
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		12	.5	.1
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		8	6.8	5.9
		10	6.8	6.8
		12	12.8	13.7
	1	1	35.3	34.0
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		3	24.6	24.2
		4	19.5	19.9
		5	28.3	28.3
		6	7.5	6.3
		7	15.2	14.6
		8	17.2	17.1
		9	4.2	5.7
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		11	11.3	11.2
		12	3.0	1.4
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-6	3	12	.5	5.0
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		4	12.4	12.7
		5	3.8	5.1
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		11	8.7	9.7
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		8	5.9	5.0
		9	5.4	2.2
		10	1.2	.3
		11	.6	.8
		12	.5	1.9
	9	1	.5	4.2
		2	5.1	4.4
		3	.5	2.6
		4	5.6	5.0
		5	4.0	5.4
		6	4.2	5.2
		7	.5	.2
		8	2.6	1.5
		9	.4	3.0
		10	.6	2.7
		11	.4	4.8
	10	1	4.5	4.9
		2	2.8	1.2
		3	4.0	2.2
		4	8.5	9.6
		5	.5	.0
		7	.5	.0
		9	.5	2.3
		10	.6	1.1
		11	.4	3.1
-2	0	2	69.9	69.8
		4	14.1	13.7
		6	3.6	3.0
		8	28.1	28.4
		10	3.9	4.4
		12	4.2	3.6
	1	1	86.9	85.7
		2	132.2	131.5
		3	99.7	98.3
		4	25.0	23.5
		5	24.3	25.2
		6	36.2	38.0
		7	12.0	12.1
		8	1.4	.6
		9	3.9	2.8
		10	2.6	1.7
		11	5.0	5.6
		12	5.9	5.1
	2	1	77.9	79.2
		2	39.8	39.0
		3	98.4	99.0
		4	12.7	13.0
		5	26.7	25.7
		6	42.3	43.1
		7	.4	2.0
		8	.4	2.9
		9	2.5	2.6
		10	2.7	3.4
		11	7.4	7.0
		12	4.8	1.8
	3	1	.4	2.3
		2	4.6	8.3
		3	20.9	21.3
		4	7.5	6.9
		5	25.2	24.8
		6	11.0	11.1
		7	16.8	16.4
		8	4.8	5.9
		9	9.6	9.4
		10	10.2	11.2
		11	.5	4.9
		12	.4	2.5
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		3	14.0	13.0
		4	37.4	37.4
		5	6.5	7.1
		6	10.8	11.9
		7	11.0	11.5
		8	.4	2.3
		9	.5	2.8
		10	7.9	8.0
		11	.7	1.6
	5	1	30.8	31.5
		2	9.6	9.6
		3	16.9	15.2
		4	.4	3.3
		5	7.6	6.5
		6	4.1	5.0
		7	21.4	21.6
		8	10.3	10.6
		9	6.6	6.7
		10	12.8	12.3
		11	6.1	6.8
		12	4.2	5.0
	6	1	12.7	12.5
		2	.4	3.6
		3	6.0	5.2
		4	5.2	5.0
		5	8.1	7.3
		6	2.2	1.1
		7	4.5	5.5
		8	16.3	17.0
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		10	.5	1.0
		11	.4	2.1
		12	.5	2.0
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		2	11.1	10.9
		3	3.9	4.2
		4	12.0	12.7
		5	8.7	7.9
		6	17.5	18.0
		7	11.5	11.6
		8	2.5	1.9
		9	4.8	2.5
-2	7	10	3.0	4.1
		11	.6	1.1
		12	4.2	1.9
	8	1	.4	1.4
		2	5.2	4.9
		3	7.9	8.7
		4	4.0	5.4
		5	21.5	21.2
		6	.4	3.8
		7	4.2	4.2
		8	.5	2.6
		9	4.5	2.5
		10	.5	.6
		11	.8	1.0
		12	1.4	.7
	9	1	4.3	1.6
		2	10.0	10.3
		3	5.7	6.9
		4	4.7	5.2
		5	.4	2.1
		6	8.4	7.8
		7	.4	2.5
		8	6.9	7.4
		10	.6	1.1
		11	.5	3.2
		12	.7	1.4
	10	1	7.8	8.9
		2	.5	.0
		3	4.7	3.0
		4	5.4	4.6
		5	1.1	1.9
		6	.6	1.5
		7	.5	.7
		8	.5	3.5
		9	3.1	1.9
		10	.4	3.0
		11	5.9	5.7
-1	0	3	85.5	87.4
		5	38.6	39.4
		7	.4	3.6
		11	12.3	13.2
		2	6.8	5.0
		3	83.4	84.3
		4	61.1	60.7
		5	26.7	27.3
		6	26.5	27.8
		7	22.0	22.7
		8	37.7	37.9
		9	.4	1.7
		10	18.8	19.2
		11	9.0	9.2
		12	6.7	7.2
	2	1	12.3	13.3
		2	36.5	37.5
		3	136.8	140.9
		4	13.8	11.3
		5	15.9	15.3
		6	5.8	6.1
		7	8.3	8.9
		8	12.6	12.7
		9	11.0	10.6
		10	1.7	2.5
		11	.4	3.9
		12	.4	1.5
	3	1	23.4	22.7
		2	9.7	7.8
		3	8.2	8.7
		4	40.1	40.1
		5	28.1	27.1
		6	22.9	23.5
		7	3.5	2.3
		8	3.9	2.3
		9	13.7	13.0
		10	4.5	5.6
		11	4.5	1.2
		12	.8	.5
	4	1	41.0	41.6
		2	20.6	20.1
		3	11.1	10.8
		4	33.4	32.5
		5	8.4	8.6
		6	6.5	6.8
		7	9.0	9.6
		8	.4	1.7
		9	.4	2.8
		10	2.8	3.4
		11	.5	3.2
		12	.5	.2
	5	1	10.2	9.8
		2	26.2	29.1
		3	20.2	21.1
		4	6.3	5.2
		6	6.1	7.2
		7	11.6	12.1
		8	6.1	7.3
		9	8.1	8.0
		10	.4	3.0
		11	.5	2.6
		12	.4	1.8
	6	1	5.9	3.9
		2	5.1	4.9
		3	9.1	9.7
		4	4.0	3.6
		5	7.2	7.8
		6	2.0	3.9
		7	10.1	8.9
		8	8.1	8.7
		9	.5	2.9
		10	6.4	7.3
		12	.4	2.5
	7	1	4.8	4.2
		2	11.5	12.3
		3	11.9	11.5
		4	8.1	7.5
		5	26.8	27.7
		6	16.9	17.1
		7	9.6	9.5
		8	9.3	9.2
		9	.4	3.0
		10	6.4	6.7
		12	4.9	3.5
	8	1	6.2	5.9
		2	4.2	4.5
		3	.6	2.0
		4	.4	4.6
		5	9.7	8.9
		6	.7	1.2
		7	9.0	9.4
		8	8.6	9.1
		9	2.9	3.2
		10	.4	.1
		11	.6	3.0
		12	.4	.3
	9	1	4.4	3.7
		2	4.6	2.5
		3	11.3	10.3
		4	.4	1.5
		5	.4	3.2
		6	.4	2.9
		7	5.9	4.8
		8	.5	.2
		9	6.3	6.9
		10	.6	2.2
		11	5.4	6.7
		12	.5	1.6
	10	1	5.3	5.5
		2	2.9	5.5
		3	4.6	4.4
		4	4.2	4.2
		5	.6	1.7
		6	.7	.4
		7	.7	.4
		9	.5	1.5
		10	.5	4.5
		11	.7	1.5
0	0	2	88.5	87.4
		4	30.4	29.2
		6	11.1	12.3
		8	50.7	50.7
		10	8.7	8.3
		12	.6	.9
	1	2	31.3	28.5
		3	82.0	82.5
		4	30.1	30.8
		5	.4	1.2
		7	15.8	17.7
		8	7.1	6.8
		9	7.6	7.3
		10	7.1	7.4
		11	7.3	7.9
		12	5.5	7.0
	2	0	15.9	13.3

Table 5. *Interatomic distances* (Å) *in OPBC, with their standard deviations in parentheses*

C(1)—C(2)	1·510 (5)	C(10)–C(11)	1·381 (6)
C(1)—O(3)	1·383 (5)	C(11)–C(12)	1·383 (7)
O(3)—N(2)	1·427 (4)	C(12)–C(13)	1·370 (8)
N(2)—C(9)	1·284 (5)	C(13)–C(14)	1·367 (9)
C(9)—C(10)	1·474 (5)	C(14)–C(15)	1·385 (7)
		C(15)–C(10)	1·397 (6)
C(1)—N(1)	1·617 (6)		
N(1)—O(1)	1·165 (7)	C(3)—H(C3)	0·90 (5)
N(1)—O(2)	1·126 (6)	C(4)—H(C4)	0·96 (4)
C(1)—C(8)	1·491 (6)	C(5)—H(C5)	0·98 (5)
C(8)—N(3)	1·113 (6)	C(6)—H(C6)	0·97 (5)
C(9)—C(16)	1·462 (6)	C(7)—H(C7)	0·97 (4)
C(16)–N(4)	1·127 (6)	C(11)–H(C11)	0·95 (5)
C(2)—C(3)	1·398 (6)	C(12)–H(C12)	0·97 (6)
C(3)—C(4)	1·379 (6)	C(13)–H(C13)	0·92 (5)
C(4)—C(5)	1·367 (7)	C(14)–H(C14)	0·94 (6)
C(5)—C(6)	1·375 (8)	C(15)–H(C15)	0·97 (4)
C(6)—C(7)	1·380 (7)		
C(7)—C(2)	1·389 (6)		

1·617 Å. There are a number of reports of C–N(O_2) distances longer than the accepted average 1·50 Å, but they do not exceed 1·53 Å (Saunder, 1946). In view of the large number and good quality of the measured reflexions and also of the fact that all the other distances are very reasonable, this long distance has to be significant. Mass spectral data of the compound agree with this result. No peak corresponding to the molecular ion M^+ could be observed but instead there was a peak corresponding to an M^+–46 ion, which suggests very easy abstraction of the NO_2 group from the molecular ion M^+. Hence, the bond between C(1) and the nitro group has to be very weak, as it would in the case of a long C(1)–N(1) bond. It should be noted here that the temperature factors of the two O atoms of the nitro group are considerably larger than those of the other atoms (Table 2).

Fig. 2 shows the molecular packing of OPBC in

Table 7. *Least-squares planes in OPBC, with displacements of atoms from the planes* (Å)

The equation for a plane is in the form $AX+BY+CZ=D$ and refers to orthogonal axes. The coordinates X,Y,Z are expressed in Å; D is the distance of the plane from the origin. Asterisks indicate atoms not included in the calculation of the plane. Mean estimated standard deviations of the atoms defining a plane are given in parentheses attached to the distance of the first atom.

(*B*1) Benzene ring 1 [attached to C(1)]

$$-0{\cdot}44896X+0{\cdot}66762Y+0{\cdot}59390Z=5{\cdot}88875$$

C(2)	−0·003 (4)	C(1)*	0·037
C(3)	0·004		
C(4)	0·000		
C(5)	−0·004		
C(6)	0·005		
C(7)	−0·002		

(*B*2) Benzene ring 2 [attached to C(9)]

$$-0{\cdot}49383X-0{\cdot}27287Y+0{\cdot}82564Z=9{\cdot}92239$$

C(10)	−0·017 (12)	C(9)*	−0·026
C(11)	0·014		
C(12)	0·000		
C(13)	−0·011		
C(14)	0·008		
C(15)	0·006		

(*P*1) Plane of the nitro group

$$0{\cdot}33805X-0{\cdot}71564Y+0{\cdot}61285Z=5{\cdot}01160$$

C(1)	−0·003 (10)
N(1)	0·015
O(1)	−0·006
O(2)	−0·006

(*P*2) Main chain

$$-0{\cdot}69046X+0{\cdot}37397Y+0{\cdot}61920Z=6{\cdot}26029$$

C(1)	−0·007 (9)	C(2)*	−0·192
O(3)	0·007	C(10)*	−0·015
N(2)	0·008	C(16)*	−0·090
C(9)	−0·008	N(4)*	−0·171

Dihedral angles between planes (°)

$B1\wedge B2$	58·0	$B2\wedge P1$	57·6	$P1\wedge P2$	83·1
$B1\wedge P1$	74·7	$B2\wedge P2$	41·4		
$B1\wedge P2$	22·0				

Table 6. *Bond angles in OPBC, with their standard deviations in parentheses* (°)

C(2)—C(1)—N(1)	107·9 (0·3)	C(4)—C(5)—C(6)	120·3 (0·4)	C(4)—C(5)—H(C5)	118·6 (2·9)
C(2)—C(1)—C(8)	112·7 (0·3)	C(5)—C(6)—C(7)	120·4 (0·5)	C(6)—C(5)—H(C5)	121·1 (2·9)
C(2)—C(1)—O(3)	109·9 (0·3)	C(6)—C(7)—C(2)	119·4 (0·4)	C(5)—C(6)—H(C6)	123·0 (2·7)
C(8)—C(1)—O(3)	112·0 (0·3)	C(7)—C(2)—C(3)	120·1 (0·4)	C(7)—C(6)—H(C6)	116·3 (2·7)
N(1)—C(1)—O(3)	108·9 (0·3)	C(1)—C(2)—C(3)	119·9 (0·4)	C(6)—C(7)—H(C7)	121·1 (2·6)
C(8)—C(1)—N(1)	105·3 (0·3)	C(1)—C(2)—C(7)	119·9 (0·3)	C(2)—C(7)—H(C7)	119·5 (2·6)
C(1)—O(3)—N(2)	109·2 (0·3)	C(10)–C(11)–C(12)	120·2 (0·4)	C(10)–C(11)–H(C11)	115·8 (3·2)
O(3)—N(2)—C(9)	110·7 (0·3)	C(11)–C(12)–C(13)	119·9 (0·5)	C(12)–C(11)–H(C11)	123·6 (3·2)
N(2)—C(9)—C(10)	130·9 (0·3)	C(12)–C(13)–C(14)	120·9 (0·5)	C(11)–C(12)–H(C12)	117·9 (2·9)
N(2)—C(9)—C(16)	111·1 (0·3)	C(13)–C(14)–C(15)	119·8 (0·5)	C(13)–C(12)–H(C12)	122·2 (2·9)
C(10)–C(9)—C(16)	117·9 (0·4)	C(14)–C(15)–C(10)	119·9 (0·4)	C(12)–C(13)–H(C13)	122·4 (3·6)
C(1)—N(1)—O(1)	113·0 (0·4)	C(15)–C(10)–C(11)	119·2 (0·4)	C(14)–C(13)–H(C13)	116·7 (3·6)
C(1)—N(1)—O(2)	116·9 (0·4)	C(9)—C(10)–C(11)	119·3 (0·4)	C(13)–C(14)–H(C14)	124·7 (3·3)
O(1)—N(1)—O(2)	130·0 (0·5)	C(9)—C(10)–C(15)	121·4 (0·3)	C(15)–C(14)–H(C14)	115·4 (3·4)
C(1)—C(8)—N(3)	176·1 (0·5)	C(2)—C(3)—H(C3)	119·2 (2·5)	C(14)–C(15)–H(C15)	119·7 (2·1)
C(9)—C(16)–N(4)	178·4 (0·5)	C(4)—C(3)—H(C3)	121·4 (2·5)	C(10)–C(15)–H(C15)	120·4 (2·1)
C(2)—C(3)—C(4)	119·0 (0·4)	C(3)—C(4)—H(C4)	119·6 (2·7)		
C(3)—C(4)—C(5)	120·8 (0·4)	C(5)—C(4)—H(C4)	119·5 (2·7)		

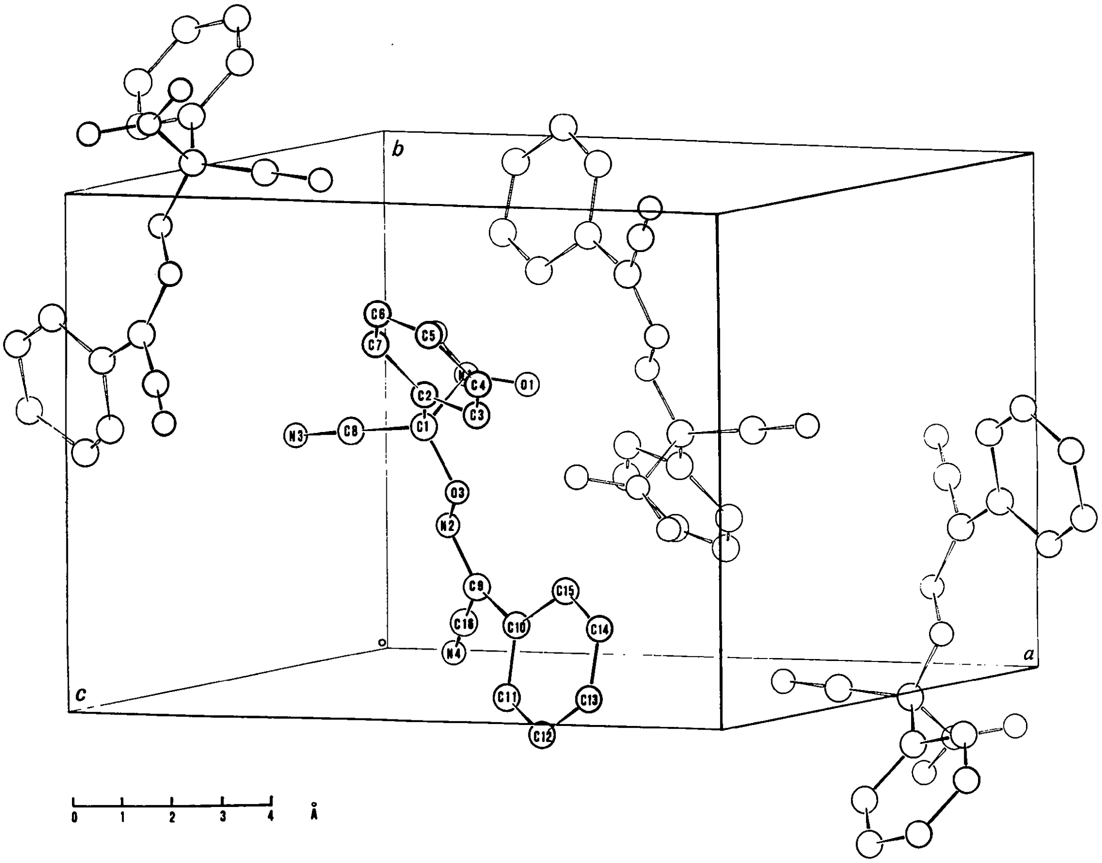

Fig. 2. Clinographic projection of the unit cell, showing the molecular packing.

clinographic projection. The various intermolecular distances are normal.

Thanks are due to Professor N. E. Alexandrou and Mr P. S. Lianis, Laboratory of Organic Chemistry, Aristotle University of Thessaloniki, Greece, for providing the OPBC crystals and the mass spectral data. We also thank the University of Thessaloniki for the use of its UNIVAC 1106 computer.

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