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2,3,8,12,13-Pentamethoxy-5*H*-dibenzo-[*c*,*n*]acridin-7(6*H*)-one toluene solvate

Marlon R. Lutz Jr,^a Matthias Zeller^b and Daniel P. Becker^a*

^aDepartment of Chemistry, Loyola University, 6525 North Sheridan Road, Chicago, IL 60626, USA, and ^bDepartment of Chemistry, Youngstown State University, One University Plaza, Youngstown, OH 44555, USA Correspondence e-mail: dbecke3@luc.edu

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Key indicators: single-crystal X-ray study; T = 100 K; mean σ (C–C) = 0.003 Å; R factor = 0.076; wR factor = 0.199; data-to-parameter ratio = 28.9.

The title compound, $C_{26}H_{25}NO_6 \cdot C_7H_8$, formed by an unexpected tandem reaction of Beckmann rearrangement, electrophilic aromatic addition and subsequent demethylation, was crystallized as its toluene solvate. The crystal under investigation was found to be nonmerohedrally twinned by a rotation around the reciprocal axis [100]; the twin ratio refined to 0.688 (2):0.312 (2). The molecule exhibits an unusual helical arrangement of three six-membered rings that are all connected at one central C atom. The helix effectively performs one full turn around this atom, and the thread pitch, as defined by the distance of the terminal C atoms of the helix, is 4.98 (3) Å. The angles around the central atom are between 104.7 (2) and 115.2 (2)°. The middle ring, a cyclohexa-2,4-dienimine ring containing only one saturated C atom, is essentially planar, with an r.m.s. deviation from the mean plane of only 0.035 Å. The other two rings have conformations best described as between envelope and screw-boat, with puckering amplitudes of 0.527 (2) and 0.544 (2) Å, respectively. The packing appears to be dominated by a combination of simple dispersion forces, weak C-H···O hydrogen bonds and $C - H \cdots \pi$ interactions.

Related literature

For the use of crown-shaped [1.1.1]orthocyclophane cyclotriveratrylene (CTV, hexamethoxytribenzocyclononene) as a scaffold in supramolecular chemistry, see: Collet (1987). For crown and saddle conformers of CTV oxime, see: Lutz *et al.* (2007). For other related literature, see: Boeyens (1978); Cremer & Pople (1975); Herbstein (2000).



V = 2757.1 (12) Å³

Mo $K\alpha$ radiation

 $0.60 \times 0.19 \times 0.09 \text{ mm}$

40178 measured reflections

10641 independent reflections

7887 reflections with $I > 2\sigma(I)$ R_{int} not defined due to twin pairing

errors (Herbst-Irmer, 2006)

 $\mu = 0.09 \text{ mm}^{-1}$

T = 100 (2) K

Z = 4

Experimental

Crystal data

 $\begin{array}{l} C_{26}H_{25}NO_6\cdot C_7H_8\\ M_r = 539.60\\ Monoclinic, P2_1/c\\ a = 14.952 \ (4) \ {\rm \AA}\\ b = 7.1736 \ (18) \ {\rm \AA}\\ c = 25.787 \ (6) \ {\rm \AA}\\ \beta = 94.571 \ (7)^\circ \end{array}$

Data collection

Bruker SMART APEX CCD diffractometer Absorption correction: multi-scan (*TWINABS*; Bruker, 2003) $T_{\rm min} = 0.773, T_{\rm max} = 1.000$ (expected range = 0.767–0.992)

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.076$ 368 parameters $wR(F^2) = 0.199$ H-atom parameters constrainedS = 1.08 $\Delta \rho_{max} = 0.67$ e Å $^{-3}$ 10641 reflections $\Delta \rho_{min} = -0.25$ e Å $^{-3}$

Table 1

Hydrogen bonding and $C-H\cdots\pi$ interactions.

*Cg*1 denotes the centroid of ring C8–C13, *Cg*2 that of C15–C20 and *Cg*3 that of C27–C32.

D−H···A	D-H	$H{\cdots}A$	D···A	D−H···A
C23 $-H23B\cdots O4^{i}$	0.98	2.41	3.354 (3)	160.4
$C26-H26B\cdots O2^{ii}$	0.98	2.59	3.210 (3)	120.9
$C26-H26C\cdots O6^{iii}$	0.98	2.58	3.526 (3)	162.2
$C12-H12\cdots Cg2^{iV}$	0.95	3.32	3.780(2)	112
$C22 - H22A \cdots Cg2^{iii}$	0.98	2.97	3.557 (3)	120
$C23-H23C\cdots Cg1^{v}$	0.98	2.99	3.902 (3)	156
$C24 - H24A \cdots Cg3^{vi}$	0.98	2.66	3.447 (3)	137
$C25-H25C\cdots Cg3$	0.98	2.63	3.487 (3)	146
Symmetry codes: (i)	-x, -y, -	z + 1; (ii)	$-x+1, y+\frac{1}{2}, -x+\frac{1}{2}$	$-z + \frac{1}{2};$ (iii)
-x + 1, -y + 2, -z + 1;	(iv) <i>x</i> , <i>y</i>	-1, z; (v)	-x, -y + 1, -	-z + 1; (vi)
$-x, y - 1/2, -z + \frac{1}{2}$				

Data collection: *SMART* (Bruker, 2002); cell refinement: *CELL_NOW* (Sheldrick, 2004) and *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2480).

References

Boeyens, J. C. A. (1978). J. Cryst. Mol. Struct. 8, 317-320.

- Bruker (2000). SHELXTL. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2002). SMART for WNT/2000. Version 5.630. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2003). SAINT-Plus. Version 6.45 (includes TWINABS as an implemented subprogram). Bruker AXS Inc., Madison, Wisconsin, USA. Collet, A. (1987). Tetrahedron, 43, 5725–5759.
- Cremer, D. & Pople, J. A. (1975). J. Am. Chem. Soc. 97, 1354–1358.
- Herbstein, F. H. (2000). Acta Cryst. B56, 547-557.
- Herbst-Irmer, R. (2006). Private Communication at the 62nd Conference of the Pittsburgh Diffraction Society, Pittsburgh, PA, USA.
- Lutz, M. R. Jr, French, D. C., Rehage, P. & Becker, D. P. (2007). *Tetrahedron Lett.* 48, 6368–6371.
- Sheldrick, G. M. (2004). CELL_NOW. University of Göttingen, Germany.

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2,3,8,12,13-Pentamethoxy-5H-dibenzo[c,n]acridin-7(6H)-one toluene solvate

M. R. Lutz Jr, M. Zeller and D. P. Becker

Comment

The crown-shaped [1.1.1]orthocyclophane cyclotriveratrylene (CTV, hexamethoxy tribenzocyclononene) molecule has been employed extensively as a scaffold in supramolecular chemistry (Collet, 1987). We are interested in new apex-modified derivatives of CTV and recently reported the isolation of the crown and saddle conformers of CTV oxime (Lutz *et al.*, 2007). In the course of studying the Beckmann rearrangement of this molecule we observed the unexpected formation of the title compound, resulting from a Beckmann rearrangement followed by an intramolecular electrophilic aromatic addition and subsequent demethylation (Fig. 1). Studies of the reaction conditions and mechanism will be discussed in detail in a separate publication.

The title compound was crystallized from methylene chloride/toluene as its toluene solvate (Figure 2). The red needle-like crystals were heavily intergrown, and the crystal that was finally selected for single-crystal data collection was found to be non-merohedrally twinned with two twin components in a ratio of 0.688 (2) to 0.312 (2) (See experimental refinement section for details of unit cell determination, data workup, refinement, and type of twinning).

The compound shows an unusual helical arrangement of three six-membered rings that are all connected at the central carbon atom C6. The helix effectively performs one full turn around C6, and the thread pitch, as defined by the distance of the terminal atoms C2 and C20 of the helix, is 4.98 (3) Å. The angles around C6 are between 104.7 (2) and 115.2 (2)°. The middle ring, a cyclohexa-2,4-dienimine with C6 being the only saturated atom in the ring, is nearly planar with an r.m.s. deviation from the mean plane of only 0.035 Å. The other two rings have conformations best described as between envelope and screw-boat (Boeyens, 1978) with puckering amplitudes of 0.527 (2) and 0.544 (2) Å, respectively (Cremer & Pople, 1975).

The packing of the title compound, illustrated in Figure 3, seems to be dominated by a combination of simple dispersion forces, and weak interactions of the methoxy methyl hydrogen bonds with both neigboring oxygen atoms and aromatic rings. All methoxy groups are involved in at least one C—H···O hydrogen bond or C—H··· π contact, and all aromatic rings act as an acceptor to one or two methoxy CH₃ groups.

Experimental

To a solution of the crown conformer of CTV oxime (10,15-dihydro-2,3,7,8,12,13-hexamethoxy-5*H*-tribenzo[a,d,g]cyclononen-5-oxime, 200 mg, 0.417 mmol) in 4 ml diethyl ether and 1 ml of dichloromethane at 273 K was added thionyl chloride (1.88 g, 15.8 mmol) dropwise over 1 minute. The reaction mixture was stirred for 5 minutes at 273 K, then poured over ice and extracted with methylene chloride. The organic layer was washed successively with saturated aqueous sodium bicarbonate, water and brine, and then dried over sodium sulfate. Concentration gave a residue which was chromatographed on silica gel eluting with ethyl acetate/methylene chloride (30/70) to afford 0.028 g of a solid which was recrystallized from toluene/dichloromethane to give 0.023 g (23%) of the product as red-bronze crystals.

Refinement

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now (Sheldrick, 2004), and the two components were integrated using Saint+ (Bruker, 2003), resulting in a total of 40178 reflections. 12959 reflections (5474 unique) involved component 1 only (mean I/sigma = 5.5), 12616 reflections (5374 unique ones) involved component 2 only (mean I/sigma = 3.7), and 14603 reflections (7998 unique ones) involved both components (mean I/sigma = 6.4). The exact twin matrix identified by the integration program was found to be 0.99876 - 0.00396 - 0.00012, $0.00212 \ 0.99889 \ 0.00875$, $-0.00309 - 0.11163 \ 0.99795$, which is for this structure equivalent to a 180° rotation around the reciprocal axis [1 0 0].

The data were corrected for absorption using Twinabs (Bruker, 2003), and the structure was solved using direct methods with only the non-overlapping reflections of component 1. The structure was refined using the hklf 5 routine with all reflections of component 1 (including the overlapping ones) below a *d*-spacing threshold of 3/4, resulting in a BASF value of 0.312 (2). Due to "twin pairing errors" in Saint+ (equivalent reflections being counted as overlapping for one reflection, but as not overlapping for an eqivalent one) no accurate R_{int} value can be given. This also results in an incomplete merging of equivalent reflections in Twinabs, thus resulting in too many independent reflections. (Herbst-Irmer, 2006)

Hydrogen atoms were added in calculated positions with C—H distances of 0.95, 0.99 and 0.98 Å for aromatic, methylene and methyl H atoms, respectively, and were refined with $U_{iso}(H) = x U_{eq}(C)$ (x = 1.2 for C—H and CH₂, 1.5 for CH₃).

The s.u. values of the cell parameters are taken from the software recognizing that the values are unreasonably small (Herbstein, 2000).

Figures



Fig. 1. Synthesis of the title compound.

Fig. 2. The molecular structure of the title compound with the atomic numbering scheme. Thermal displacement parameters are at the 50% probabilty level.

Fig. 3. Partially expanded packing diagram of the title compound with 50% probability thermal ellipsoids. C—H···O hydrogen bonds are indicated by broken turquoise lines, C—H··· π contacts by dashed blue lines.

2,3,8,12,13-Pentamethoxy-5H-dibenzo[c,n]acridin-7(6H)-one toluene solvate

 $F_{000} = 1144$

 $D_{\rm x} = 1.300 {\rm ~Mg} {\rm ~m}^{-3}$

Cell parameters from 6322 reflections

Mo Kα radiation

 $\lambda = 0.71073 \text{ Å}$

 $\theta = 3.0 - 30.5^{\circ}$

 $\mu = 0.09 \text{ mm}^{-1}$

T = 100 (2) K

 $0.60 \times 0.19 \times 0.09 \text{ mm}$

Rod, red

C₂₆H₂₅NO₆·C₇H₈ $M_r = 539.60$ Monoclinic, $P2_1/c$ Hall symbol: -P 2ybc a = 14.952 (4) Å b = 7.1736 (18) Å c = 25.787 (6) Å $\beta = 94.571$ (7)° V = 2757.1 (12) Å³ Z = 4

Data collection

Bruker SMART APEX CCD diffractometer	10641 independent reflections
Radiation source: fine-focus sealed tube	7887 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = not defined due to twin pairing errors, Herbst- Irmer, 2006
T = 100(2) K	$\theta_{\text{max}} = 28.3^{\circ}$
ω scans	$\theta_{\min} = 1.4^{\circ}$
Absorption correction: multi-scan (TWINABS; Bruker, 2003)	$h = -19 \rightarrow 19$
$T_{\min} = 0.773, T_{\max} = 1.000$	$k = 0 \rightarrow 9$
40178 measured reflections	$l = 0 \rightarrow 34$

Refinement

Refinement on F^2

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.076$$

 $wR(F^2) = 0.199$

S = 1.08

10641 reflections

368 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained $w = 1/[\sigma^2(F_0^2) + (0.0913P)^2 + 1.3281P]$ where $P = (F_0^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 0.67 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{min} = -0.25 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Special details

Experimental. The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, and the two components were integrated using Saint, resulting in a total of 40178 reflections. 12959 reflections (5474 unique ones) involved component 1 only (mean I/sigma = 5.5), 12616 reflections (5374 unique ones) involved component 2 only (mean I/sigma = 3.7), and 14603 reflections (7998 unique ones) involved both components (mean I/sigma = 6.4). The exact twin matrix identified by the integration program was found to be 0.99876 - 0.00396 - 0.00012, $0.00212 \ 0.99889 \ 0.00875$, $-0.00309 - 0.11163 \ 0.99795$.

The data were corrected for absorption using twinabs, and the structure was solved using direct methods with only the non-overlapping reflections of component 1. The structure was refined using the hklf 5 routine with all reflections of component 1 (including the overlapping ones) below a *d*-spacing threshold of 3/4, resulting in a BASF value of 0.312 (2).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2 , conventional *R*-factors *R* are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2 \operatorname{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
C1	0.36910 (14)	0.6758 (3)	0.48902 (8)	0.0190 (4)
H1A	0.3447	0.5551	0.4757	0.023*
H1B	0.4282	0.6947	0.4751	0.023*
C2	0.38116 (14)	0.6689 (3)	0.54776 (8)	0.0202 (4)
C3	0.38050 (14)	0.8509 (3)	0.57581 (8)	0.0193 (4)
C4	0.36991 (14)	1.0121 (3)	0.54819 (8)	0.0192 (4)
H4	0.3771	1.1280	0.5659	0.023*
C5	0.34790 (13)	1.0112 (3)	0.49225 (7)	0.0164 (4)
C6	0.30468 (14)	0.8353 (3)	0.46952 (7)	0.0161 (4)
C7	0.21107 (14)	0.7989 (3)	0.48916 (8)	0.0175 (4)
H7A	0.2157	0.7918	0.5276	0.021*
H7B	0.1696	0.9016	0.4782	0.021*
C8	0.17650 (14)	0.6175 (3)	0.46620 (8)	0.0174 (4)
С9	0.12927 (14)	0.4885 (3)	0.49419 (8)	0.0193 (4)
H9	0.1164	0.5165	0.5288	0.023*
C10	0.10097 (14)	0.3203 (3)	0.47201 (8)	0.0191 (4)
C11	0.11910 (14)	0.2807 (3)	0.42046 (8)	0.0183 (4)
C12	0.16534 (13)	0.4081 (3)	0.39220 (7)	0.0169 (4)
H12	0.1769	0.3814	0.3573	0.020*
C13	0.19494 (13)	0.5765 (3)	0.41539 (7)	0.0165 (4)
C14	0.28966 (13)	0.8315 (3)	0.40988 (7)	0.0156 (4)
C15	0.32871 (13)	0.9817 (3)	0.37944 (7)	0.0159 (4)
C16	0.32393 (13)	0.9731 (3)	0.32478 (7)	0.0159 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A^2)

111.6	0.0070	0.0(70	0.0074	0.010#
HI6	0.2972	0.8679	0.3074	0.019*
C17	0.35782 (13)	1.1168 (3)	0.29594 (8)	0.0160 (4)
C18	0.39549 (13)	1.2758 (3)	0.32219 (8)	0.0167 (4)
C19	0.39815 (13)	1.2865 (3)	0.37567 (8)	0.0172 (4)
H19	0.4221	1.3948	0.3929	0.021*
C20	0.36590 (13)	1.1392 (3)	0.40523 (8)	0.0156 (4)
C21	0.37340 (14)	1.1502 (3)	0.46147 (8)	0.0180 (4)
H21	0.3974	1.2606	0.4774	0.022*
C22	0.41041 (17)	1.0041 (3)	0.65651 (8)	0.0256 (5)
H22A	0.4633	1.0682	0.6452	0.038*
H22B	0.4197	0.9764	0.6938	0.038*
H22C	0.3576	1.0843	0.6501	0.038*
C23	0.05158 (16)	0.2025 (3)	0.55146 (8)	0.0254 (5)
H23A	0.1125	0.2149	0.5681	0.038*
H23B	0.0231	0.0913	0.5649	0.038*
H23C	0.0164	0.3131	0.5590	0.038*
C24	0.09328 (15)	0.0706 (3)	0.34878 (8)	0.0221 (5)
H24A	0.0601	0.1665	0.3281	0.033*
H24B	0.0664	-0.0517	0.3408	0.033*
H24C	0.1560	0.0701	0.3403	0.033*
C25	0.32396 (16)	0.9605 (3)	0.21512 (8)	0.0251 (5)
H25A	0.3573	0.8492	0.2274	0.038*
H25B	0.3303	0.9779	0.1779	0.038*
H25C	0.2604	0.9451	0.2208	0.038*
C26	0.46204 (15)	1.5756 (3)	0.31657 (8)	0.0209 (5)
H26A	0.4142	1.6355	0.3344	0.031*
H26B	0.4837	1.6616	0.2908	0.031*
H26C	0.5116	1.5426	0.3421	0.031*
C27	0.14872 (15)	0.6018 (3)	0.21337 (8)	0.0239 (5)
C28	0.14841 (16)	0.6401 (4)	0.16066 (9)	0.0299 (6)
H28	0.1748	0.5535	0.1385	0.036*
C29	0.11040 (18)	0.8023 (4)	0.13957 (9)	0.0365 (6)
H29	0.1103	0.8252	0.1033	0.044*
C30	0.07272 (17)	0.9308 (4)	0.17138 (10)	0.0335 (6)
H30	0.0471	1.0426	0.1571	0.040*
C31	0.07257 (16)	0.8953 (3)	0.22406 (9)	0.0271 (5)
H31	0.0467	0.9829	0.2461	0.033*
C32	0.11011 (15)	0.7325 (3)	0.24480 (8)	0.0233 (5)
H32	0.1095	0.7094	0.2810	0.028*
C33	0.18935 (19)	0.4249 (4)	0.23630 (10)	0.0384 (6)
H33A	0.2126	0.3497	0.2086	0.058*
H33B	0.1434	0.3541	0.2529	0.058*
H33C	0.2385	0.4561	0.2623	0.058*
N1	0.24151 (11)	0.7050 (2)	0.38542 (6)	0.0174 (4)
01	0.39663 (10)	0.8337 (2)	0.62800 (5)	0.0222 (3)
02	0.35886 (10)	1.1202 (2)	0.24319 (5)	0.0203 (3)
03	0.42770 (10)	1.4094 (2)	0.29075 (5)	0.0210 (3)
04	0.08931 (10)	0.1096 (2)	0.40264 (5)	0.0222 (3)
05	0.05546 (10)	0.1852 (2)	0.49660 (5)	0.0239 (4)
	0.000 10 (10)	0.1002 (2)		0.0207(1)

\lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) \lambda^2) <th>O6</th> <th>0.39527 (12)</th> <th>0.5216 (2)</th> <th>0.571</th> <th>17 (6)</th> <th>0.0308 (4)</th> <th></th>	O6	0.39527 (12)	0.5216 (2)	0.571	17 (6)	0.0308 (4)	
The second constrained and the second secon	Atomic displ	accoment parameters	(λ^2)				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Atomic dispi		(A)	* 33	r 12	z 13	± ²³
C1 0021 (11) 0015 (10) 0021 (10) 00001 (9) 0001 (8) -0001 (8) C2 0019 (11) 0015 (11) 0022 (11) -0003 (9) 0001 (8) -0001 (8) C3 00202 (11) 0019 (11) 00202 (11) -0003 (9) 00018 (8) -0001 (8) C4 00223 (11) 00151 (10) 00204 (10) -0005 (8) 00027 (8) -00030 (8) C6 00193 (10) 00131 (10) 0019 (10) -0005 (8) 00027 (8) -00020 (8) C6 00193 (10) 00131 (10) 00160 (9) -00019 (9) 00018 (8) 00002 (7) C7 00206 (10) 00148 (10) 00176 (10) -00024 (9) 00018 (8) -00029 (8) C8 00168 (10) 00150 (10) 0023 (10) 00002 (9) 00007 (8) -00029 (8) C9 00238 (11) 00180 (10) 00167 (10) -00024 (9) 00027 (8) -00021 (8) C10 00201 (10) 00166 (10) 00207 (10) -00024 (9) 00027 (8) 00000 (8) C12 00187 (10) 00166 (10) 00126 (10) -00033 (9) -00023 (8) 00009 (8) C12 00187 (10) 00166 (10) 00128 (10) -00033 (9) -00023 (8) 00009 (8) C13 00163 (10) 00148 (10) 00182 (10) -00033 (9) -00023 (8) 00009 (8) C14 00160 (10) 00122 (10) 00128 (10) -00003 (9) -00021 (8) 00009 (8) C15 00144 (10) 00124 (10) 00195 (10) -00004 (8) 00027 (7) 00020 (8) C16 00144 (9) 00126 (10) 0027 (10) -00009 (8) 00019 (8) -00021 (8) C17 00138 (10) 00161 (10) 00124 (10) -00003 (8) 00026 (7) 00020 (8) C18 00143 (10) 00144 (10) 00214 (10) -00003 (8) 00024 (7) -00001 (8) C20 00145 (9) 00126 (10) 0024 (10) -00003 (8) 00024 (8) -00022 (8) C19 00161 (10) 00110 (9) 00224 (10) -0003 (8) 00021 (8) -00002 (8) C21 00266 (10) 00113 (9) 00224 (10) -00033 (8) 00022 (8) -00007 (8) C22 00352 (13) 00216 (11) 00226 (11) -00033 (9) 00022 (8) -00007 (8) C23 00396 (12) 00254 (12) 00226 (11) -00039 (9) 00048 (9) 00002 (8) C24 00225 (11) 00230 (11) 00225 (11) -00039 (9) 00048 (9) 00002 (8) C24 00235 (11) 00230 (12) 00275 (12) -00040 (10) 00038 (9) -00038 (9) C24 00235 (11) 00203 (11) 00222 (11) -00039 (9) 00048 (9) 00007 (8) C27 00216 (11) 00134 (10) 00222 (11) -00039 (10) 00032 (8) -00016 (9) C33 00398 (15) 00341 (14) 00012 (12) -00036 (11) 00038 (10) -00038 (7) C10 00296 (8) 00186 (8) 00180 (7) -00089 (7) 00038 (6) -00007 (6) C3 00235 (1) 00166 (8) 00210 (7) -00089 (7) 00038 (6) -000	01	U^{11}	$U^{}$	U^{33}	U^{12}	U^{22}	U^{22}
$\begin{array}{ccccc} 2 & 0.0192 (11) & 0.0185 (11) & 0.022 (11) & -0.0013 (9) & -0.0014 (8) & 0.0001 (8) \\ \hline C3 & 0.0202 (11) & 0.0151 (10) & 0.0204 (10) & -0.0038 (9) & 0.0018 (8) & -0.0023 (8) \\ \hline C4 & 0.0223 (11) & 0.0151 (10) & 0.0193 (10) & -0.0005 (8) & 0.0027 (8) & -0.0036 (8) \\ \hline C5 & 0.0171 (10) & 0.0131 (10) & 0.0160 (9) & -0.0019 (9) & 0.0018 (8) & -0.0022 (8) \\ \hline C7 & 0.0206 (10) & 0.0148 (10) & 0.0176 (10) & -0.0014 (9) & 0.0043 (8) & -0.0029 (8) \\ \hline C8 & 0.0168 (10) & 0.0150 (10) & 0.0203 (10) & 0.0002 (9) & 0.0017 (8) & -0.0009 (8) \\ \hline C9 & 0.0238 (11) & 0.0180 (10) & 0.0167 (10) & -0.0024 (9) & 0.0077 (8) & -0.0009 (8) \\ \hline C10 & 0.0201 (10) & 0.0166 (10) & 0.0207 (10) & -0.0022 (9) & -0.0002 (8) & 0.0009 (8) \\ \hline C12 & 0.0187 (10) & 0.0166 (10) & 0.0224 (10) & -0.0033 (9) & -0.0002 (8) & 0.0009 (8) \\ \hline C13 & 0.0163 (10) & 0.0144 (10) & 0.0182 (10) & -0.0013 (9) & -0.0009 (8) & 0.0007 (8) \\ \hline C14 & 0.0160 (10) & 0.0123 (10) & 0.0187 (10) & -0.0004 (8) & 0.0019 (8) & -0.0022 (8) \\ \hline C15 & 0.0144 (10) & 0.0142 (10) & -0.0031 (9) & -0.0009 (8) & 0.0027 (8) \\ \hline C16 & 0.0145 (10) & 0.0144 (10) & 0.0182 (10) & -0.0004 (8) & 0.0024 (7) & -0.0002 (8) \\ \hline C17 & 0.0138 (10) & 0.0160 (10) & 0.0182 (9) & 0.0013 (8) & 0.0024 (7) & -0.0002 (8) \\ \hline C18 & 0.0143 (10) & 0.0124 (10) & -0.0003 (8) & 0.0022 (8) & 0.0007 (7) \\ \hline C20 & 0.0145 (10) & 0.0113 (9) & 0.0212 (10) & -0.0003 (8) & 0.0022 (8) & -0.0012 (8) \\ \hline C22 & 0.0352 (13) & 0.0216 (11) & 0.0198 (11) & -0.0003 (8) & 0.0022 (8) & -0.0012 (8) \\ \hline C23 & 0.0350 (12) & 0.0224 (12) & -0.0003 (10) & 0.0022 (8) & -0.0012 (8) \\ \hline C24 & 0.0235 (11) & 0.0214 (10) & 0.0222 (11) & -0.0003 (8) & 0.0022 (8) & -0.0012 (8) \\ \hline C24 & 0.0235 (11) & 0.0134 (10) & 0.0223 (11) & -0.0003 (10) & 0.0022 (8) & -0.0012 (9) \\ \hline C34 & 0.0235 (11) & 0.0249 (12) & 0.0203 (11) & -0.0053 (10) & 0.0022 (8) & -0.0012 (9) \\ \hline C33 & 0.0357 (13) & 0.034 (14) & 0.0025 (11) & -0.0003 (10) & 0.0023 (8) & -0.00012 (9) \\ \hline C33 & 0.0357 (13) & 0.034 (14) & 0.0017 (10) & 0.0018 (10) & -0.0003 (10) \\ \hline C33 & 0.$		0.0221 (11)	0.0138 (10)	0.0210 (10)	0.0001 (9)	0.0014 (8)	-0.0018 (8)
C3 00.02 (11) 00.012 (11) 00.012 (10) -00.018 (10) -00.0038 (9) 00.013 (8) -00.013 (8) C4 00.223 (11) 00.0151 (10) 00.204 (10) -00.0138 (9) 00.013 (8) -00.023 (8) C5 00.0171 (10) 00.0131 (10) 00.0160 (9) -0.0019 (9) 00.013 (8) -0.0023 (8) C7 00.206 (10) 00.0144 (10) 00.0160 (9) -0.0019 (9) 00.013 (8) -0.0029 (8) C8 00.0238 (11) 00.0150 (10) 0.0203 (10) 0.0002 (9) 00.017 (8) -0.0029 (8) C10 00.201 (10) 00.0166 (10) 0.0207 (10) -0.0026 (9) 0.0027 (8) 0.0034 (8) C11 00.195 (10) 00.166 (10) 0.0224 (10) -0.0026 (9) 0.0027 (8) 0.0034 (8) C12 00.187 (10) 00.166 (10) 0.0224 (10) -0.0033 (9) -0.0020 (8) 0.0009 (8) C13 00.163 (10) 0.0148 (10) 0.0155 (9) -0.0003 (9) 0.0023 (8) 0.0009 (8) C14 00.160 (10) 0.0123 (10) 0.0187 (10) -0.0004 (8) 0.0019 (8) -0.0021 (8) C15 00.144 (10) 0.0124 (10) 0.0182 (10) -0.0009 (8) 0.0019 (8) -0.0021 (8) C16 00.145 (9) 0.0126 (10) 0.0274 (10) -0.0009 (8) 0.0019 (8) -0.0022 (8) C17 00.138 (10) 0.0144 (10) 0.0182 (10) -0.0009 (8) 0.0019 (8) -0.0022 (8) C18 00.143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) -0.0002 (8) C19 0.0161 (10) 0.0112 (10) 0.0224 (10) -0.0003 (8) 0.0022 (8) -0.0002 (8) C19 0.0161 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0003 (8) 0.0022 (8) -0.0013 (8) C22 0.0352 (13) 0.0216 (11) 0.0182 (10) -0.0013 (8) 0.0022 (8) -0.0013 (8) C22 0.0352 (11) 0.0203 (11) 0.0206 (10) -0.0023 (9) 0.0022 (8) -0.0013 (8) C23 0.0330 (13) 0.0214 (10) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0013 (8) C24 0.0225 (11) 0.0203 (11) 0.0206 (10) -0.0023 (9) 0.0022 (8) -0.0013 (8) C25 0.0330 (13) 0.0214 (10) 0.0226 (11) -0.0039 (10) 0.0022 (8) -0.0014 (8) C25 0.0333 (13) 0.0214 (10) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0014 (8) C25 0.0333 (13) 0.0214 (10) 0.0226 (11) -0.0033 (10) 0.0022 (8) -0.0042 (8) C25 0.0235 (11) 0.0276 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0023 (9) C24 0.0225 (8) 0.0187 (8) 0.0173 (7) -0.0037 (11) 0.0085 (10) -0.0058 (10) C32 0.0255 (8) 0.0187 (8) 0.0173 (7) -0.0058 (7) 0.0005	C2	0.0192 (11)	0.0185 (11)	0.0225 (11)	-0.0013 (9)	-0.0014 (8)	0.0001 (8)
C4 0.023 (11) 0.0151 (10) 0.0020 (10) -0.0038 (9) 0.0021 (8) -0.0028 (8) C5 0.0171 (10) 0.0131 (10) 0.0193 (10) -0.0005 (8) 0.0027 (8) -0.0030 (8) C6 0.0193 (10) 0.0148 (10) 0.0160 (9) -0.0019 (9) 0.0018 (8) -0.0029 (8) C8 0.0168 (10) 0.0150 (10) 0.0203 (10) 0.0002 (9) 0.0017 (8) -0.0009 (8) C9 0.0238 (11) 0.0180 (10) 0.0167 (10) -0.0026 (9) 0.0027 (8) -0.0009 (8) C10 0.0201 (10) 0.0128 (10) 0.0207 (10) -0.0026 (9) 0.0027 (8) 0.0009 (8) C11 0.0195 (10) 0.0128 (10) 0.0224 (10) -0.0023 (9) -0.0002 (8) 0.0009 (8) C12 0.0183 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C13 0.0163 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) 0.0019 (8) 0.0019 (8) -0.0021 (8) C15 0.0144 (10) 0.0144 (10) 0.0187 (10) -0.0004 (8) 0.0026 (7) -0.0002 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0004 (8) 0.0022 (7) -0.0002 (8) C17 0.0138 (10) 0.0146 (10) 0.0182 (9) 0.0013 (8) 0.0024 (7) -0.0001 (8) C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) -0.0022 (8) C19 0.0161 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0002 (8) C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0002 (8) C21 0.0206 (10) 0.0134 (10) 0.0207 (10) -0.003 (8) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.003 (10) 0.0022 (8) -0.0018 (8) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0044 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.003 (10) 0.0022 (8) -0.0014 (8) C25 0.0333 (13) 0.0244 (12) 0.0233 (11) -0.0033 (10) 0.0023 (8) -0.0023 (9) C24 0.0235 (11) 0.0134 (10) 0.0226 (11) -0.0033 (10) 0.0023 (8) -0.00028 (9) C25 0.0336 (13) 0.0244 (12) 0.0226 (11) -0.0033 (10) 0.0028 (10) -0.0038 (10) C30 0.0327 (14) 0.023 (12) 0.0275 (12) -0.0040 (10) 0.0014 (9) -0.0038 (10) C30 0.0327 (14) 0.0271 (2) 0.0198 (9) -0.0025 (7) 0.0038 (7) 0.0005 (1) C31 0.0226 (8) 0.0184 (8) 0.0118 (7) -0.0054 (7) 0.0058 (7) 0.0005 (6) C33 0.0257 (8) 0.0164 (8) 0.0118 (7) -0.0058 (7) 0.0005 (6) -0.0016 (6) C41 0.0331	C3	0.0202 (11)	0.0192 (11)	0.0184 (10)	-0.0038 (9)	0.0018 (8)	-0.0013 (8)
CS 0.0171 (10) 0.0131 (10) 0.019 (10) -0.009 (8) 0.0021 (8) -0.009 (8) C6 0.0193 (10) 0.0131 (10) 0.0160 (9) -0.0019 (9) 0.0018 (8) 0.0002 (7) C7 0.0206 (10) 0.0150 (10) 0.0203 (10) 0.0002 (9) 0.0017 (8) -0.0009 (8) C9 0.0238 (11) 0.0180 (10) 0.0167 (10) -0.0026 (9) 0.0055 (8) -0.0021 (8) C10 0.0201 (10) 0.0166 (10) 0.0207 (10) -0.0026 (9) 0.0027 (8) 0.0004 (8) C11 0.0195 (10) 0.0166 (10) 0.0207 (10) -0.0023 (9) -0.0002 (8) 0.0009 (8) C12 0.0187 (10) 0.0166 (10) 0.0187 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C13 0.0163 (10) 0.0144 (10) 0.0187 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C15 0.0144 (10) 0.0141 (10) 0.0195 (10) -0.0004 (8) 0.0026 (7) 0.0022 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0004 (8) 0.0027 (7) -0.0001 (8) C17 0.0138 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0002 (8) C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0002 (8) C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0216 (11) -0.0003 (8) 0.0022 (8) 0.0007 (7) C22 0.0352 (13) 0.0216 (11) 0.0226 (11) -0.003 (8) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0226 (11) -0.003 (9) 0.0022 (8) -0.0018 (8) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0039 (9) 0.0042 (9) -0.0048 (9) C24 0.0235 (11) 0.0230 (11) 0.0226 (11) -0.0039 (9) 0.0042 (9) -0.0048 (9) C25 0.0303 (13) 0.249 (12) 0.0225 (11) -0.0039 (9) 0.0048 (9) 0.0007 (8) C27 0.0211 (1) 0.0233 (12) 0.0225 (11) -0.0039 (9) 0.0048 (9) 0.0007 (8) C26 0.0236 (11) 0.0143 (10) 0.0225 (12) -0.0040 (10) 0.0018 (9) -0.0043 (9) C33 0.0397 (14) 0.0270 (12) 0.0194 (10) -0.0023 (10) -0.0038 (12) -0.0043 (9) C33 0.0398 (15) 0.0315 (14) 0.0427 (15) 0.0056 (13) 0.0085 (12) -0.0043 (12) N1 0.0189 (9) 0.0146 (8) 0.0180 (7) -0.0051 (7) 0.0046 (10) -0.0023 (8) C10 0.0255 (8) 0.0188 (8) 0.0180 (7) -0.0054 (7) 0.0056 (6) -0.0007 (6) C3 0.0257 (8) 0.0	C4	0.0223 (11)	0.0151 (10)	0.0204 (10)	-0.0038 (9)	0.0031 (8)	-0.0028 (8)
C6 0.0131 (10) 0.0131 (10) 0.0131 (10) 0.0130 (10) -0.0010 (9) 0.0013 (8) 0.0002 (7) C7 0.0206 (10) 0.0144 (10) 0.0176 (10) -0.0014 (9) 0.0043 (8) -0.0029 (8) C8 0.0168 (10) 0.0150 (10) 0.0023 (10) -0.0026 (9) 0.0027 (8) -0.0021 (8) C10 0.0201 (10) 0.0166 (10) 0.0224 (10) -0.0026 (9) -0.0022 (8) 0.0009 (8) C11 0.0195 (10) 0.0128 (10) -0.013 (9) -0.0021 (8) 0.0009 (8) C12 0.0187 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0021 (8) -0.0021 (8) C14 0.0163 (10) 0.0148 (10) 0.0187 (10) -0.0014 (8) -0.0021 (8) C15 0.0144 (10) 0.0195 (10) -0.0004 (8) 0.0022 (7) -0.0018 (8) C17 0.0138 (10) 0.0144 (10) 0.0214 (10) -0.0001 (8) 0.0022 (8) -0.0002 (8) C17 0.0138 (10) 0.0141 (10) 0.0214 (10) -0.0013 (8) 0.0011 (8) 0.00022 (8) 0.0022 (8) 0	C5	0.0171 (10)	0.0131 (10)	0.0193 (10)	-0.0005 (8)	0.0027 (8)	-0.0030 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.0193 (10)	0.0131 (10)	0.0160 (9)	-0.0019 (9)	0.0018 (8)	0.0002 (7)
C8 0.018 (10) 0.0150 (10) 0.0203 (10) 0.0002 (9) 0.0017 (8) -0.0009 (8) C9 0.0233 (11) 0.0180 (10) 0.0167 (10) -0.0026 (9) 0.0057 (8) 0.0003 (8) C10 0.0201 (10) 0.0128 (10) 0.0224 (10) -0.0032 (9) -0.0022 (8) 0.0009 (8) C12 0.0187 (10) 0.0166 (10) 0.0126 (9) -0.0003 (9) 0.0002 (8) 0.0009 (8) C12 0.0187 (10) 0.0166 (10) 0.0126 (10) -0.0013 (9) -0.0003 (8) 0.0009 (8) C13 0.0163 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) -0.0019 (8) 0.0027 (7) 0.0020 (8) C15 0.0144 (10) 0.0141 (10) 0.0195 (10) -0.0004 (8) 0.0025 (7) 0.0020 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0004 (8) 0.0025 (7) -0.0002 (8) C17 0.0138 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) -0.0002 (8) C18 0.0143 (10) 0.0160 (10) 0.0121 (10) -0.0003 (8) 0.0022 (8) 0.0002 (8) C19 0.0161 (10) 0.0114 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0128 (11) -0.0023 (9) 0.0022 (8) -0.0018 (8) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0013 (10) 0.0048 (9) -0.0028 (9) C24 0.0235 (11) 0.0203 (11) 0.0225 (11) -0.0039 (10) 0.0022 (8) -0.0018 (8) C25 0.0303 (13) 0.0249 (12) 0.0206 (11) -0.0039 (10) 0.0022 (8) -0.0042 (8) C27 0.0211 (11) 0.0230 (11) 0.0225 (11) -0.0039 (10) 0.0022 (8) -0.0032 (9) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0039 (10) 0.0025 (9) -0.0032 (9) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0039 (10) 0.0025 (9) -0.0032 (9) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0039 (10) 0.0025 (9) -0.0032 (9) C26 0.0236 (11) 0.0210 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0003 (10) C28 0.0273 (13) 0.034 (14) 0.0325 (11) -0.0039 (10) 0.0003 (10) -0.0058 (10) C32 0.0236 (11) 0.0270 (13) 0.0430 (12) -0.0003 (11) 0.0008 (10) -0.0058 (10) C32 0.0255 (8) 0.0187 (8) 0.0173 (7) -0.0058 (7) 0.0003 (7) 0.0005 (7) O1 0.0225 (8) 0.0186 (8) 0.0110 (7) -0.0058 (7) 0.0003 (7) 0.0005 (7) O1 0.0255 (8) 0.0186 (8) 0.0210 (7) -0.0058 (7) 0.0005 (6) -0.0002 (6) C3 0	C7	0.0206 (10)	0.0148 (10)	0.0176 (10)	-0.0014 (9)	0.0043 (8)	-0.0029 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.0168 (10)	0.0150 (10)	0.0203 (10)	0.0002 (9)	0.0017 (8)	-0.0009 (8)
C10 0.020 (10) 0.0166 (10) 0.0207 (10) -0.0026 (9) 0.0027 (8) 0.0027 (8) C11 0.0195 (10) 0.0128 (10) 0.0224 (10) -0.0032 (9) -0.0002 (8) 0.0009 (8) C12 0.0187 (10) 0.0166 (10) 0.0156 (9) -0.0003 (9) 0.0023 (8) 0.0009 (8) C13 0.0163 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) 0.0019 (8) 0.0009 (8) -0.0021 (8) C15 0.0144 (10) 0.0141 (10) 0.0195 (10) -0.0004 (8) 0.0026 (7) 0.0002 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0009 (8) 0.0191 (8) -0.0002 (8) C17 0.0138 (10) 0.0160 (10) 0.0121 (10) -0.0003 (8) 0.0025 (8) 0.0022 (8) C19 0.0161 (10) 0.0114 (10) 0.0214 (10) -0.0033 (8) 0.0025 (8) 0.0022 (8) C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0030 (10) 0.0022 (8) -0.0048 (9) C24 0.0235 (11) 0.0203 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0330 (13) 0.0249 (12) 0.0203 (11) -0.0060 (10) 0.0022 (8) -0.0042 (8) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C27 0.0211 (11) 0.0230 (12) 0.0275 (12) -0.0030 (10) 0.0022 (8) -0.0042 (8) C28 0.0273 (13) 0.0344 (14) 0.0301 (12) -0.0030 (10) 0.0023 (8) -0.0032 (9) C28 0.0273 (13) 0.0345 (14) 0.0301 (12) -0.0030 (11) 0.0088 (10) -0.0058 (10) C33 0.0327 (14) 0.0270 (13) 0.0443 (14) 0.0006 (12) -0.0077 (11) 0.0076 (11) C31 0.0268 (12) 0.0220 (12) 0.0323 (12) 0.0025 (7) 0.0038 (7) 0.0003 (8) -0.0005 (7) C10 0.0255 (8) 0.0187 (8) 0.0173 (7) -0.0054 (7) 0.0038 (7) 0.0005 (7) C13 0.0255 (8) 0.0187 (8) 0.0173 (7) -0.0054 (7) 0.0058 (6) -0.00027 (10) C32 0.0255 (8) 0.0187 (8) 0.0210 (7) -0.0058 (7) 0.0046 (6) -0.0021 (6) C4 0.0301 (9) 0.0165 (8) 0.0210 (7) -0.0058 (7) 0.0046 (6) -0.0021 (6) C4 0.0321 (9) 0.0165 (8) 0.0214 (7) -0.0058 (7) 0.0046 (6) -0.0	C9	0.0238 (11)	0.0180 (10)	0.0167 (10)	-0.0026 (9)	0.0065 (8)	-0.0021 (8)
C11 0.0195 (10) 0.0128 (10) 0.0224 (10) -0.0032 (9) -0.0002 (8) 0.0000 (8) C12 0.0187 (10) 0.0166 (10) 0.0156 (9) -0.0003 (9) 0.0023 (8) 0.0009 (8) C13 0.0163 (10) 0.0148 (10) 0.0187 (10) 0.0019 (8) 0.0023 (8) 0.0009 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) 0.0019 (8) 0.0026 (7) 0.0022 (8) C15 0.0144 (10) 0.0126 (10) 0.0207 (10) -0.0009 (8) 0.0019 (8) -0.0002 (8) C16 0.0145 (9) 0.0126 (10) 0.0217 (10) -0.0009 (8) 0.0019 (8) -0.0002 (8) C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0022 (7) -0.0000 (8) C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0022 (8) C19 0.0161 (10) 0.0113 (9) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0113 (9) 0.0224 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0048 (9) 0.0022 (8) C24 0.0235 (11) 0.0230 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0032 (9) C24 0.0235 (11) 0.0230 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0032 (9) C25 0.0333 (13) 0.0249 (12) 0.0273 (12) -0.0040 (10) 0.0012 (9) -0.0032 (9) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0030 (10) 0.0022 (8) -0.0003 (10) C27 0.0211 (11) 0.0230 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0032 (9) C28 0.0273 (13) 0.034 (14) 0.0023 (12) -0.0016 (13) 0.0048 (10) -0.0005 (10) C33 0.0327 (14) 0.0270 (13) 0.0403 (14) 0.0006 (12) -0.0007 (11) 0.0076 (11) C31 0.0268 (12) 0.0220 (12) 0.0323 (12) 0.0001 (10) 0.0013 (10) -0.0058 (10) C32 0.0255 (8) 0.0187 (8) 0.0173 (7) -0.0058 (7) 0.0038 (7) 0.0005 (7) O1 0.0296 (8) 0.0187 (8) 0.0173 (7) -0.0054 (7) 0.0038 (7) 0.0005 (7) O1 0.0296 (8) 0.0186 (8) 0.0180 (7) -0.0058 (7) 0.00038 (7) 0.00056 (7) O1 0.0296 (8) 0.0187 (8) 0.0210 (7) -0.0058 (7) 0.0040 (6) -0.0021 (6) O5 0.0332 (9) 0.0193 (8) 0.0212 (7) -0.0089 (7) 0.0048 (6) -0.0012 (6) O5 0.0323 (9) 0.0193 (8) 0.0212 (7) -0.0058 (7) 0.0048 (6) -0.0016 (6) O4 0.031 (9) 0.016	C10	0.0201 (10)	0.0166 (10)	0.0207 (10)	-0.0026 (9)	0.0027 (8)	0.0034 (8)
C12 0.0187 (10) 0.0166 (10) 0.0156 (9) -0.0003 (9) 0.0023 (8) 0.0009 (8) C13 0.0163 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0166 (10) 0.0123 (10) 0.0187 (10) 0.0019 (8) 0.0026 (7) 0.0020 (8) C15 0.0144 (10) 0.0126 (10) 0.0207 (10) -0.0009 (8) 0.0019 (8) -0.0021 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0009 (8) 0.0024 (7) -0.0001 (8) C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0022 (8) -0.0022 (8) C19 0.0161 (10) 0.0114 (10) 0.0214 (10) -0.0003 (8) 0.0022 (8) 0.0022 (8) C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0023 (9) 0.0022 (8) -0.0018 (8) C23 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C24 0.0235 (11) 0.0234 (12) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C26 0.0236 (11) 0.0133 (10) 0.0222 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0230 (11) -0.0060 (10) 0.0023 (9) -0.0032 (9) C26 0.0236 (11) 0.0133 (10) 0.0252 (11) -0.0039 (10) 0.0028 (9) -0.0013 (9) C28 0.0273 (13) 0.0334 (14) 0.0301 (12) -0.0060 (10) 0.0018 (9) -0.0018 (9) C29 0.0406 (15) 0.0467 (16) 0.0224 (12) -0.0016 (13) 0.0046 (10) 0.0100 (11) C30 0.0327 (14) 0.0270 (12) 0.0125 (12) -0.00016 (13) 0.0046 (10) 0.0108 (10) C31 0.0268 (12) 0.0220 (12) 0.0323 (12) 0.0001 (10) 0.0013 (10) -0.0058 (10) C32 0.0235 (11) 0.0216 (13) 0.0403 (14) 0.0006 (12) -0.0007 (11) 0.0076 (11) C31 0.0268 (12) 0.0220 (12) 0.0134 (10) -0.0025 (7) 0.0038 (7) 0.0005 (7) O1 0.0268 (8) 0.0186 (8) 0.0180 (7) -0.0025 (7) 0.0038 (7) 0.0005 (7) O1 0.0257 (8) 0.0187 (8) 0.0173 (7) -0.0058 (7) 0.0003 (6) -0.0002 (6) O2 0.0255 (8) 0.0187 (8) 0.0121 (7) -0.0058 (7) 0.0038 (6) -0.0007 (6) O3 0.0257 (8) 0.0187 (8) 0.0121 (7) -0.0058 (7) 0.0038 (6) -0.0002 (6) O4 0.0301 (9) 0.0165 (8) 0.0204 (7) -0.0058 (7) 0.0038 (6) -0.0002 (6)	C11	0.0195 (10)	0.0128 (10)	0.0224 (10)	-0.0032 (9)	-0.0002 (8)	0.0000 (8)
C13 0.0163 (10) 0.0148 (10) 0.0182 (10) -0.0013 (9) -0.0009 (8) 0.0027 (8) C14 0.0160 (10) 0.0123 (10) 0.0187 (10) 0.0019 (8) 0.0019 (8) -0.0021 (8) C15 0.0144 (10) 0.0141 (10) 0.0195 (10) -0.0004 (8) 0.0026 (7) 0.0020 (8) C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.0009 (8) 0.0019 (8) -0.0002 (8) C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0025 (8) 0.0022 (8) C19 0.0161 (10) 0.0110 (9) 0.0245 (10) -0.0003 (8) 0.0022 (8) 0.0002 (8) C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0023 (9) 0.0022 (8) -0.0018 (8) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0044 (9) -0.0048 (9) C24 0.0235 (11) 0.0203 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0225 (11) -0.0039 (10) 0.0022 (8) -0.0042 (8) C26 0.0235 (11) 0.0143 (10) 0.0225 (11) -0.0039 (10) 0.0022 (9) -0.0032 (9) C26 0.0235 (11) 0.0143 (10) 0.0252 (11) -0.0039 (10) 0.0022 (9) -0.0032 (9) C26 0.0235 (11) 0.0143 (10) 0.0252 (11) -0.0039 (10) 0.0022 (9) -0.0032 (9) C28 0.0273 (13) 0.0334 (14) 0.0301 (12) -0.0040 (10) 0.0018 (9) -0.0058 (10) C29 0.0406 (15) 0.0467 (16) 0.0224 (12) -0.0016 (13) 0.0044 (9) -0.0058 (10) C29 0.0406 (15) 0.0467 (16) 0.0224 (12) -0.0003 (11) 0.0088 (10) -0.0058 (10) C30 0.0327 (14) 0.0270 (13) 0.0403 (14) 0.0006 (12) -0.0007 (11) 0.0076 (11) C31 0.0226 (12) 0.0131 (10) -0.0058 (13) 0.0048 (10) -0.0058 (10) C32 0.0235 (11) 0.0270 (12) 0.0198 (9) -0.0025 (7) 0.0038 (7) 0.0005 (7) O1 0.0296 (8) 0.0186 (8) 0.0180 (7) -0.0058 (7) 0.00006 (6) -0.0007 (6) C3 0.0327 (14) 0.0270 (12) 0.0198 (9) -0.0052 (7) 0.0038 (7) 0.0005 (6) C4 0.0255 (8) 0.0186 (8) 0.0180 (7) -0.0058 (7) 0.0005 (6) -0.0007 (6) C3 0.0257 (8) 0.0193 (8) 0.0212 (7) -0.0058 (7) 0.0004 (6) -0.0007 (6) C4 0.0255 (8) 0.0186 (8) 0.0282 (9) -0.0052 (7) 0.0085 (6) 0.00016 (6) C4 0.0321	C12	0.0187 (10)	0.0166 (10)	0.0156 (9)	-0.0003 (9)	0.0023 (8)	0.0009 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13	0.0163 (10)	0.0148 (10)	0.0182 (10)	-0.0013 (9)	-0.0009 (8)	0.0027 (8)
C15 0.0144 (10) 0.0141 (10) 0.0195 (10) -0.0004 (8) 0.0026 (7) 0.0020 (8) C16 0.0145 (9) 0.0166 (10) 0.0207 (10) -0.0009 (8) 0.0019 (8) -0.0002 (8) C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0024 (7) -0.0001 (8) C18 0.0143 (10) 0.0114 (10) 0.0212 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0023 (9) 0.0022 (8) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0044 (9) -0.0042 (8) C24 0.0235 (11) 0.0203 (11) -0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0231 (11) -0.0030 (10) 0.0021 (8) -0.0001 (9) C26 0.0236 (11) 0.0143 (10)	C14	0.0160 (10)	0.0123 (10)	0.0187 (10)	0.0019 (8)	0.0019 (8)	-0.0021 (8)
C16 0.0145 (9) 0.0126 (10) 0.0207 (10) -0.009 (8) 0.0019 (8) -0.0002 (8) C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0024 (7) -0.0001 (8) C18 0.0143 (10) 0.0144 (10) 0.0245 (10) -0.0013 (8) 0.0022 (8) 0.0022 (8) C19 0.0161 (10) 0.0113 (9) 0.0245 (10) -0.003 (8) 0.0022 (8) -0.0018 (8) C20 0.0145 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0048 (9) 0.0022 (9) C24 0.0235 (11) 0.0203 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0203 (11) -0.0030 (10) 0.0022 (9) -0.0021 (9) C24 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0039 (9) 0	C15	0.0144 (10)	0.0141 (10)	0.0195 (10)	-0.0004 (8)	0.0026 (7)	0.0020 (8)
C17 0.0138 (10) 0.0160 (10) 0.0182 (9) 0.0013 (8) 0.0024 (7) -0.0001 (8) C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0025 (8) 0.0022 (8) C19 0.0161 (10) 0.0113 (9) 0.0245 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0023 (9) 0.0022 (8) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0048 (9) 0.0028 (9) C24 0.0235 (11) 0.0230 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0203 (11) -0.0060 (10) 0.0025 (9) -0.0032 (9) C24 0.0235 (11) 0.0230 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0017 (8) C27 0.0211 (11) 0.0230 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0016 (13) C28 0.027	C16	0.0145 (9)	0.0126 (10)	0.0207 (10)	-0.0009 (8)	0.0019 (8)	-0.0002 (8)
C18 0.0143 (10) 0.0144 (10) 0.0214 (10) -0.0003 (8) 0.0025 (8) 0.0022 (8) C19 0.0161 (10) 0.0110 (9) 0.0245 (10) -0.0013 (8) 0.0011 (8) 0.0005 (8) C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) -0.0018 (8) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0224 (12) 0.0206 (11) -0.011 (10) 0.0048 (9) 0.0022 (8) C24 0.0235 (11) 0.0203 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.303 (13) 0.0249 (12) 0.0203 (11) -0.0060 (10) 0.0025 (9) -0.0042 (8) C27 0.0211 (11) 0.0230 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0007 (8) C38 0.0273 (13) 0.0346 (14) 0.0301 (12) -0.0003 (11) 0.0088 (10) -0.0001 (9) 0.018 (9) -0.0058 (10)	C17	0.0138 (10)	0.0160 (10)	0.0182 (9)	0.0013 (8)	0.0024 (7)	-0.0001 (8)
C190.0161 (10)0.0110 (9)0.0245 (10)-0.0013 (8)0.0011 (8)0.0005 (8)C200.0145 (10)0.0113 (9)0.0212 (10)-0.0003 (8)0.0022 (8)0.0007 (7)C210.0206 (10)0.0134 (10)0.0200 (10)-0.0023 (9)0.0022 (8)-0.0018 (8)C220.0352 (13)0.0216 (11)0.0198 (11)-0.0029 (11)0.0004 (9)-0.0048 (9)C230.0306 (12)0.0254 (12)0.0206 (11)-0.0101 (10)0.0048 (9)0.0028 (9)C240.0235 (11)0.0203 (11)0.0226 (11)-0.0030 (10)0.0022 (8)-0.0042 (8)C250.0303 (13)0.0249 (12)0.023 (11)-0.0060 (10)0.0025 (9)-0.0042 (9)C260.0236 (11)0.0143 (10)0.0252 (11)-0.0039 (9)0.0048 (9)0.0007 (8)C270.0211 (11)0.0230 (12)0.0275 (12)-0.0040 (10)0.0018 (9)-0.0058 (10)C280.0273 (13)0.0334 (14)0.0301 (12)-0.0003 (11)0.0088 (10)-0.0058 (10)C300.0327 (14)0.0270 (13)0.0403 (14)0.0066 (12)-0.0007 (11)0.0076 (11)C310.0268 (12)0.0220 (12)0.0323 (12)0.0001 (10)0.0013 (10)-0.0058 (10)C320.0235 (11)0.0270 (12)0.0194 (10)-0.0025 (7)0.0038 (7)0.0005 (7)C310.0268 (12)0.0210 (7)-0.0025 (7)0.0038 (7)0.0005 (7)0.0016 (1)C320.0235 (11)0.0270 (12)0.0194 (10) <td>C18</td> <td>0.0143 (10)</td> <td>0.0144 (10)</td> <td>0.0214 (10)</td> <td>-0.0003 (8)</td> <td>0.0025 (8)</td> <td>0.0022 (8)</td>	C18	0.0143 (10)	0.0144 (10)	0.0214 (10)	-0.0003 (8)	0.0025 (8)	0.0022 (8)
C20 0.0145 (10) 0.0113 (9) 0.0212 (10) -0.0003 (8) 0.0022 (8) 0.0007 (7) C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0022 (8) -0.0042 (8) C24 0.0235 (11) 0.0203 (11) 0.0262 (11) -0.0030 (10) 0.0025 (9) -0.0032 (9) C26 0.0303 (13) 0.0249 (12) 0.0203 (11) -0.0060 (10) 0.0018 (9) -0.0002 (8) C27 0.0211 (11) 0.0133 (12) 0.0275 (12) -0.0040 (10) 0.0018 (9) -0.0007 (8) C27 0.0211 (11) 0.0133 (12) 0.0077 (13) 0.0403 (12) -0.003 (11) 0.0088 (10) -0.0058 (10) C28 0.0273 (13) 0.0467 (16) 0.0224 (12) -0.0016 (13) 0.0046 (10) 0.0100 (11) C30 0.327 (14) 0.0270 (12) 0.0194 (10) -0.0027 (11) 0.0076 (11) C31 <	C19	0.0161 (10)	0.0110 (9)	0.0245 (10)	-0.0013 (8)	0.0011 (8)	0.0005 (8)
C21 0.0206 (10) 0.0134 (10) 0.0200 (10) -0.0023 (9) 0.0022 (8) -0.0018 (8) C22 0.0352 (13) 0.0216 (11) 0.0198 (11) -0.0029 (11) 0.0004 (9) -0.0048 (9) C23 0.0306 (12) 0.0254 (12) 0.0206 (11) -0.0101 (10) 0.0048 (9) 0.0022 (8) C24 0.0235 (11) 0.0203 (11) 0.0226 (11) -0.0030 (10) 0.0022 (8) -0.0042 (8) C25 0.0303 (13) 0.0249 (12) 0.0203 (11) -0.0030 (10) 0.0025 (9) -0.0032 (9) C26 0.0236 (11) 0.0143 (10) 0.0252 (11) -0.0039 (9) 0.0048 (9) 0.0007 (8) C27 0.0211 (11) 0.0230 (12) 0.0275 (12) -0.0043 (10) 0.0018 (9) -0.00058 (10) C28 0.0273 (13) 0.0344 (14) 0.0301 (12) -0.0003 (11) 0.0018 (10) -0.0058 (10) C29 0.406 (15) 0.467 (16) 0.0224 (12) -0.0016 (13) 0.0046 (10) 0.0100 (11) C30 0.327 (14) 0.0270 (12) 0.0194 (10) -0.0023 (8) -0.0005 (11) <t< td=""><td>C20</td><td>0.0145 (10)</td><td>0.0113 (9)</td><td>0.0212 (10)</td><td>-0.0003 (8)</td><td>0.0022 (8)</td><td>0.0007 (7)</td></t<>	C20	0.0145 (10)	0.0113 (9)	0.0212 (10)	-0.0003 (8)	0.0022 (8)	0.0007 (7)
C22 $0.0352 (13)$ $0.0216 (11)$ $0.0198 (11)$ $-0.0029 (11)$ $0.0004 (9)$ $-0.0048 (9)$ C23 $0.0306 (12)$ $0.0254 (12)$ $0.0206 (11)$ $-0.0101 (10)$ $0.0048 (9)$ $0.0028 (9)$ C24 $0.0235 (11)$ $0.0203 (11)$ $0.0226 (11)$ $-0.0030 (10)$ $0.0022 (8)$ $-0.0042 (8)$ C25 $0.0303 (13)$ $0.0249 (12)$ $0.0203 (11)$ $-0.0060 (10)$ $0.0025 (9)$ $-0.0032 (9)$ C26 $0.0236 (11)$ $0.0143 (10)$ $0.0252 (11)$ $-0.0039 (9)$ $0.0048 (9)$ $0.0007 (8)$ C27 $0.0211 (11)$ $0.0230 (12)$ $0.0275 (12)$ $-0.0040 (10)$ $0.0018 (9)$ $-0.0001 (9)$ C28 $0.0273 (13)$ $0.0334 (14)$ $0.0301 (12)$ $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 $0.0406 (15)$ $0.0467 (16)$ $0.0224 (12)$ $-0.0016 (13)$ $0.0048 (10)$ $0.0100 (11)$ C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ <td< td=""><td>C21</td><td>0.0206 (10)</td><td>0.0134 (10)</td><td>0.0200 (10)</td><td>-0.0023 (9)</td><td>0.0022 (8)</td><td>-0.0018 (8)</td></td<>	C21	0.0206 (10)	0.0134 (10)	0.0200 (10)	-0.0023 (9)	0.0022 (8)	-0.0018 (8)
C23 0.0306 (12) 0.0254 (12) 0.0206 (11) $-0.0101 (10)$ 0.0048 (9) 0.0028 (9) C24 0.0235 (11) 0.0203 (11) 0.0226 (11) $-0.0030 (10)$ 0.0022 (8) $-0.0042 (8)$ C25 0.0303 (13) 0.0249 (12) 0.0203 (11) $-0.0060 (10)$ 0.0025 (9) $-0.0032 (9)$ C26 0.0236 (11) 0.0143 (10) 0.0252 (11) $-0.0039 (9)$ 0.0048 (9) $0.0007 (8)$ C27 0.0211 (11) 0.0230 (12) 0.0275 (12) $-0.0040 (10)$ $0.0018 (9)$ $-0.0001 (9)$ C28 0.0273 (13) 0.0334 (14) 0.0301 (12) $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 0.0406 (15) 0.0467 (16) 0.0224 (12) $-0.0016 (13)$ $0.0007 (11)$ $0.0076 (11)$ C30 0.0327 (14) 0.0270 (13) 0.0403 (14) $0.0001 (10)$ $0.0101 (11)$ C31 0.0268 (12) 0.0220 (12) 0.0323 (12) $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 0.0325 (11) 0.0270 (12) 0.0194 (10) $-0.0025 (7)$ $0.0038 (7)$ $0.0010 (9)$	C22	0.0352 (13)	0.0216 (11)	0.0198 (11)	-0.0029 (11)	0.0004 (9)	-0.0048 (9)
C24 $0.0235 (11)$ $0.0203 (11)$ $0.0226 (11)$ $-0.0030 (10)$ $0.0022 (8)$ $-0.0042 (8)$ C25 $0.0303 (13)$ $0.0249 (12)$ $0.0203 (11)$ $-0.0060 (10)$ $0.0025 (9)$ $-0.0032 (9)$ C26 $0.0236 (11)$ $0.0143 (10)$ $0.0252 (11)$ $-0.0039 (9)$ $0.0048 (9)$ $0.0007 (8)$ C27 $0.0211 (11)$ $0.0230 (12)$ $0.0275 (12)$ $-0.0040 (10)$ $0.0018 (9)$ $-0.0001 (9)$ C28 $0.0273 (13)$ $0.0334 (14)$ $0.0301 (12)$ $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 $0.0406 (15)$ $0.0467 (16)$ $0.0224 (12)$ $-0.0016 (13)$ $0.0046 (10)$ $0.0100 (11)$ C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0225 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0003 (6)$ $-0.0002 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0210 (7)$ $-0.0054 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$	C23	0.0306 (12)	0.0254 (12)	0.0206 (11)	-0.0101 (10)	0.0048 (9)	0.0028 (9)
C25 $0.0303 (13)$ $0.0249 (12)$ $0.0203 (11)$ $-0.0060 (10)$ $0.0025 (9)$ $-0.0032 (9)$ C26 $0.0236 (11)$ $0.0143 (10)$ $0.0252 (11)$ $-0.0039 (9)$ $0.0048 (9)$ $0.0007 (8)$ C27 $0.0211 (11)$ $0.0230 (12)$ $0.0275 (12)$ $-0.0040 (10)$ $0.018 (9)$ $-0.0001 (9)$ C28 $0.0273 (13)$ $0.0334 (14)$ $0.0301 (12)$ $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 $0.0406 (15)$ $0.0467 (16)$ $0.0224 (12)$ $-0.0016 (13)$ $0.0046 (10)$ $0.0100 (11)$ C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0000 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0005 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0193 (8)$ 0.021	C24	0.0235 (11)	0.0203 (11)	0.0226 (11)	-0.0030 (10)	0.0022 (8)	-0.0042 (8)
C260.0236 (11)0.0143 (10)0.0252 (11) $-0.0039 (9)$ 0.0048 (9)0.0007 (8)C270.0211 (11)0.0230 (12)0.0275 (12) $-0.0040 (10)$ 0.0018 (9) $-0.0001 (9)$ C280.0273 (13)0.0334 (14)0.0301 (12) $-0.0003 (11)$ 0.0088 (10) $-0.0058 (10)$ C290.0406 (15)0.0467 (16)0.0224 (12) $-0.0016 (13)$ 0.0046 (10)0.0100 (11)C300.0327 (14)0.0270 (13)0.0403 (14)0.0006 (12) $-0.0007 (11)$ 0.0076 (11)C310.0268 (12)0.0220 (12)0.0323 (12)0.0001 (10)0.0013 (10) $-0.0058 (10)$ C320.0235 (11)0.0270 (12)0.0194 (10) $-0.0029 (10)$ 0.0023 (8) $-0.0010 (9)$ C330.0398 (15)0.0315 (14)0.0447 (15)0.0056 (13)0.0085 (12)0.0043 (12)N10.0189 (9)0.0140 (9)0.0198 (9) $-0.0025 (7)$ 0.0038 (7)0.0002 (6)O20.0257 (8)0.0187 (8)0.0173 (7) $-0.0054 (7)$ 0.0050 (6) $-0.0021 (6)$ O30.0257 (8)0.0169 (8)0.0210 (7) $-0.0082 (7)$ 0.0040 (6) $-0.0021 (6)$ O40.0301 (9)0.0165 (8)0.0212 (7) $-0.0089 (7)$ 0.0085 (6)0.0006 (6)O50.0323 (9)0.0193 (8)0.0212 (7) $-0.0089 (7)$ 0.0085 (6)0.0004 (7)C1=-C21.512 (3)C19, H19 $-0.0050 (8)$ $-0.0069 (7)$ 0.0044 (7)	C25	0.0303 (13)	0.0249 (12)	0.0203 (11)	-0.0060 (10)	0.0025 (9)	-0.0032 (9)
C27 $0.0211 (11)$ $0.0230 (12)$ $0.0275 (12)$ $-0.0040 (10)$ $0.0018 (9)$ $-0.0001 (9)$ C28 $0.0273 (13)$ $0.0334 (14)$ $0.0301 (12)$ $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 $0.0406 (15)$ $0.0467 (16)$ $0.0224 (12)$ $-0.0016 (13)$ $0.0046 (10)$ $0.0100 (11)$ C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0296 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0000 (6)$ $-0.0002 (6)$ O2 $0.0257 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0050 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0165 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0173 (8)$ $0.0212 (7)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$ Geometric parameters (\hat{A}, \circ) $(1512 (3))$ $(19$	C26	0.0236 (11)	0.0143 (10)	0.0252 (11)	-0.0039 (9)	0.0048 (9)	0.0007 (8)
C28 $0.0273 (13)$ $0.0334 (14)$ $0.0301 (12)$ $-0.0003 (11)$ $0.0088 (10)$ $-0.0058 (10)$ C29 $0.0406 (15)$ $0.0467 (16)$ $0.0224 (12)$ $-0.0016 (13)$ $0.0046 (10)$ $0.0100 (11)$ C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0296 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0000 (6)$ $-0.0002 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0050 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0165 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0044 (7)$ Geometric parameters $(\hat{A}, °)$ $(1512 (3))$ $C19, H19$ $-0.0069 (7)$ $0.0044 (7)$	C27	0.0211 (11)	0.0230 (12)	0.0275 (12)	-0.0040 (10)	0.0018 (9)	-0.0001 (9)
C29 $0.0406(15)$ $0.0467(16)$ $0.0224(12)$ $-0.0016(13)$ $0.0046(10)$ $0.0100(11)$ C30 $0.0327(14)$ $0.0270(13)$ $0.0403(14)$ $0.0006(12)$ $-0.0007(11)$ $0.0076(11)$ C31 $0.0268(12)$ $0.0220(12)$ $0.0323(12)$ $0.0001(10)$ $0.0013(10)$ $-0.0058(10)$ C32 $0.0235(11)$ $0.0270(12)$ $0.0194(10)$ $-0.0029(10)$ $0.0023(8)$ $-0.0010(9)$ C33 $0.0398(15)$ $0.0315(14)$ $0.0447(15)$ $0.0056(13)$ $0.0085(12)$ $0.0043(12)$ N1 $0.0189(9)$ $0.0140(9)$ $0.0198(9)$ $-0.0025(7)$ $0.0038(7)$ $0.0005(7)$ O1 $0.0296(8)$ $0.0186(8)$ $0.0180(7)$ $-0.0058(7)$ $0.0000(6)$ $-0.0002(6)$ O2 $0.0255(8)$ $0.0187(8)$ $0.0173(7)$ $-0.0054(7)$ $0.0050(6)$ $-0.0007(6)$ O3 $0.0257(8)$ $0.0169(8)$ $0.0210(7)$ $-0.0082(7)$ $0.0040(6)$ $-0.0021(6)$ O4 $0.0301(9)$ $0.0173(8)$ $0.0212(7)$ $-0.0089(7)$ $0.0085(6)$ $0.0006(6)$ O6 $0.0452(11)$ $0.0174(8)$ $0.0282(9)$ $-0.0005(8)$ $-0.0069(7)$ $0.0044(7)$	C28	0.0273 (13)	0.0334 (14)	0.0301 (12)	-0.0003 (11)	0.0088 (10)	-0.0058 (10)
C30 $0.0327 (14)$ $0.0270 (13)$ $0.0403 (14)$ $0.0006 (12)$ $-0.0007 (11)$ $0.0076 (11)$ C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0296 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0000 (6)$ $-0.0002 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0050 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0155 (8)$ $0.0210 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0044 (7)$ Geometric parameters (Å, °)	C29	0.0406 (15)	0.0467 (16)	0.0224 (12)	-0.0016 (13)	0.0046 (10)	0.0100 (11)
C31 $0.0268 (12)$ $0.0220 (12)$ $0.0323 (12)$ $0.0001 (10)$ $0.0013 (10)$ $-0.0058 (10)$ C32 $0.0235 (11)$ $0.0270 (12)$ $0.0194 (10)$ $-0.0029 (10)$ $0.0023 (8)$ $-0.0010 (9)$ C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0296 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0000 (6)$ $-0.0002 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0050 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0071 (7)$ $0.0050 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0165 (8)$ $0.0204 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0006 (6)$ O6 $0.0452 (11)$ $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$	C30	0.0327 (14)	0.0270 (13)	0.0403 (14)	0.0006 (12)	-0.0007 (11)	0.0076 (11)
C320.0235 (11)0.0270 (12)0.0194 (10) $-0.0029 (10)$ 0.0023 (8) $-0.0010 (9)$ C330.0398 (15)0.0315 (14)0.0447 (15)0.0056 (13)0.0085 (12)0.0043 (12)N10.0189 (9)0.0140 (9)0.0198 (9) $-0.0025 (7)$ 0.0038 (7)0.0005 (7)O10.0296 (8)0.0186 (8)0.0180 (7) $-0.0058 (7)$ 0.0000 (6) $-0.0002 (6)$ O20.0255 (8)0.0187 (8)0.0173 (7) $-0.0054 (7)$ 0.0050 (6) $-0.0007 (6)$ O30.0257 (8)0.0169 (8)0.0210 (7) $-0.0071 (7)$ 0.0050 (6) $-0.0021 (6)$ O40.0301 (9)0.0165 (8)0.0212 (7) $-0.0082 (7)$ 0.0043 (6) $-0.0021 (6)$ O50.0323 (9)0.0193 (8)0.0212 (7) $-0.0089 (7)$ 0.0085 (6)0.0006 (6)O60.0452 (11)0.0174 (8)0.0282 (9) $-0.0005 (8)$ $-0.0069 (7)$ 0.0044 (7)	C31	0.0268 (12)	0.0220 (12)	0.0323 (12)	0.0001 (10)	0.0013 (10)	-0.0058 (10)
C33 $0.0398 (15)$ $0.0315 (14)$ $0.0447 (15)$ $0.0056 (13)$ $0.0085 (12)$ $0.0043 (12)$ N1 $0.0189 (9)$ $0.0140 (9)$ $0.0198 (9)$ $-0.0025 (7)$ $0.0038 (7)$ $0.0005 (7)$ O1 $0.0296 (8)$ $0.0186 (8)$ $0.0180 (7)$ $-0.0058 (7)$ $0.0000 (6)$ $-0.0002 (6)$ O2 $0.0255 (8)$ $0.0187 (8)$ $0.0173 (7)$ $-0.0054 (7)$ $0.0050 (6)$ $-0.0007 (6)$ O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0071 (7)$ $0.0050 (6)$ $-0.0021 (6)$ O4 $0.0301 (9)$ $0.0165 (8)$ $0.0204 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0006 (6)$ O6 $0.0452 (11)$ $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$	C32	0.0235 (11)	0.0270 (12)	0.0194 (10)	-0.0029 (10)	0.0023 (8)	-0.0010 (9)
N1 $0.0189(9)$ $0.0140(9)$ $0.0198(9)$ $-0.0025(7)$ $0.0038(7)$ $0.0005(7)$ O1 $0.0296(8)$ $0.0186(8)$ $0.0180(7)$ $-0.0058(7)$ $0.0000(6)$ $-0.0002(6)$ O2 $0.0255(8)$ $0.0187(8)$ $0.0173(7)$ $-0.0054(7)$ $0.0050(6)$ $-0.0007(6)$ O3 $0.0257(8)$ $0.0169(8)$ $0.0210(7)$ $-0.0071(7)$ $0.0050(6)$ $-0.0021(6)$ O4 $0.0301(9)$ $0.0165(8)$ $0.0204(7)$ $-0.0082(7)$ $0.0040(6)$ $-0.0021(6)$ O5 $0.0323(9)$ $0.0193(8)$ $0.0212(7)$ $-0.0089(7)$ $0.0085(6)$ $0.0006(6)$ O6 $0.0452(11)$ $0.0174(8)$ $0.0282(9)$ $-0.0005(8)$ $-0.0069(7)$ $0.0044(7)$	C33	0.0398 (15)	0.0315 (14)	0.0447 (15)	0.0056 (13)	0.0085 (12)	0.0043 (12)
O1 $0.0296(8)$ $0.0186(8)$ $0.0180(7)$ $-0.0058(7)$ $0.0000(6)$ $-0.0002(6)$ O2 $0.0255(8)$ $0.0187(8)$ $0.0173(7)$ $-0.0054(7)$ $0.0050(6)$ $-0.0007(6)$ O3 $0.0257(8)$ $0.0169(8)$ $0.0210(7)$ $-0.0071(7)$ $0.0050(6)$ $0.0016(6)$ O4 $0.0301(9)$ $0.0165(8)$ $0.0204(7)$ $-0.0082(7)$ $0.0040(6)$ $-0.0021(6)$ O5 $0.0323(9)$ $0.0193(8)$ $0.0212(7)$ $-0.0089(7)$ $0.0085(6)$ $0.0006(6)$ O6 $0.0452(11)$ $0.0174(8)$ $0.0282(9)$ $-0.0005(8)$ $-0.0069(7)$ $0.0044(7)$	N1	0.0189 (9)	0.0140 (9)	0.0198 (9)	-0.0025 (7)	0.0038 (7)	0.0005 (7)
O2 $0.0255(8)$ $0.0187(8)$ $0.0173(7)$ $-0.0054(7)$ $0.0050(6)$ $-0.0007(6)$ O3 $0.0257(8)$ $0.0169(8)$ $0.0210(7)$ $-0.0071(7)$ $0.0050(6)$ $0.0016(6)$ O4 $0.0301(9)$ $0.0165(8)$ $0.0204(7)$ $-0.0082(7)$ $0.0040(6)$ $-0.0021(6)$ O5 $0.0323(9)$ $0.0193(8)$ $0.0212(7)$ $-0.0089(7)$ $0.0085(6)$ $0.0006(6)$ O6 $0.0452(11)$ $0.0174(8)$ $0.0282(9)$ $-0.0005(8)$ $-0.0069(7)$ $0.0044(7)$	O1	0.0296 (8)	0.0186 (8)	0.0180 (7)	-0.0058 (7)	0.0000 (6)	-0.0002 (6)
O3 $0.0257 (8)$ $0.0169 (8)$ $0.0210 (7)$ $-0.0071 (7)$ $0.0050 (6)$ $0.0016 (6)$ O4 $0.0301 (9)$ $0.0165 (8)$ $0.0204 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ O5 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0006 (6)$ O6 $0.0452 (11)$ $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$	02	0.0255 (8)	0.0187 (8)	0.0173 (7)	-0.0054 (7)	0.0050 (6)	-0.0007 (6)
04 $0.0301 (9)$ $0.0165 (8)$ $0.0204 (7)$ $-0.0082 (7)$ $0.0040 (6)$ $-0.0021 (6)$ 05 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0006 (6)$ 06 $0.0452 (11)$ $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$ Geometric parameters (Å, °) C10 H19 0.0500	O3	0.0257 (8)	0.0169 (8)	0.0210 (7)	-0.0071 (7)	0.0050 (6)	0.0016 (6)
O5 $0.0323 (9)$ $0.0193 (8)$ $0.0212 (7)$ $-0.0089 (7)$ $0.0085 (6)$ $0.0006 (6)$ O6 $0.0452 (11)$ $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$ Geometric parameters (Å, °) C19 H19 0.0500	O4	0.0301 (9)	0.0165 (8)	0.0204 (7)	-0.0082 (7)	0.0040 (6)	-0.0021 (6)
0.0452 (11) $0.0174 (8)$ $0.0282 (9)$ $-0.0005 (8)$ $-0.0069 (7)$ $0.0044 (7)$ Geometric parameters (Å, °) $1.512 (3)$ $C19$ H19 0.0500	05	0.0323 (9)	0.0193 (8)	0.0212 (7)	-0.0089 (7)	0.0085 (6)	0.0006 (6)
Geometric parameters (\mathring{A}, \circ) C1-C2 $1.512 (3)$ $C10$ H10 0.0500	O6	0.0452 (11)	0.0174 (8)	0.0282 (9)	-0.0005 (8)	-0.0069 (7)	0.0044 (7)
C1 = C2 1 512 (3) C10 H10 0 0500	Geometric p	arameters (Å, °)					
0.1 - 0.2 $1.312(3)$ $0.17 - 0.17$	C1—C2		1.512 (3)	C19–	-H19	0.95	00

C1—C6	1.553 (3)	C20—C21	1.448 (3)
C1—H1A	0.9900	C21—H21	0.9500
C1—H1B	0.9900	C22—O1	1.433 (2)
C2—O6	1.227 (2)	C22—H22A	0.9800
C2—C3	1.493 (3)	C22—H22B	0.9800
C3—O1	1.354 (2)	C22—H22C	0.9800
C3—C4	1.361 (3)	C23—O5	1.426 (2)
C4—C5	1.454 (3)	C23—H23A	0.9800
C4—H4	0.9500	С23—Н23В	0.9800
C5—C21	1.348 (3)	С23—Н23С	0.9800
C5—C6	1.515 (3)	C24—O4	1.423 (2)
C6—C14	1.537 (3)	C24—H24A	0.9800
C6—C7	1.548 (3)	C24—H24B	0.9800
С7—С8	1.504 (3)	C24—H24C	0.9800
С7—Н7А	0.9900	C25—O2	1.431 (2)
С7—Н7В	0.9900	C25—H25A	0.9800
C8—C13	1.392 (3)	С25—Н25В	0.9800
C8—C9	1.399 (3)	С25—Н25С	0.9800
C9—C10	1.387 (3)	C26—O3	1.440 (2)
С9—Н9	0.9500	C26—H26A	0.9800
C10—O5	1.369 (2)	С26—Н26В	0.9800
C10—C11	1.407 (3)	C26—H26C	0.9800
C11—O4	1.372 (2)	C27—C28	1.386 (3)
C11—C12	1.387 (3)	C27—C32	1.394 (3)
C12—C13	1.404 (3)	C27—C33	1.507 (3)
C12—H12	0.9500	C28—C29	1.387 (3)
C13—N1	1.420 (2)	C28—H28	0.9500
C14—N1	1.291 (3)	C29—C30	1.383 (4)
C14—C15	1.480 (3)	С29—Н29	0.9500
C15—C20	1.403 (3)	C30—C31	1.382 (3)
C15—C16	1.407 (3)	С30—Н30	0.9500
C16—C17	1.390 (3)	C31—C32	1.385 (3)
C16—H16	0.9500	C31—H31	0.9500
C17—O2	1.362 (2)	С32—Н32	0.9500
C17—C18	1.420 (3)	С33—Н33А	0.9800
C18—O3	1.368 (2)	С33—Н33В	0.9800
C18—C19	1.379 (3)	С33—Н33С	0.9800
C19—C20	1.411 (3)		
C2—C1—C6	111.71 (16)	C15—C20—C19	119.14 (18)
C2—C1—H1A	109.3	C15—C20—C21	120.99 (18)
C6—C1—H1A	109.3	C19—C20—C21	119.86 (18)
C2—C1—H1B	109.3	C5—C21—C20	123.13 (19)
C6—C1—H1B	109.3	C5—C21—H21	118.4
H1A—C1—H1B	107.9	C20—C21—H21	118.4
O6—C2—C3	121.48 (19)	O1—C22—H22A	109.5
O6—C2—C1	121.57 (19)	O1—C22—H22B	109.5
C3—C2—C1	116.85 (18)	H22A—C22—H22B	109.5
O1—C3—C4	127.01 (19)	O1—C22—H22C	109.5
O1—C3—C2	113.21 (18)	H22A—C22—H22C	109.5

C4—C3—C2	119.65 (18)	H22B—C22—H22C	109.5
C3—C4—C5	121.56 (19)	O5—C23—H23A	109.5
С3—С4—Н4	119.2	O5—C23—H23B	109.5
С5—С4—Н4	119.2	H23A—C23—H23B	109.5
C21—C5—C4	121.93 (19)	O5—C23—H23C	109.5
C21—C5—C6	121.36 (17)	H23A—C23—H23C	109.5
C4—C5—C6	116.32 (17)	H23B—C23—H23C	109.5
C5—C6—C14	115.20 (16)	O4—C24—H24A	109.5
C5—C6—C7	112.52 (16)	O4—C24—H24B	109.5
C14—C6—C7	105.10 (16)	H24A—C24—H24B	109.5
C5—C6—C1	104.72 (16)	O4—C24—H24C	109.5
C14—C6—C1	110.39 (16)	H24A—C24—H24C	109.5
C7—C6—C1	108.88 (16)	H24B—C24—H24C	109.5
C8—C7—C6	107.96 (16)	O2—C25—H25A	109.5
С8—С7—Н7А	110.1	O2—C25—H25B	109.5
С6—С7—Н7А	110.1	H25A—C25—H25B	109.5
С8—С7—Н7В	110.1	O2—C25—H25C	109.5
С6—С7—Н7В	110.1	H25A—C25—H25C	109.5
H7A—C7—H7B	108.4	H25B—C25—H25C	109.5
C13—C8—C9	119.48 (19)	O3—C26—H26A	109.5
C13—C8—C7	117.74 (18)	O3—C26—H26B	109.5
C9—C8—C7	122.76 (17)	H26A—C26—H26B	109.5
C10—C9—C8	120.85 (18)	O3—C26—H26C	109.5
С10—С9—Н9	119.6	H26A—C26—H26C	109.5
С8—С9—Н9	119.6	H26B—C26—H26C	109.5
O5—C10—C9	124.88 (18)	C28—C27—C32	117.9 (2)
O5—C10—C11	115.76 (18)	C28—C27—C33	121.4 (2)
C9—C10—C11	119.36 (18)	C32—C27—C33	120.7 (2)
O4—C11—C12	125.11 (18)	C27—C28—C29	121.3 (2)
O4—C11—C10	114.56 (17)	С27—С28—Н28	119.3
C12—C11—C10	120.31 (19)	С29—С28—Н28	119.3
C11—C12—C13	119.77 (18)	C30—C29—C28	120.0 (2)
С11—С12—Н12	120.1	С30—С29—Н29	120.0
С13—С12—Н12	120.1	С28—С29—Н29	120.0
C8—C13—C12	120.21 (18)	C31—C30—C29	119.5 (2)
C8—C13—N1	121.20 (18)	С31—С30—Н30	120.2
C12—C13—N1	118.56 (17)	С29—С30—Н30	120.2
N1—C14—C15	118.74 (17)	C30—C31—C32	120.2 (2)
N1-C14-C6	122.18 (18)	С30—С31—Н31	119.9
C15—C14—C6	119.04 (17)	C32—C31—H31	119.9
C20-C15-C16	119.78 (18)	C31—C32—C27	121.1 (2)
C20—C15—C14	119.54 (17)	C31—C32—H32	119.5
C16—C15—C14	120.57 (18)	С27—С32—Н32	119.5
C17—C16—C15	120.79 (18)	С27—С33—Н33А	109.5
C17—C16—H16	119.6	С27—С33—Н33В	109.5
C15—C16—H16	119.6	H33A—C33—H33B	109.5
O2—C17—C16	125.53 (18)	С27—С33—Н33С	109.5
O2—C17—C18	115.24 (17)	H33A—C33—H33C	109.5
C16—C17—C18	119.23 (18)	H33B—C33—H33C	109.5

O3—C18—C19	124.78 (18)	C14—N1—C13	117.94 (17)
O3—C18—C17	115.18 (17)	C3—O1—C22	116.05 (16)
C19—C18—C17	120.04 (18)	C17—O2—C25	117.29 (15)
C18—C19—C20	120.98 (19)	C18—O3—C26	115.81 (15)
С18—С19—Н19	119.5	C11—O4—C24	117.74 (16)
С20—С19—Н19	119.5	C10—O5—C23	117.31 (16)
C6—C1—C2—O6	148.9 (2)	N1-C14-C15-C20	167.52 (18)
C6—C1—C2—C3	-34.6 (3)	C6-C14-C15-C20	-10.2 (3)
O6—C2—C3—O1	-0.1 (3)	N1-C14-C15-C16	-8.6 (3)
C1—C2—C3—O1	-176.55 (17)	C6-C14-C15-C16	173.70 (18)
O6—C2—C3—C4	176.1 (2)	C20-C15-C16-C17	1.7 (3)
C1—C2—C3—C4	-0.4 (3)	C14—C15—C16—C17	177.83 (18)
O1—C3—C4—C5	-176.57 (19)	C15—C16—C17—O2	178.08 (18)
C2—C3—C4—C5	7.9 (3)	C15-C16-C17-C18	-1.6 (3)
C3—C4—C5—C21	-151.1 (2)	O2—C17—C18—O3	-0.2 (3)
C3—C4—C5—C6	21.7 (3)	C16—C17—C18—O3	179.55 (18)
C21—C5—C6—C14	-2.0 (3)	O2—C17—C18—C19	-179.77 (18)
C4—C5—C6—C14	-174.90 (17)	C16—C17—C18—C19	0.0 (3)
C21—C5—C6—C7	-122.5 (2)	O3—C18—C19—C20	-177.93 (18)
C4—C5—C6—C7	64.6 (2)	C17—C18—C19—C20	1.6 (3)
C21—C5—C6—C1	119.4 (2)	C16—C15—C20—C19	-0.1 (3)
C4—C5—C6—C1	-53.5 (2)	C14—C15—C20—C19	-176.29 (18)
C2-C1-C6-C5	58.7 (2)	C16—C15—C20—C21	-178.69 (19)
C2-C1-C6-C14	-176.78 (17)	C14—C15—C20—C21	5.1 (3)
C_{2} — C_{1} — C_{6} — C_{7}	-61 9 (2)	C18 - C19 - C20 - C15	-15(3)
$C_{5} - C_{6} - C_{7} - C_{8}$	-17745(16)	$C_{18} - C_{19} - C_{20} - C_{21}$	177 05 (19)
C14—C6—C7—C8	56 4 (2)	C4-C5-C21-C20	169 34 (19)
C1 - C6 - C7 - C8	-61.8(2)	$C_{6} = C_{5} = C_{21} = C_{20}$	-32(3)
C6-C7-C8-C13	-37.5(2)	$C_{15} - C_{20} - C_{21} - C_{5}$	17(3)
C6-C7-C8-C9	140.8 (2)	$C_{19} - C_{20} - C_{21} - C_{5}$	-1768(2)
$C_{13} - C_{8} - C_{9} - C_{10}$	0.2(3)	C_{32} C_{27} C_{28} C_{29}	-0.5(3)
C7-C8-C9-C10	-178.02(19)	$C_{33} = C_{27} = C_{28} = C_{29}$	1795(2)
C8 - C9 - C10 - O5	179 2 (2)	$C_{27} - C_{28} - C_{29} - C_{30}$	0.7(4)
$C_{8} = C_{9} = C_{10} = C_{11}$	-0.9(3)	$C_{28} = C_{29} = C_{30} = C_{31}$	-0.6(4)
05-C10-C11-O4	-0.9(3)	$C_{20} = C_{20} = C_{30} = C_{31} = C_{32}$	0.0(4)
$C_{2} = C_{10} = C_{11} = C_{14}$	179 11 (18)	$C_{2}^{30} = C_{31}^{31} = C_{32}^{32} = C_{27}^{32}$	0.2(4)
05-010-011-04	-179.63(18)	$C_{30} = C_{31} = C_{32} = C_{27}$	0.1(3)
$C_{10} = C_{11} = C_{12}$	0.4(3)	$C_{23} = C_{27} = C_{32} = C_{31}$	-180.0(2)
$04 C_{11} C_{12} C_{13}$	-177.02(10)	$C_{33} = C_{27} = C_{32} = C_{31}$	-171.83(17)
$C_{10} - C_{11} - C_{12} - C_{13}$	0.7(3)	C6-C14-N1-C13	5 8 (3)
$C_{10} = C_{11} = C_{12} = C_{13}$	0.7(3)	$C_{0} = C_{1}^{1} = N_{1}^{1} = C_{1}^{1}$	20.8(3)
$C_{7} = C_{8} = C_{13} = C_{12}$	179 18 (18)	C_{12} C_{13} N_{12} C_{14}	-160.95(18)
$C_{1} = C_{1} = C_{1} = C_{1} = C_{1}$	179.03 (10)	$C_{12} = C_{13} = 11 = C_{14}$	-19(3)
C7 - C8 - C13 - N1	-26(3)	$C_{2}^{2} = C_{3}^{2} = 0_{1}^{2} = C_{2}^{2}$	170 91 (18)
C_{11} C_{12} C_{13} C_{8}	-13(3)	$C_2 = C_3 = 01 = 022$	-15(3)
$C_{11} - C_{12} - C_{13} - C_{0}$	-179 52 (18)	$C_{10} = C_{17} = 02 = C_{23}$	178 24 (17)
C_{5} C_{6} C_{14} N_{1}	-169 12 (18)	C19 - C18 - O3 - C26	-34(3)
C_{7} C_{6} C_{14} N_{1}	-44.7(2)	$C_{17} - C_{18} - C_{20} - C_{20}$	יד. ד. (ג) 177 01 (17)
$C_1 = C_0 = C_1 + I_1 + I_1 + I_2 + I_1 + I_2 $	тт./ (<i>2)</i> 72 6 (2)	$C_{17} - C_{10} - O_{5} - C_{20}$	-104(2)
C1-C0-C14-INI	12.0 (2)	C12 - C11 - C4 - C24	10.4 (3)

C5—C6—C14—C15		8.5 (3)	C10-C11-O4-C24	170.96 (18)
C7—C6—C14—C15		132.91 (18)	C9-C10-O5-C23	-12.3 (3)
C1—C6—C14—C15		-109.8 (2)	C11—C10—O5—C23	167.70 (19)
Table 1. Hydrogen bond	ling and C-H	$I \cdots \pi$ interactions		
D—H···A	D—H	Н…А	D…A	D—H···A
C23—H23B…O4 ⁱ	0.98	2.41	3.354 (3)	160.4
C26—H26B····O2 ⁱⁱ	0.98	2.59	3.210 (3)	120.9
C26—H26C…O6 ⁱⁱⁱ	0.98	2.58	3.526 (3)	162.2
C12—H12····Cg2 ^{iV}	0.95	3.3199	3.780 (2)	112.02
C22—H22A…Cg2 ⁱⁱⁱ	0.98	2.9687	3.557 (3)	119.73
C23—H23C… <i>Cg</i> 1 ^v	0.98	2.9869	3.902 (3)	155.82
C24—H24A…Cg3 ^{vi}	0.98	2.6627	3.447 (3)	137.12
C25—H25C…Cg3	0.98	2.6327	3.487 (3)	145.87

*Cg*1 denotes the centroid of ring C8–C13, *Cg*2 that of C15–C20, and *Cg*3 that of C27–C32. Symmetry codes: (i) -x, -y, -z + 1; (ii) -x + 1, y + 1/2, -z + 1/2; (iii) -x + 1, -y + 2, -z + 1; (iv) x, y - 1, z; (v) -x, -y + 1, -z + 1; (vi) -x, y - 1/2, -z + 1/2.







