

Data collection

Nonius CAD-4 diffractometer	440 observed reflections
$\theta/2\theta$ scans	$[I > 2\sigma(I)]$
Absorption correction:	$R_{\text{int}} = 0.053$
by integration from crystal shape	$\theta_{\text{max}} = 69.80^\circ$
$T_{\text{min}} = 0.24$, $T_{\text{max}} = 0.61$	$h = 0 \rightarrow 11$
1502 measured reflections	$k = 0 \rightarrow 12$
467 independent reflections	$l = -5 \rightarrow 5$
	6 standard reflections
	frequency: 30 min
	intensity decay: 0.7%

Refinement

Refinement on F^2	$\Delta\rho_{\text{max}} = 0.49 \text{ e } \text{\AA}^{-3}$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$\Delta\rho_{\text{min}} = -0.60 \text{ e } \text{\AA}^{-3}$
$wR(F^2) = 0.109$	Extinction correction:
$S = 1.12$	SHELXL93 (Sheldrick, 1993)
467 reflections	Extinction coefficient:
39 parameters	0.0043 (18)
All H-atom parameters refined	Atomic scattering factors from <i>International Tables for Crystallography</i> (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
$w = 1/[\sigma^2(F_o^2) + (0.0845P)^2]$	
where $P = (F_o^2 + 2F_c^2)/3$	
$(\Delta/\sigma)_{\text{max}} = -0.03$	

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1258). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j$$

	x	y	z	U_{eq}
Cl	0.23662 (7)	0	0.50616 (13)	0.0467 (4)
N1	0.4255 (2)	-0.1499 (2)	0.1468 (3)	0.0397 (5)
H1	0.373 (3)	-0.124 (2)	0.253 (5)	0.045 (6)
C2	1/2	-0.0719 (2)	0	0.0339 (6)
C3	0.4536 (3)	-0.2799 (2)	0.0916 (5)	0.0508 (6)
H3	0.415 (3)	-0.351 (4)	0.182 (5)	0.068 (9)

Table 2. Selected geometric parameters (\AA , $^\circ$)

N1—C2	1.328 (2)	C2—C2'	1.442 (5)
N1—C3	1.366 (3)	C3—C3''	1.338 (5)
N1—H1	0.81 (3)	C3—H3	0.94 (4)
C2—N1—C3	108.9 (2)	N1—C2—C2'	126.1 (1)
C2—N1—H1	125 (2)	C3''—C3—N1	107.2 (1)
C3—N1—H1	126 (2)	C3''—C3—H3	131 (2)
N1''—C2—N1	107.8 (2)	N1—C3—H3	122 (2)

Symmetry codes: (i) $1 - x, -y, -z$; (ii) $1 - x, y, -z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *NRC Crystallographic Computer Programs* (Ahmed, Hall, Pippy & Huber, 1973). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976; Gabe, Le Page, Charland, Lee & White, 1989). Software used to prepare material for publication: *SHELXL93*.

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1,2-[3,4-Dihydro-2-(4-methoxyphenyl)-2H-pyrrolo][60]fullerene Carbon Disulfide

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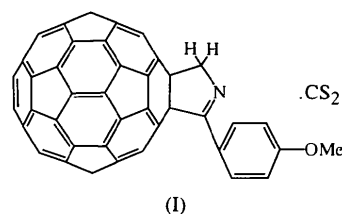
Abstract

The title fullerene, C₆₀H₉NO.CS₂, is a low-symmetry derivative of C₆₀ and does not show the known disorder of the unsubstituted fullerene molecule. Contrary to spectroscopic investigations, the C_s symmetry of the molecule is no longer present in the crystal. The two bridging atoms, C1 and C2, 'stand out' of the C₆₀ surface.

Comment

Disorder plays a crucial role when investigating solid structures of fullerenes, and a number of static and

dynamic disorder models have been discussed (Chow, Jiang, Reiter, Wochner, Moss, Axe, Hanson, McMullan, Meng & Chu, 1992; Bürgi, Restori & Schwarzenbach, 1993; Bensch, Werner, Bartl & Schlögel, 1994; Boeyens, Ramm, Zobel & Luger, 1996). Two ways seem to be possible to suppress the adverse influence of the molecular dynamics in the solid state. The first is to crystallize host-guest complexes (Roth & Adelman, 1993; Fedurco, Olmstead & Fawcett, 1995). The second involves the use of low-symmetry derivatives either as substituted compounds (Osterodt, Nieger & Vögtle, 1994; Irgartinger, Köhler, Huber-Patz & Krätschmer, 1994) or metal-organic compounds (Balch, Catalano, Lee & Olmstead, 1992). Functionalization by cycloaddition reactions represents a useful strategy to modify fullerenes (Hirsch, 1995) and to obtain molecules with lower symmetry. 1,2-(3,4-dihydro-2*H*-pyrrolo)[60]fullerenes can be obtained by photocycloaddition (Averdung & Mattay, 1996). Extensive spectroscopic investigations of these compounds [¹H NMR, ¹³C NMR, UV-visible, LDTOF MS (laser desorption time of flight mass spectroscopy)] showed that the data were only compatible with a spatial substituent position, thus satisfying overall molecular C_s symmetry. In the crystal of the title derivative (I), however, this symmetry is no longer present. While the pyrroline ring lies in the mirror plane of the C₆₀ molecule, it encloses an angle of about 33.8(2)° with the phenyl ring plane (Fig. 1).



The increased bond length between the two bridged C atoms, C1 and C2, of 1.597(4) Å, is in good agreement with comparable bond lengths found for methanofullerenes [1.574(3)–1.614(7) Å (Anderson, Boudon, Diederich, Gisselbrecht, Gross & Seiler, 1994; Osterodt, Nieger & Vögtle, 1994; Paulus & Bingel, 1995), a Diels–Alder adduct [1.62(4); Rubin, Khan, Freedberg & Yerezian, 1993] and a [3+2] cycloaddition adduct [1.584(5) Å; Irgartinger, Köhler, Huber-Patz & Krätschmer, 1994]. The two *sp*³–*sp*² bonds involving C1 and C2 are slightly elongated. The 5–6 and 6–6 bond lengths in the C₆₀ sphere range from 1.389(5) (C14–C22) to 1.497(5) Å (C51–C53) and from 1.320(5) (C43–C55) to 1.422(5) Å (C40–C41), respectively. The average values of 1.446(5) and 1.378(5) Å, respectively, correspond to those of 1.458(6) and 1.40(1) Å determined by electron diffraction (Hedberg, Hedberg, Bethune, Brown, Dorn, Johnson & de Vries, 1991). The distances of the C atoms, except C1 and C2, from the centre of the molecule vary between 3.492(3) (C16) and 3.557(3) Å (C57),

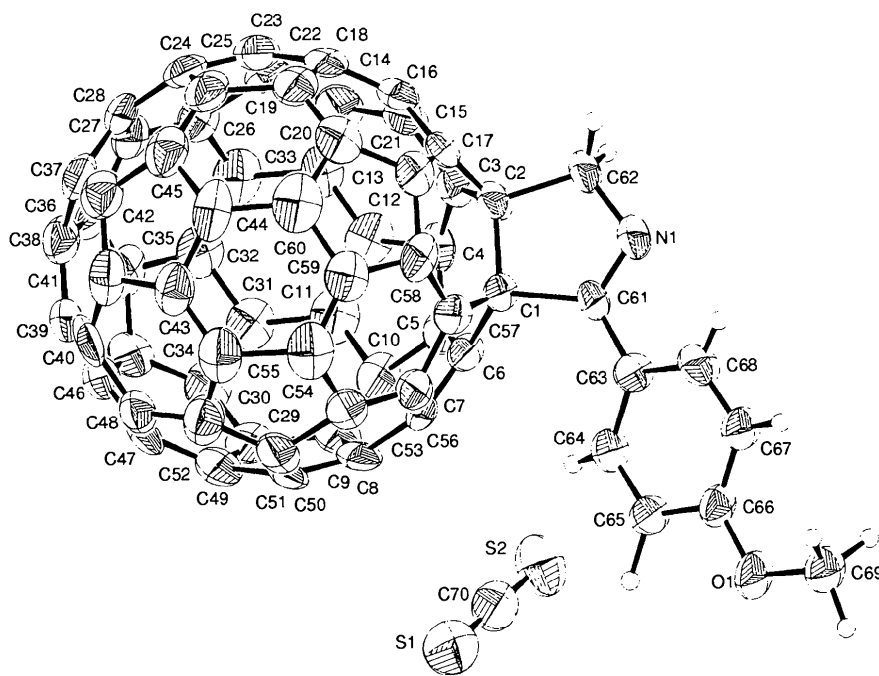


Fig. 1. ORTEP (Johnson, 1971) drawing of the asymmetric unit showing the crystallographic numbering scheme (50% probability displacement ellipsoids).

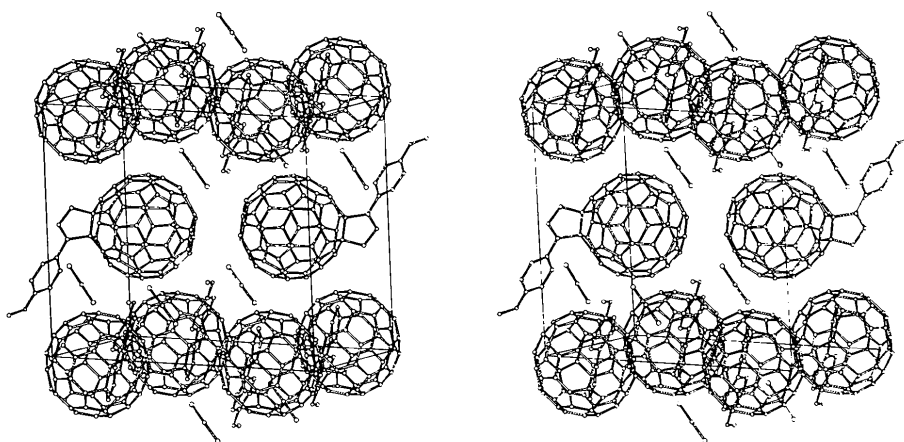


Fig. 2. *SCHAKAL92* (Keller, 1992) drawing of the arrangement of the molecules in the unit cell.

with an average value of 3.522 (3) Å. The distances of C1 [3.837 (3) Å] and C2 [3.820 (3) Å] are considerably longer. Hence, as in other derivatives of fullerene (Anderson, Boudon, Diederich, Gisselbrecht, Gross & Seiler, 1994; Irgartinger, Köhler, Huber-Patz & Krätschmer, 1994), C1 and C2 stand out of the C₆₀ surface by approximately 0.3 Å.

All five- and six-membered rings of the C₆₀ sphere, except those containing C1 and C2, are planar, with average distances of the atoms from the least-squares planes of 0.005 (2) and 0.006 (2) Å, respectively. Deviations from the least-squares planes including C1 and C2 amount to 0.069 (2) and 0.052 (2) Å, respectively.

The arrangement of the molecules in the unit cell is shown in Fig. 2. If the fullerene molecules are regarded as forming a 'coordination polyhedron', a coordination number of 10 could be envisaged. The centre-to-centre distances are in the range 9.941 (5)–13.318 (6) Å.

Experimental

A solution of C₆₀ and 2-(4-methoxyphenyl)-2H-azirine in toluene was irradiated in a quartz tube. The solution was filtered, concentrated in vacuo and then chromatographed (Averdung & Matthey, 1996). The dark-brown solid was dissolved in carbon disulfide. Slow evaporation yielded crystals of the title compound.

Crystal data

C₆₉H₉NO.CS₂
M_r = 943.90
 Monoclinic
*P*2₁/*n*
a = 21.094 (4) Å
b = 10.022 (3) Å
c = 17.293 (4) Å
 β = 90.18 (2)°

Cu *K*α radiation
 λ = 1.54178 Å
 Cell parameters from 61 reflections
 θ = 15–36°
 μ = 1.829 mm⁻¹
T = 293 (1) K
 Prism

V = 3655.8 (15) Å³

Z = 4

D_s = 1.715 Mg m⁻³

D_m not measured

0.40 × 0.24 × 0.12 mm

Black

Data collection

Stoe AED diffractometer

$\omega/2\theta$ scans

Absorption correction:

none

5642 measured reflections

5436 independent reflections

3098 observed reflections

[*I* > 2σ(*I*)]

*R*_{int} = 0.0125

θ_{\max} = 60.09°

h = -23 → 23

k = 0 → 11

l = 0 → 19

3 standard reflections

frequency: 90 min

intensity decay: 1.2%

Refinement

Refinement on *F*²

R[*F*² > 2σ(*F*²)] = 0.0451

wR(*F*²) = 0.1211

S = 0.881

5436 reflections

692 parameters

H atoms: see text

w = 1/[σ²(*F*_o²) + (0.0779*P*)²]

where *P* = (*F*_o² + 2*F*_c²)/3

(Δ/σ)_{max} = 0.007

Δρ_{max} = 0.349 e Å⁻³

Δρ_{min} = -0.251 e Å⁻³

Extinction correction:

SHELXL93 (Sheldrick, 1993)

Extinction coefficient:

0.00010 (6)

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

	$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
S1	0.93495 (6)	0.6725 (1)	0.81099 (7)	0.0922 (4)
S2	1.02412 (6)	0.6575 (1)	0.67178 (7)	0.0849 (4)
O1	1.0336 (1)	1.2026 (2)	0.7993 (1)	0.0651 (7)
N1	0.9186 (1)	1.1157 (3)	0.4646 (2)	0.0573 (7)
C1	0.8546 (2)	0.9405 (3)	0.5196 (2)	0.0454 (8)
C2	0.8368 (2)	0.9522 (3)	0.4300 (2)	0.0477 (8)
C3	0.8430 (1)	0.8269 (3)	0.3832 (2)	0.0422 (7)
C4	0.8728 (2)	0.7147 (3)	0.4101 (2)	0.0493 (8)
C5	0.8906 (2)	0.7031 (3)	0.4905 (2)	0.0545 (9)

C6	0.8780 (1)	0.7986 (3)	0.5418 (2)	0.0433 (7)	C1—C2	1.597 (4)	C32—C35	1.441 (5)
C7	0.8513 (2)	0.7656 (3)	0.6162 (2)	0.0484 (8)	C2—C3	1.501 (4)	C34—C46	1.382 (5)
C8	0.8420 (2)	0.6343 (3)	0.6393 (2)	0.062 (1)	C2—C17	1.506 (4)	C34—C35	1.435 (5)
C9	0.8577 (2)	0.5295 (3)	0.5846 (2)	0.061 (1)	C2—C62	1.592 (4)	C35—C36	1.368 (5)
C10	0.8810 (2)	0.5626 (3)	0.5138 (2)	0.059 (1)	C3—C4	1.369 (4)	C36—C38	1.434 (5)
C11	0.8591 (2)	0.4934 (3)	0.4435 (2)	0.066 (1)	C3—C15	1.419 (4)	C37—C42	1.366 (5)
C12	0.8531 (2)	0.5838 (3)	0.3819 (2)	0.0598 (9)	C4—C5	1.443 (4)	C37—C38	1.459 (5)
C13	0.8046 (2)	0.5732 (3)	0.3280 (2)	0.0553 (9)	C4—C12	1.460 (4)	C38—C39	1.379 (5)
C14	0.7714 (2)	0.6929 (3)	0.3016 (2)	0.061 (1)	C5—C6	1.332 (4)	C39—C46	1.399 (5)
C15	0.7916 (2)	0.8164 (3)	0.3304 (2)	0.0547 (9)	C5—C10	1.478 (4)	C39—C40	1.452 (5)
C16	0.7456 (2)	0.9127 (3)	0.3501 (2)	0.0488 (8)	C6—C7	1.445 (4)	C40—C41	1.422 (5)
C17	0.7680 (2)	0.9850 (3)	0.4163 (2)	0.0469 (8)	C7—C8	1.390 (4)	C40—C48	1.432 (5)
C18	0.6818 (2)	0.8851 (3)	0.3419 (2)	0.057 (1)	C7—C56	1.469 (4)	C41—C42	1.428 (5)
C19	0.6381 (2)	0.9253 (3)	0.3994 (2)	0.0583 (9)	C8—C50	1.425 (5)	C41—C43	1.461 (5)
C20	0.6595 (2)	0.9938 (3)	0.4634 (2)	0.063 (1)	C8—C9	1.452 (5)	C42—C45	1.429 (5)
C21	0.7273 (2)	1.0239 (3)	0.4723 (2)	0.0539 (9)	C9—C10	1.361 (5)	C43—C55	1.320 (5)
C22	0.7073 (2)	0.6636 (3)	0.2932 (2)	0.0598 (9)	C9—C29	1.462 (5)	C43—C44	1.457 (5)
C23	0.6603 (2)	0.7562 (4)	0.3130 (2)	0.0588 (9)	C10—C11	1.473 (5)	C44—C60	1.405 (5)
C24	0.6056 (2)	0.7165 (3)	0.3528 (2)	0.0566 (9)	C11—C31	1.401 (5)	C44—C45	1.481 (5)
C25	0.5894 (2)	0.8220 (3)	0.4071 (2)	0.062 (1)	C11—C12	1.404 (5)	C46—C47	1.442 (5)
C26	0.6958 (2)	0.5230 (3)	0.3159 (2)	0.0567 (9)	C12—C13	1.386 (5)	C47—C49	1.415 (5)
C27	0.6436 (2)	0.4867 (3)	0.3545 (2)	0.0567 (9)	C13—C33	1.420 (5)	C47—C58	1.435 (5)
C28	0.5956 (2)	0.5857 (3)	0.3756 (2)	0.0566 (9)	C13—C14	1.461 (5)	C48—C52	1.394 (5)
C29	0.8099 (2)	0.4252 (3)	0.5943 (3)	0.075 (1)	C14—C22	1.389 (5)	C49—C50	1.470 (5)
C30	0.7900 (2)	0.3580 (3)	0.5262 (3)	0.074 (1)	C14—C15	1.401 (4)	C50—C51	1.356 (5)
C31	0.8146 (2)	0.3907 (3)	0.4521 (2)	0.061 (1)	C15—C16	1.411 (4)	C51—C52	1.427 (5)
C32	0.7618 (2)	0.3810 (3)	0.3976 (2)	0.066 (1)	C16—C18	1.381 (4)	C51—C53	1.497 (4)
C33	0.7586 (2)	0.4709 (3)	0.3367 (2)	0.068 (1)	C16—C17	1.434 (4)	C52—C55	1.466 (5)
C34	0.7226 (2)	0.3265 (3)	0.5189 (2)	0.073 (1)	C17—C21	1.354 (4)	C53—C56	1.349 (5)
C35	0.7056 (2)	0.3419 (3)	0.4390 (2)	0.064 (1)	C18—C19	1.418 (5)	C53—C54	1.446 (5)
C36	0.6478 (2)	0.3938 (3)	0.4191 (2)	0.058 (1)	C18—C23	1.456 (5)	C54—C59	1.376 (5)
C37	0.5713 (2)	0.5535 (3)	0.4511 (2)	0.0599 (9)	C19—C20	1.378 (5)	C54—C55	1.491 (5)
C38	0.6038 (2)	0.4335 (3)	0.4778 (2)	0.062 (1)	C19—C25	1.464 (5)	C56—C57	1.417 (4)
C39	0.6213 (2)	0.4184 (3)	0.5543 (2)	0.062 (1)	C20—C60	1.433 (5)	C57—C58	1.359 (4)
C40	0.6052 (2)	0.5235 (4)	0.6086 (2)	0.065 (1)	C20—C21	1.469 (5)	C58—C59	1.431 (5)
C41	0.5745 (2)	0.6404 (4)	0.5809 (2)	0.065 (1)	C21—C58	1.456 (5)	C59—C60	1.466 (5)
C42	0.5573 (2)	0.6544 (3)	0.5014 (2)	0.0605 (9)	C22—C23	1.402 (5)	C61—C63	1.464 (4)
C43	0.5939 (2)	0.7691 (4)	0.6128 (2)	0.0601 (9)	C22—C26	1.483 (4)	C63—C68	1.388 (4)
C44	0.5895 (2)	0.8628 (3)	0.5486 (2)	0.064 (1)	C23—C24	1.402 (5)	C63—C64	1.393 (4)
C45	0.5667 (2)	0.7904 (4)	0.4792 (2)	0.066 (1)	C24—C28	1.386 (5)	C64—C65	1.352 (4)
C46	0.6803 (2)	0.3662 (3)	0.5753 (2)	0.064 (1)	C24—C25	1.456 (5)	C65—C66	1.399 (4)
C47	0.7015 (2)	0.4360 (3)	0.6436 (2)	0.070 (1)	C25—C45	1.375 (5)	C66—C67	1.387 (4)
C48	0.6556 (2)	0.5356 (4)	0.6639 (2)	0.061 (1)	C26—C27	1.339 (5)	C67—C68	1.348 (4)
C49	0.7668 (2)	0.4650 (3)	0.6521 (2)	0.071 (1)	C26—C33	1.468 (5)		
C50	0.7863 (2)	0.5971 (3)	0.6804 (2)	0.058 (1)				
C51	0.7408 (2)	0.6867 (4)	0.6995 (2)	0.069 (1)	C66—O1—C69	118.2 (2)	C28—C24—C25	117.8 (3)
C52	0.6747 (2)	0.6599 (4)	0.6915 (2)	0.068 (1)	C61—N1—C62	112.5 (3)	C23—C24—C25	107.8 (3)
C53	0.7521 (2)	0.8288 (3)	0.6768 (2)	0.060 (1)	C57—C1—C6	101.9 (2)	C45—C25—C24	120.1 (3)
C54	0.6908 (2)	0.8831 (4)	0.6562 (2)	0.065 (1)	C57—C1—C61	112.3 (2)	C45—C25—C19	119.6 (3)
C55	0.6410 (2)	0.7781 (4)	0.6629 (2)	0.068 (1)	C6—C1—C61	114.3 (2)	C24—C25—C19	106.8 (3)
C56	0.8038 (2)	0.8666 (3)	0.6367 (2)	0.0487 (8)	C57—C1—C2	116.1 (3)	C27—C26—C33	121.5 (3)
C57	0.8008 (2)	0.9614 (3)	0.5760 (2)	0.0433 (7)	C6—C1—C2	112.4 (2)	C27—C26—C22	121.8 (3)
C58	0.7435 (2)	1.0106 (3)	0.5538 (2)	0.0508 (8)	C61—C1—C2	100.5 (2)	C33—C26—C22	104.7 (3)
C59	0.6879 (2)	0.9706 (3)	0.5950 (2)	0.0553 (9)	C3—C2—C17	100.5 (2)	C26—C27—C36	120.6 (3)
C60	0.6359 (2)	0.9620 (3)	0.5388 (2)	0.068 (1)	C3—C2—C62	113.6 (3)	C26—C27—C28	120.6 (3)
C61	0.9070 (2)	1.0523 (3)	0.5264 (2)	0.0466 (8)	C17—C2—C62	110.7 (2)	C36—C27—C28	106.3 (3)
C62	0.8810 (2)	1.0705 (3)	0.4008 (2)	0.0522 (9)	C3—C2—C1	116.2 (2)	C24—C28—C37	121.7 (3)
C63	0.9383 (2)	1.0913 (3)	0.5986 (2)	0.0456 (8)	C17—C2—C1	113.1 (3)	C24—C28—C27	117.6 (3)
C64	0.9543 (2)	1.0024 (3)	0.6573 (2)	0.058 (1)	C62—C2—C1	103.1 (2)	C37—C28—C27	108.9 (3)
C65	0.9850 (2)	1.0412 (3)	0.7223 (2)	0.0582 (9)	C4—C3—C15	120.5 (3)	C49—C29—C30	122.2 (4)
C66	1.0021 (2)	1.1749 (3)	0.7326 (2)	0.0478 (8)	C4—C3—C2	120.0 (3)	C49—C29—C9	109.0 (4)
C67	0.9852 (2)	1.2656 (3)	0.6756 (2)	0.0560 (9)	C15—C3—C2	110.0 (3)	C30—C29—C9	116.5 (4)
C68	0.9530 (2)	1.2242 (3)	0.6125 (2)	0.0542 (9)	C3—C4—C5	120.8 (3)	C29—C30—C31	122.1 (4)
C69	1.0545 (2)	1.3359 (3)	0.8119 (2)	0.0596 (9)	C3—C4—C12	119.6 (3)	C29—C30—C34	117.4 (4)
C70	0.9793 (2)	0.6634 (3)	0.7404 (2)	0.072 (1)	C5—C4—C12	108.8 (3)	C31—C30—C34	109.2 (4)
					C6—C5—C4	122.1 (3)	C11—C31—C30	120.7 (3)
					C6—C5—C10	118.3 (3)	C11—C31—C32	119.4 (3)
					C4—C5—C10	107.8 (3)	C30—C31—C32	106.7 (3)
					C5—C6—C7	120.5 (3)	C33—C32—C35	121.0 (4)
					C5—C6—C1	123.9 (3)	C33—C32—C31	118.8 (3)
					C7—C6—C1	107.8 (3)	C35—C32—C31	109.0 (3)
					C8—C7—C6	121.9 (3)	C32—C33—C13	121.1 (4)
					C8—C7—C56	119.1 (3)	C32—C33—C26	117.3 (4)
					C6—C7—C56	109.0 (3)	C13—C33—C26	109.5 (3)
					C7—C8—C50	120.6 (3)	C46—C34—C35	119.3 (4)
					C7—C8—C9	117.8 (3)	C46—C34—C30	120.4 (4)
					C50—C8—C9	109.1 (3)	C35—C34—C30	107.5 (4)
					C10—C9—C8	119.5 (3)	C36—C35—C34	120.1 (4)
S1—C70	1.543 (4)	C27—C36	1.457 (4)					
S2—C70	1.521 (4)	C27—C28	1.465 (5)					
O1—C66	1.358 (4)	C28—C37	1.440 (5)					
O1—C69	1.424 (3)	C29—C49	1.411 (6)					
N1—C61	1.267 (4)	C29—C30	1.418 (5)					
N1—C62	1.431 (4)	C30—C31	1.422 (5)					
C1—C57	1.514 (4)	C30—C34	1.463 (5)					
C1—C6	1.553 (4)	C31—C32	1.460 (5)					
C1—C61	1.577 (4)	C32—C33	1.388 (5)					

Table 2. Selected geometric parameters (\AA , $^\circ$)

C10—C9—C29	121.9 (4)	C36—C35—C32	120.4 (4)
C8—C9—C29	106.4 (4)	C34—C35—C32	107.7 (3)
C9—C10—C11	120.9 (3)	C35—C36—C38	120.4 (4)
C9—C10—C5	121.8 (3)	C35—C36—C27	119.1 (4)
C11—C10—C5	105.4 (3)	C38—C36—C27	109.1 (3)
C31—C11—C12	119.7 (4)	C42—C37—C28	119.3 (3)
C31—C11—C10	117.8 (4)	C42—C37—C38	120.7 (3)
C12—C11—C10	110.5 (3)	C28—C37—C38	107.6 (3)
C13—C12—C11	121.7 (3)	C39—C38—C36	118.4 (3)
C13—C12—C4	120.2 (3)	C39—C38—C37	121.2 (4)
C11—C12—C4	107.5 (3)	C36—C38—C37	108.0 (3)
C12—C13—C33	119.2 (3)	C38—C39—C46	121.7 (4)
C12—C13—C14	120.0 (3)	C38—C39—C40	118.6 (4)
C33—C13—C14	107.4 (3)	C46—C39—C40	108.2 (3)
C22—C14—C15	121.2 (4)	C41—C40—C48	119.4 (3)
C22—C14—C13	108.9 (3)	C41—C40—C39	119.1 (3)
C15—C14—C13	117.9 (3)	C48—C40—C39	108.7 (3)
C14—C15—C16	118.8 (3)	C40—C41—C42	121.3 (3)
C14—C15—C3	121.7 (3)	C40—C41—C43	118.3 (4)
C16—C15—C3	108.6 (3)	C42—C41—C43	110.3 (3)
C18—C16—C15	120.5 (3)	C37—C42—C41	119.1 (3)
C18—C16—C17	120.2 (3)	C37—C42—C45	120.3 (4)
C15—C16—C17	108.2 (3)	C41—C42—C45	108.5 (3)
C21—C17—C16	120.6 (3)	C55—C43—C44	120.1 (3)
C21—C17—C2	124.3 (3)	C55—C43—C41	121.2 (4)
C16—C17—C2	109.3 (3)	C44—C43—C41	105.4 (3)
C16—C18—C19	120.5 (3)	C60—C44—C43	120.3 (4)
C16—C18—C23	121.0 (3)	C60—C44—C45	118.3 (4)
C19—C18—C23	106.8 (3)	C43—C44—C45	108.7 (3)
C20—C19—C18	119.5 (3)	C25—C45—C42	120.8 (4)
C20—C19—C25	120.5 (4)	C25—C45—C44	120.4 (3)
C18—C19—C25	108.7 (3)	C42—C45—C44	107.2 (3)
C19—C20—C60	120.4 (3)	C34—C46—C39	119.9 (4)
C19—C20—C21	120.2 (4)	C34—C46—C47	121.3 (4)
C60—C20—C21	106.9 (3)	C39—C46—C47	107.7 (4)
C17—C21—C58	121.2 (3)	C49—C47—C48	119.3 (3)
C17—C21—C20	119.1 (3)	C49—C47—C46	118.9 (4)
C58—C21—C20	107.9 (3)	C48—C47—C46	109.3 (3)
C14—C22—C23	121.6 (3)	C52—C48—C40	121.2 (4)
C14—C22—C26	109.5 (3)	C52—C48—C47	120.7 (4)
C23—C22—C26	116.6 (3)	C40—C48—C47	106.1 (3)
C22—C23—C24	120.1 (3)	C29—C49—C47	119.8 (4)
C22—C23—C18	116.8 (3)	C29—C49—C50	108.1 (4)
C24—C23—C18	109.9 (3)	C47—C49—C50	119.4 (4)
C28—C24—C23	122.3 (3)	C51—C50—C8	122.2 (3)
C51—C50—C49	118.7 (4)	C57—C58—C21	120.8 (3)
C8—C50—C49	107.4 (4)	C59—C58—C21	108.5 (3)
C50—C51—C52	123.0 (3)	C54—C59—C58	121.8 (3)
C50—C51—C53	116.9 (3)	C54—C59—C60	120.3 (3)
C52—C51—C53	108.0 (4)	C58—C59—C60	107.4 (3)
C48—C52—C51	118.9 (4)	C44—C60—C20	120.7 (4)
C48—C52—C55	117.9 (3)	C44—C60—C59	118.8 (4)
C51—C52—C55	110.7 (3)	C20—C60—C59	109.2 (3)
C56—C53—C54	119.4 (3)	N1—C61—C63	119.8 (3)
C56—C53—C51	122.1 (4)	N1—C61—C1	115.5 (3)
C54—C53—C51	106.3 (3)	C63—C61—C1	124.5 (3)
C59—C54—C53	117.8 (3)	N1—C62—C2	108.3 (3)
C59—C54—C55	118.7 (4)	C68—C63—C64	115.7 (3)
C53—C54—C55	110.2 (3)	C68—C63—C61	120.3 (3)
C43—C55—C52	121.9 (4)	C64—C63—C61	124.0 (3)
C43—C55—C54	121.8 (4)	C65—C64—C63	122.5 (3)
C52—C55—C54	104.8 (3)	C64—C65—C66	120.3 (3)
C53—C56—C57	122.4 (3)	O1—C66—C67	126.4 (3)
C53—C56—C7	118.9 (3)	O1—C66—C65	115.4 (3)
C57—C56—C7	108.2 (3)	C67—C66—C65	118.1 (3)
C58—C57—C56	119.3 (3)	C68—C67—C66	120.1 (3)
C58—C57—C1	122.4 (3)	C67—C68—C63	123.2 (3)
C56—C57—C1	110.7 (3)	S2—C70—S1	178.4 (3)
C57—C58—C59	119.2 (3)		

and that the structure has, in reality, the centrosymmetric space group $P2_1/n$. All H atoms were refined except H691, H692 and H693 which were included as riding atoms. The bond length involving H622 (C62—H622) was restrained.

Data collection: Stoe diffractometer software. Cell refinement: Stoe diffractometer software. Data reduction: Stoe diffractometer software. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1971), *SCHAKAL92* (Keller, 1992). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1208). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Although the systematic absences and the intensity statistics favoured the centrosymmetric space group, the phase problem could be solved only in the non-centrosymmetric space group $P2_1$ with two molecules in the asymmetric unit. In the course of the refinement, it was found that one molecule of the fullerene crystallizes with one molecule of carbon disulfide