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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55602 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI1026]

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Structures of Two (1:1) Adducts of [α,α-Bis(3,3,3-trifluoropropynyl)]benzyl Benzoate and Furan

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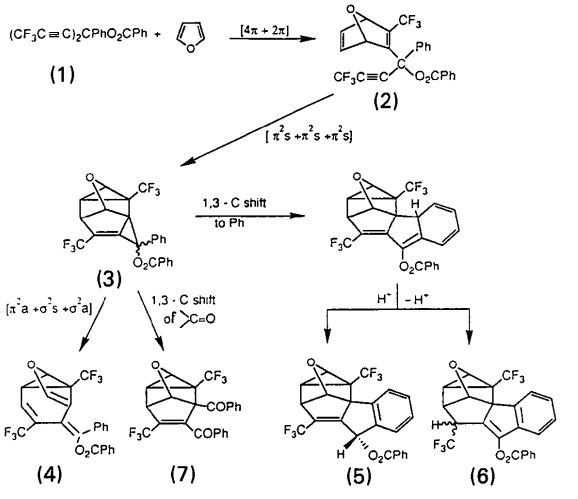
Abstract

[(*Z*)-5-(Benzoyloxybenzylidene)]-1,4-bis(trifluoromethyl)-8-oxatricyclo[4.3.0.$0^{2,9}$]nona-3,6-diene (4) and 11,12-benzo-10-benzoyloxy-2,8-bis(trifluoromethyl)-5-oxapentacyclo[7.3.0.$0^{1,6}$.$0^{2,4}$.$0^{3,7}$]dodec-8-ene (5) are two of four main (1:1) adducts of the title reactants. The crystallographical characterization of (4) and (5) assists in establishing the mechanistic pathways of the reaction. The ring strain in isomer (4) is particularly marked at double-bonded C6 where the three angles sum to 344.4 (7)°; in the three-membered ring, C2—C9 [1.542 (7) Å] is significantly longer than C1—C2 and C1—C9 [1.479 (6) and 1.470 (6) Å respectively] and the angles C2—C1—C9, C1—C2—C9 and C1—C9—C2 [63.1 (3), 58.2 (3) and 58.8 (3)° respectively] are all significantly different from 60°. The strain in isomer (5), which has two molecules of the same chirality in the asymmetric unit, does not distort the three-membered ring but gives rise to a long bond [C1—C6 = 1.59 (2) and 1.62 (2) Å in molecules 1 and 2, respectively], angles around C1 considerably distorted from tetrahedral, and a large angle at double-bonded C9 [C8—C9—C10 = 142 (1), 138 (1)°].

Comment

When [α,α-bis(3,3,3-trifluoropropynyl)]benzyl benzoate (1) undergoes Diels–Alder reaction with furan, four major (1:1) adducts $C_{24}H_{14}F_6O_3$ (4)–(7) can be isolated (besides minor components) from a solid product; crystallographic identification of (4) and (5) confirms the participation of the unstable intermediate adduct (3) formed by intramolecular ($\pi^2s + \pi^2s + \pi^2s$) cycloaddition from the initial alkyne Diels–Alder adduct (2) (Barlow, Tajammal & Tipping, 1989). Adducts (6) and (7) were identified by ^{1}H, ^{13}C and ^{19}F NMR; details of the preparation of all the materials have been given by Tajammal (1991). After chromatographic separation of (4)–(7) from the initial solid, (4) was recrystallized slowly from a mixture of petroleum ether (b.p. 313–333 K) and dichloromethane (3:5:1 *v*/*v*), and (5) from pentane.



A crystal structure determination of a saturated 7-oxa lactone derivative of the tricyclic ring system in (4) has been reported (Dulcere & Crandall, 1990). No other crystal structure with the ring system of (5) appears to have been reported.

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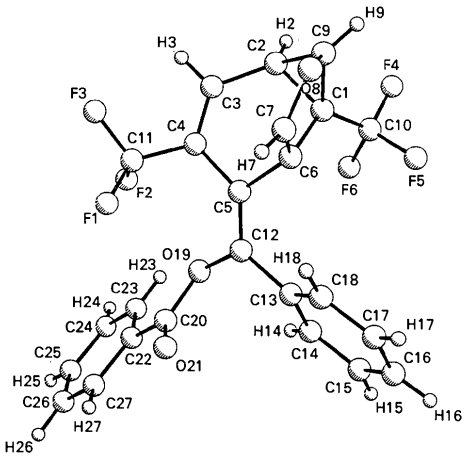

Fig. 1. View of (4) showing atom labelling; F7, F8 and F9, the lesser components of the disordered CF_3 at C10, are omitted for clarity.

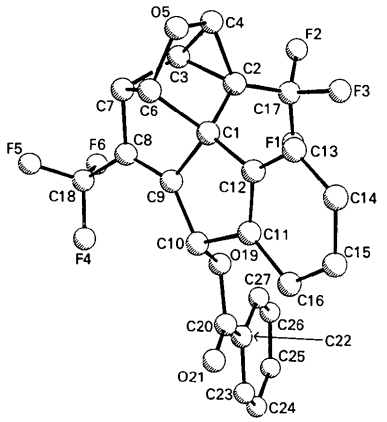

Fig. 2. View of one of the two independent molecules of (5) showing the atom labelling; H atoms are omitted for clarity. The other molecule, which has identical labelling suffixed with *A*, is not significantly different.

Experimental

Compound (4)

Crystal data

$C_{24}H_{14}F_6O_3$
M_r = 464.36
Monoclinic
$P2_1/c$
a = 9.526 (2) Å
b = 20.167 (2) Å
c = 11.067 (2) Å
β = 90.00 (2)°
V = 2126 (1) Å^3
Z = 4
D_x = 1.451 (1) Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 7.99–12.15°
μ = 0.123 mm^{-1}
T = 296 K
Blocks
0.3 × 0.3 × 0.2 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3144 measured reflections
1741 independent reflections
1246 observed reflections [$I>2.00\sigma(I)$]
R_{int} = 0.021
θ_{max} = 23.0°
$h = -10 \rightarrow 5$
$k = 0 \rightarrow 21$
$l = -12 \rightarrow 11$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F
Final R = 0.046
wR = 0.026
S = 3.52
1246 reflections
306 parameters
$w = 4F_o^2/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Program(s) used to solve structure: *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *SHELXS*86 (Sheldrick, 1985) and *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976) and *TEXSAN* (Molecular Structure Corporation, 1985). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978).

Compound (5)

Crystal data

$C_{24}H_{14}F_6O_3$
M_r = 464.36
Monoclinic
Cc
a = 13.138 (2) Å
b = 13.897 (2) Å
c = 21.912 (2) Å
β = 91.77 (2)°
V = 3999 (1) Å^3
Z = 8
D_x = 1.543 (1) Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 9.94–15.67°
μ = 0.131 mm^{-1}
T = 296 K
Blocks
0.4 × 0.4 × 0.3 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3690 measured reflections
3516 independent reflections
2454 observed reflections [$I>2.00\sigma(I)$]
R_{int} = 0.017
θ_{max} = 25.0°
$h = 0 \rightarrow 15$
$k = 0 \rightarrow 16$
$l = -24 \rightarrow 25$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F
Final R = 0.085
wR = 0.059
S = 5.89
2454 reflections
593 parameters
$w = 4F_o^2/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max}$ = 0.076
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
(4)				
F1	0.8536 (3)	0.66210 (15)	0.3752 (3)	9.5 (2)
F2	0.7715 (3)	0.68539 (12)	0.2030 (3)	9.3 (2)
F3	0.6393 (3)	0.69123 (13)	0.3570 (4)	11.2 (2)
F4	0.5062 (4)	0.4036 (4)	0.0647 (5)	13.0 (4)
F5	0.6877 (8)	0.3598 (2)	0.1348 (3)	12.4 (4)
F6	0.7001 (5)	0.4489 (2)	0.0454 (3)	9.6 (3)
O8	0.5550 (3)	0.43092 (13)	0.4442 (3)	5.9 (2)
O19	0.9837 (3)	0.58870 (12)	0.1934 (2)	4.4 (1)
O21	1.1688 (3)	0.59249 (14)	0.3202 (3)	6.3 (2)
C1	0.6027 (4)	0.4516 (2)	0.2390 (4)	4.4 (2)
C2	0.4998 (5)	0.5054 (2)	0.2594 (4)	5.1 (2)
C3	0.5620 (5)	0.5709 (2)	0.2894 (4)	5.2 (2)
C4	0.6973 (5)	0.5845 (2)	0.2912 (4)	4.8 (2)
C5	0.8023 (4)	0.5294 (2)	0.2843 (4)	4.2 (2)
C6	0.7244 (4)	0.4683 (2)	0.3184 (4)	4.1 (2)
C7	0.6851 (5)	0.4562 (2)	0.4303 (4)	5.2 (3)
C9	0.4926 (5)	0.4393 (2)	0.3293 (5)	5.7 (3)
C10	0.6223 (6)	0.4159 (3)	0.1218 (5)	6.0 (3)
C11	0.7418 (6)	0.6544 (3)	0.3069 (6)	7.5 (4)
C12	0.9344 (5)	0.5299 (2)	0.2459 (4)	4.1 (2)
C13	1.0255 (4)	0.4717 (2)	0.2320 (4)	4.2 (2)
C14	1.1032 (4)	0.4648 (2)	0.1287 (4)	4.8 (2)
C15	1.1823 (5)	0.4085 (3)	0.1096 (5)	6.3 (3)
C16	1.1853 (5)	0.3579 (2)	0.1917 (6)	7.5 (3)
C17	1.1100 (5)	0.3655 (2)	0.2968 (5)	7.7 (3)
C18	1.0319 (5)	0.4223 (2)	0.3183 (4)	6.0 (3)
C20	1.1061 (5)	0.6147 (2)	0.2349 (4)	4.2 (2)
C22	1.1514 (4)	0.6725 (2)	0.1620 (4)	4.0 (2)
C23	1.0775 (4)	0.6942 (2)	0.0639 (4)	5.2 (2)
C24	1.1252 (5)	0.7485 (2)	−0.0018 (4)	6.3 (3)
C25	1.2439 (6)	0.7807 (2)	0.0332 (4)	6.6 (3)
C26	1.3192 (5)	0.7599 (2)	0.1305 (5)	6.9 (3)
C27	1.2714 (5)	0.7054 (2)	0.1973 (4)	5.5 (3)
F7	0.754 (2)	0.4058 (14)	0.095 (2)	4.1 (6)
F8	0.559 (2)	0.3578 (10)	0.135 (2)	4.1 (6)
F9	0.560 (3)	0.4485 (9)	0.035 (2)	4.1 (6)
(5)				
F1	0.143	0.7404 (8)	0.763	6.5 (6)
F2	0.0060 (10)	0.6702 (7)	0.7283 (7)	6.7 (5)
F3	0.0038 (12)	0.8201 (8)	0.7586 (7)	9.3 (7)
F4	0.3214 (9)	0.5895 (6)	0.9584 (7)	6.8 (6)
F5	0.2059 (10)	0.4922 (8)	0.9859 (7)	8.7 (7)
F6	0.2538 (9)	0.4869 (7)	0.8951 (7)	8.3 (7)
O5	−0.1076 (9)	0.6869 (7)	0.9071 (7)	5.5 (6)
O19	0.3195 (8)	0.7701 (6)	0.8691 (7)	3.7 (4)
O21	0.4259 (10)	0.8679 (7)	0.9230 (7)	4.7 (5)
C1	0.0601 (11)	0.7504 (9)	0.8908 (8)	3.6 (7)
C2	0.0166 (11)	0.7007 (10)	0.8316 (9)	3.8 (7)
C3	0.0062 (11)	0.5963 (9)	0.8505 (9)	4.0 (7)
C4	−0.0858 (12)	0.6601 (10)	0.8468 (9)	4.6 (8)
C6	−0.0059 (11)	0.6856 (10)	0.9347 (9)	4.2 (7)
C7	0.0437 (12)	0.5897 (9)	0.9184 (9)	3.7 (7)
C8	0.1529 (11)	0.6174 (9)	0.9236 (8)	3.1 (7)
C9	0.1654 (10)	0.7083 (9)	0.9104 (8)	3.2 (7)
C10	0.2432 (11)	0.7869 (9)	0.9136 (8)	3.5 (7)
C11	0.1782 (11)	0.8773 (9)	0.9000 (8)	3.3 (7)
C12	0.0760 (12)	0.8588 (9)	0.8919 (8)	3.8 (7)
C13	0.0049 (12)	0.9263 (11)	0.8848 (9)	4.6 (8)
C14	0.0391 (15)	1.0221 (12)	0.8867 (10)	6 (1)
C15	0.1432 (13)	1.0474 (12)	0.8925 (10)	6 (1)
C16	0.2182 (14)	0.9755 (11)	0.9007 (10)	5.1 (9)
C17	0.044 (2)	0.7313 (13)	0.7719 (10)	6 (1)
C18	0.2330 (14)	0.5480 (10)	0.9428 (10)	4.5 (8)
C20	0.4125 (11)	0.8163 (10)	0.8798 (10)	4.2 (8)
C22	0.4877 (11)	0.7846 (9)	0.8343 (9)	4.0 (7)
C23	0.5864 (12)	0.8195 (10)	0.8424 (9)	4.8 (8)
C24	0.6603 (12)	0.7969 (12)	0.8056 (11)	6 (1)
C25	0.6390 (13)	0.7418 (13)	0.7542 (10)	5 (1)
C26	0.540 (2)	0.7066 (14)	0.7432 (11)	7 (1)
C27	0.4676 (13)	0.7321 (11)	0.7810 (10)	5 (1)
F1*A*	0.6816 (8)	0.4780 (8)	0.7124 (5)	7.2 (6)
F2*A*	0.8122 (11)	0.4141 (8)	0.7540 (7)	8.2 (7)
F3*A*	0.8122 (10)	0.5598 (7)	0.7262 (7)	7.7 (6)
F4*A*	0.5250 (9)	0.3436 (6)	0.5145 (7)	5.9 (5)
F5*A*	0.6371 (10)	0.2472 (7)	0.4834 (8)	9.2 (7)
F6*A*	0.5894 (10)	0.2356 (7)	0.5732 (7)	7.9 (7)
O5*A*	0.9535 (9)	0.4261 (7)	0.5819 (7)	5.7 (6)
O19*A*	0.5290 (9)	0.5255 (6)	0.6044 (7)	3.8 (5)
O21*A*	0.4225 (10)	0.6184 (7)	0.5437 (8)	5.3 (6)
C1*A*	0.7854 (11)	0.4937 (9)	0.5902 (8)	3.3 (7)
C2*A*	0.8169 (11)	0.4426 (10)	0.6503 (9)	3.7 (7)
C3*A*	0.8268 (11)	0.3348 (10)	0.6320 (8)	4.2 (8)
C4*A*	0.9200 (13)	0.3962 (10)	0.6394 (10)	5.1 (9)
C6*A*	0.8593 (12)	0.4299 (10)	0.5487 (8)	4.3 (8)
C7*A*	0.8013 (11)	0.3348 (9)	0.5649 (9)	4.7 (8)
C8*A*	0.6912 (11)	0.3678 (9)	0.5504 (9)	3.6 (7)
C9*A*	0.6849 (11)	0.4584 (9)	0.5662 (8)	2.8 (6)
C10*A*	0.6088 (11)	0.5406 (8)	0.5604 (8)	3.1 (6)
C11*A*	0.6736 (11)	0.6270 (8)	0.5753 (8)	3.5 (7)
C12*A*	0.7725 (11)	0.5974 (9)	0.5909 (8)	3.9 (7)
C13*A*	0.8496 (12)	0.6695 (10)	0.6006 (9)	4.9 (8)
C14*A*	0.8202 (13)	0.7700 (12)	0.6001 (10)	6 (1)
C15*A*	0.7232 (15)	0.7920 (9)	0.5888 (9)	5 (1)
C16*A*	0.6408 (12)	0.7224 (11)	0.5743 (8)	3.8 (7)
C17*A*	0.7849 (13)	0.4732 (13)	0.7103 (9)	4.5 (9)
C18*A*	0.6092 (14)	0.2993 (11)	0.5317 (11)	5 (1)
C20*A*	0.4382 (11)	0.5722 (10)	0.5878 (9)	4.0 (8)
C22*A*	0.3618 (11)	0.5461 (8)	0.6368 (9)	4.0 (7)
C23*A*	0.2605 (11)	0.5739 (10)	0.6199 (10)	4.7 (8)
C24*A*	0.1881 (13)	0.5525 (12)	0.6657 (10)	6 (1)
C25*A*	0.2147 (15)	0.5063 (13)	0.7151 (10)	7 (1)
C26*A*	0.3117 (12)	0.4802 (15)	0.7296 (10)	7 (1)
C27*A*	0.3870 (12)	0.5004 (11)	0.6895 (10)	5.0 (8)

Table 2. *Selected geometric parameters* (Å, °)

Compound (4)			
O8—C7	1.349 (6)	C2—C9	1.542 (7)
O8—C9	1.414 (6)	C3—C4	1.318 (6)
O19—C12	1.402 (5)	C4—C5	1.498 (6)
O19—C20	1.359 (5)	C4—C11	1.482 (7)
O21—C20	1.203 (5)	C5—C6	1.487 (6)
C1—C2	1.479 (6)	C5—C12	1.328 (6)
C1—C6	1.493 (6)	C6—C7	1.317 (7)
C1—C9	1.470 (6)	C12—C13	1.467 (6)
C1—C10	1.496 (7)	C20—C22	1.482 (6)
C2—C3	1.484 (6)		
C7—O8—C9	103.8 (3)	C4—C5—C12	130.0 (4)
C12—O19—C20	118.3 (3)	C6—C5—C12	124.1 (4)
C2—C1—C6	105.1 (3)	C1—C6—C5	115.2 (4)
C2—C1—C9	63.1 (3)	C1—C6—C7	106.9 (4)
C2—C1—C10	124.7 (4)	C5—C6—C7	122.3 (4)
C6—C1—C9	101.1 (4)	O8—C7—C6	116.0 (4)
C6—C1—C10	121.4 (4)	O8—C9—C1	109.3 (4)
C9—C1—C10	126.7 (4)	O8—C9—C2	122.4 (4)
C1—C2—C3	115.0 (4)	C1—C9—C2	58.8 (3)
C1—C2—C9	58.2 (3)	O19—C12—C5	117.2 (3)
C3—C2—C9	132.4 (4)	O19—C12—C13	115.8 (3)
C2—C3—C4	125.4 (4)	C5—C12—C13	126.0 (4)
C3—C4—C5	119.8 (4)	O19—C20—O21	123.2 (4)
C3—C4—C11	118.7 (4)	O19—C20—C22	111.7 (3)
C5—C4—C11	121.4 (4)	O21—C20—C22	125.2 (4)
C4—C5—C6	105.6 (3)		
Compound (5)			
O5—C4	1.41 (2)	O5*A*—C4*A*	1.41 (2)
O5—C6	1.45 (1)	O5*A*—C6*A*	1.42 (2)
C1—C2	1.56 (2)	C1*A*—C2*A*	1.54 (2)
C1—C6	1.59 (2)	C1*A*—C6*A*	1.62 (2)
C1—C9	1.55 (2)	C1*A*—C9*A*	1.49 (2)
C1—C12	1.52 (2)	C1*A*—C12*A*	1.45 (2)
C2—C3	1.52 (2)	C2*A*—C3*A*	1.56 (2)
C2—C4	1.51 (2)	C2*A*—C4*A*	1.53 (2)
C2—C17	1.43 (2)	C2*A*—C17*A*	1.46 (2)
C3—C4	1.50 (2)	C3*A*—C4*A*	1.50 (2)

C3—C7	1.55 (2)	C3A—C7A	1.50 (2)
C6—C7	1.53 (2)	C6A—C7A	1.57 (2)
C7—C8	1.49 (2)	C7A—C8A	1.54 (2)
C8—C9	1.31 (2)	C8A—C9A	1.31 (2)
C8—C18	1.48 (2)	C8A—C18A	1.49 (2)
C9—C10	1.50 (2)	C9A—C10A	1.52 (2)
C10—C11	1.54 (2)	C10A—C11A	1.50 (2)
C11—C12	1.37 (2)	C11A—C12A	1.39 (2)
C4—O5—C6	100 (1)	C4A—O5A—C6A	100 (1)
C2—C1—C6	93 (1)	C2A—C1A—C6A	94 (1)
C2—C1—C9	111 (1)	C2A—C1A—C9A	111 (1)
C2—C1—C12	120 (1)	C2A—C1A—C12A	118 (1)
C6—C1—C9	97 (1)	C6A—C1A—C9A	99 (1)
C6—C1—C12	129 (1)	C6A—C1A—C12A	129 (1)
C9—C1—C12	104 (1)	C9A—C1A—C12A	103 (1)
C1—C2—C3	103 (1)	C1A—C2A—C3A	104 (1)
C1—C2—C4	107 (1)	C1A—C2A—C4A	106 (1)
C1—C2—C17	122 (1)	C1A—C2A—C17A	124 (1)
C3—C2—C4	59.4 (9)	C3A—C2A—C4A	58.1 (9)
C3—C2—C17	124 (1)	C3A—C2A—C17A	123 (1)
C4—C2—C17	124 (1)	C4A—C2A—C17A	123 (1)
C2—C3—C4	59.9 (8)	C2A—C3A—C4A	59.9 (9)
C2—C3—C7	107 (1)	C2A—C3A—C7A	104 (1)
C4—C3—C7	109 (1)	C4A—C3A—C7A	105 (1)
O5—C4—C2	108 (1)	O5A—C4A—C2A	109 (1)
O5—C4—C3	107 (1)	O5A—C4A—C3A	110 (1)
C2—C4—C3	60.6 (9)	C2A—C4A—C3A	62.0 (9)
O5—C6—C1	105 (1)	O5A—C6A—C1A	105 (1)
O5—C6—C7	107 (1)	O5A—C6A—C7A	106 (1)
C1—C6—C7	96 (1)	C1A—C6A—C7A	92 (1)
C3—C7—C6	93 (1)	C3A—C7A—C6A	97 (1)
C3—C7—C8	110 (1)	C3A—C7A—C8A	112 (1)
C6—C7—C8	100 (1)	C6A—C7A—C8A	99 (1)
C7—C8—C9	111 (1)	C7A—C8A—C9A	107 (1)
C7—C8—C18	122 (1)	C7A—C8A—C18A	122 (1)
C9—C8—C18	127 (1)	C9A—C8A—C18A	130 (1)
C1—C9—C8	108 (1)	C1A—C9A—C8A	110 (1)
C1—C9—C10	110 (1)	C1A—C9A—C10A	111 (1)
C8—C9—C10	142 (1)	C8A—C9A—C10A	138 (1)
O19—C10—C9	110 (1)	O19A—C10A—C9A	109 (1)
O19—C10—C11	113 (1)	O19A—C10A—C11A	113 (1)
C9—C10—C11	102 (1)	C9A—C10A—C11A	102.4 (9)
C10—C11—C12	114 (1)	C10A—C11A—C12A	110 (1)
C10—C11—C16	124 (1)	C10A—C11A—C16A	126 (1)
C12—C11—C16	122 (1)	C12A—C11A—C16A	125 (1)
C1—C12—C11	109 (1)	C1A—C12A—C11A	114 (1)
C1—C12—C13	127 (1)	C1A—C12A—C13A	128 (1)
C11—C12—C13	124 (1)	C11A—C12A—C13A	119 (1)

The data for compounds (4) and (5) were corrected for Lorentz and polarization effects. Most H atoms were located in $\Delta\rho$ maps, but were held fixed during refinements at calculated positions which were updated after each sequence of refinement cycles (no significant improvement in the agreement with experiment was achieved by refining hydrogen parameters). In compound (4), the F atoms at C10 are disordered. F4, F5 and F6 form the major component of the CF_3 group with a common fluorine site occupancy factor, s, which refined to 0.89(1); these atoms were otherwise refined individually and anisotropically. F7, F8 and F9 were refined as a triangular group with a group isotropic vibrational parameter; their common site occupancies were constrained to $1 - s$.

The final R of 0.085 for compound (5) (wR = 0.059) occurs because of small electron density peaks in positions attributable to a fragmented and highly disordered H-bonded water network in the cavities and between the independent molecules; the water could not be removed totally by drying.

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Lists of structure factors, anisotropic thermal parameters and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55655 (46 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL1014]

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Structure of Pentabenzylcyclopentadiene

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Abstract

The crystal structure analysis of pentabenzylcyclopentadiene {1,1′,1″,1‴,1⁗-[(1,3-cyclopentadiene-1,2,3,4,5-pentayl)pentakis(methylene)]pentakis(benzene)} shows groups of two and three benzyl substituents on opposite sides of the planar cyclopentadiene ring. The compound is monomeric.

Comment

Substituting the cyclopentadienyl ligand in organoelement and organometal compounds with the bulky pentabenzylcyclopentadienyl system $[C_5(CH_2Ph)_5]^-$

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