SUPPORTING INFORMATION

4,5-Dehydro- and 4,5,15,16-*bis*-(dehydro)octafluoro[2.2]paracyclophanes: Facile Generation and Extraordinary Diels-Alder Reactivity

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X-ray experimental: Data were collected at 173 K on a Siemens SMART PLATFORM equipped with a CCD area detector and a graphite monochromator utilizing MoK α radiation (λ = 0.71073 Å). Cell parameters were refined using up to 8192 reflections. A full sphere of data (1381 frames) was collected using the ω -scan method (0.3° frame width). The first 50 frames were remeasured at the end of data collection to monitor instrument and crystal stability (maximum correction on I was < 1 %). Absorption corrections by integration were applied based on measured indexed crystal faces.

The structure was solved by the Direct Methods in *SHELXTL5*, and refined using full-matrix least squares. The non-H atoms were treated anisotropically, whereas the hydrogen atoms were calculated in ideal positions and were riding on their respective carbon atoms. A total of 361 parameters were refined in the final cycle of refinement using 4305 reflections with $I > 2\sigma(I)$ to yield R_1 and wR_2 of 4.67% and 11.73%, respectively. Refinement was done using F^2 .

Sheldrick, G. M. (1998). *SHELXTL5*. Bruker-AXS, Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for anthracene adduct, **5**.

Identification code	yz03t	
Empirical formula	C ₂₈ H ₁₆ F ₈	
Formula weight	504.41	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.9041(5) Å	α = 101.308(1)°.
	b = 9.3253(5) Å	β = 91.161(1)°.
	c = 14.3897(8) Å	γ = 107.872(1)°.
Volume	1110.9(1) Å ³	
Z	2	
Density (calculated)	1.508 Mg/m ³	
Absorption coefficient	0.134 mm ⁻¹	
F(000)	512	
Crystal size	0.23 x 0.11 x 0.10 mm ³	
Theta range for data collection	1.45 to 27.50°.	
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18	
Reflections collected	10130	
Independent reflections	5004 [R(int) = 0.0331]	
Completeness to theta = 27.50°	97.9 %	
Absorption correction	Integration	
Max. and min. transmission	0.9915 and 0.9717	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5004 / 0 / 343	
Goodness-of-fit on F ²	1.066	
Final R indices [I > 2σ(I)]	R1 = 0.0413, wR2 = 0.1035 [3846]	
R indices (all data)	R1 = 0.0598, wR2 = 0.1162	
Largest diff. peak and hole	0.299 and -0.237 e.Å ⁻³	

$$R1 = \sum(|F_o| - |F_c|) / \sum F_o$$

$$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$$

$$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$$

$$w = 1/[\sigma^2(F_o^2) + (0.0464 \cdot p)^2 + 0.55 \cdot p], p = [\max(F_o^2, 0) + 2 \cdot F_c^2] / 3$$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for anthracene adduct, **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F1	6306(2)	4438(2)	1778(1)	54(1)
C1	3849(2)	1170(2)	2698(1)	22(1)
F2	6404(1)	2100(2)	1375(1)	44(1)
C2	2621(2)	985(2)	3310(1)	21(1)
F3	4807(2)	3541(2)	184(1)	53(1)
C3	2202(2)	2264(2)	3748(1)	24(1)
F4	3913(2)	1142(1)	295(1)	43(1)
C4	3278(2)	3725(2)	3776(1)	29(1)
F5	20(2)	4519(2)	3835(1)	56(1)
C5	4494(2)	3910(2)	3194(1)	31(1)
F6	-1839(1)	2351(2)	3295(1)	54(1)
C6	4670(2)	2637(2)	2562(1)	27(1)
F7	534(2)	2905(2)	4918(1)	46(1)
C7	5414(2)	2930(2)	1653(2)	34(1)
F8	-441(1)	757(1)	3885(1)	42(1)
C8	4137(2)	2607(2)	781(1)	36(1)
C9	2594(2)	2801(2)	1093(1)	32(1)
C10	1344(2)	1497(2)	1153(1)	31(1)
C11	229(2)	1612(2)	1794(1)	31(1)
C12	380(2)	3028(2)	2385(1)	32(1)
C13	1425(2)	4360(2)	2182(2)	37(1)
C14	2527(2)	4247(2)	1526(2)	36(1)
C15	-251(2)	3053(2)	3348(2)	37(1)
C16	552(2)	2220(2)	3999(1)	30(1)
C17	4067(2)	-360(2)	2212(1)	23(1)
C18	4412(2)	-1043(2)	3038(1)	23(1)
C19	5759(2)	-1425(2)	3218(1)	30(1)
C20	5901(2)	-1997(2)	4026(1)	33(1)
C21	4709(2)	-2193(2)	4636(1)	32(1)
C22	3355(2)	-1808(2)	4460(1)	27(1)
C23	3215(2)	-1231(2)	3659(1)	22(1)

C24	1844(2)	-712(2)	3366(1)	22(1)
C25	1255(2)	-1587(2)	2352(1)	22(1)
C26	-281(2)	-2490(2)	2017(1)	28(1)
C27	-611(2)	-3199(2)	1060(1)	34(1)
C28	581(2)	-3023(2)	448(1)	33(1)
C30	2454(2)	-1408(2)	1733(1)	23(1)
C29	2130(2)	-2135(2)	782(1)	28(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for anthracene adduct, **5**.

F1-C7	1.361(2)
C1-C6	1.393(2)
C1-C2	1.408(2)
C1-C17	1.532(2)
F2-C7	1.359(2)
C2-C3	1.395(2)
C2-C24	1.539(2)
F3-C8	1.359(2)
C3-C4	1.397(2)
C3-C16	1.511(2)
F4-C8	1.359(2)
C4-C5	1.373(3)
C4-H4A	0.9500
F5-C15	1.354(2)
C5-C6	1.399(3)
C5-H5A	0.9500
F6-C15	1.357(2)
C6-C7	1.512(3)
F7-C16	1.354(2)
C7-C8	1.594(3)
F8-C16	1.355(2)
C8-C9	1.505(3)
C9-C14	1.390(3)
C9-C10	1.393(3)
C10-C11	1.382(3)
C10-H10A	0.9500
C11-C12	1.390(3)
C11-H11A	0.9500
C12-C13	1.392(3)
C12-C15	1.505(3)
C13-C14	1.389(3)
C13-H13A	0.9500
C14-H14A	0.9500
C15-C16	1.609(3)

C17-C18	1.521(2)
C17-C30	1.525(2)
C17-H17A	1.0000
C18-C19	1.385(2)
C18-C23	1.397(2)
C19-C20	1.389(3)
C19-H19A	0.9500
C20-C21	1.383(3)
C20-H20A	0.9500
C21-C22	1.391(3)
C21-H21A	0.9500
C22-C23	1.382(2)
C22-H22A	0.9500
C23-C24	1.525(2)
C24-C25	1.520(2)
C24-H24A	1.0000
C25-C26	1.385(2)
C25-C30	1.396(2)
C26-C27	1.389(3)
C26-H26A	0.9500
C27-C28	1.384(3)
C27-H27A	0.9500
C28-C29	1.391(3)
C28-H28A	0.9500
C30-C29	1.385(2)
C29-H29A	0.9500

C6-C1-C2	119.69(15)
C6-C1-C17	127.17(15)
C2-C1-C17	113.08(14)
C3-C2-C1	119.63(15)
C3-C2-C24	127.96(15)
C1-C2-C24	112.34(14)
C2-C3-C4	117.84(16)
C2-C3-C16	124.77(16)
C4-C3-C16	115.96(15)

C5-C4-C3	120.43(16)
C5-C4-H4A	119.8
C3-C4-H4A	119.8
C4-C5-C6	120.43(16)
C4-C5-H5A	119.8
C6-C5-H5A	119.8
C1-C6-C5	118.06(16)
C1-C6-C7	123.35(16)
C5-C6-C7	116.94(16)
F2-C7-F1	106.03(15)
F2-C7-C6	113.85(15)
F1-C7-C6	109.66(16)
F2-C7-C8	107.66(16)
F1-C7-C8	106.25(15)
C6-C7-C8	112.90(15)
F4-C8-F3	106.02(16)
F4-C8-C9	110.76(16)
F3-C8-C9	112.67(16)
F4-C8-C7	106.69(15)
F3-C8-C7	107.59(16)
C9-C8-C7	112.71(16)
C14-C9-C10	119.10(18)
C14-C9-C8	120.28(18)
C10-C9-C8	118.90(17)
C11-C10-C9	119.96(17)
C11-C10-H10A	120.0
C9-C10-H10A	120.0
C10-C11-C12	119.55(18)
C10-C11-H11A	120.2
C12-C11-H11A	120.2
C11-C12-C13	119.16(18)
C11-C12-C15	118.66(18)
C13-C12-C15	120.31(18)
C14-C13-C12	119.81(18)
C14-C13-H13A	120.1
C12-C13-H13A	120.1

C13-C14-C9	119.43(18)
C13-C14-H14A	120.3
C9-C14-H14A	120.3
F5-C15-F6	106.37(15)
F5-C15-C12	110.88(17)
F6-C15-C12	112.70(17)
F5-C15-C16	106.93(16)
F6-C15-C16	106.80(16)
C12-C15-C16	112.76(14)
F7-C16-F8	106.13(15)
F7-C16-C3	112.05(15)
F8-C16-C3	111.98(14)
F7-C16-C15	107.45(14)
F8-C16-C15	106.15(15)
C3-C16-C15	112.65(15)
C18-C17-C30	106.16(13)
C18-C17-C1	103.76(13)
C30-C17-C1	107.02(13)
C18-C17-H17A	113.1
C30-C17-H17A	113.1
C1-C17-H17A	113.1
C19-C18-C23	120.38(16)
C19-C18-C17	126.68(16)
C23-C18-C17	112.92(14)
C18-C19-C20	119.06(17)
C18-C19-H19A	120.5
C20-C19-H19A	120.5
C21-C20-C19	120.40(17)
C21-C20-H20A	119.8
C19-C20-H20A	119.8
C20-C21-C22	120.82(17)
C20-C21-H21A	119.6
C22-C21-H21A	119.6
C23-C22-C21	118.84(17)
C23-C22-H22A	120.6
C21-C22-H22A	120.6

C22-C23-C18	120.49(16)
C22-C23-C24	126.14(15)
C18-C23-C24	113.36(14)
C25-C24-C23	106.63(13)
C25-C24-C2	106.15(13)
C23-C24-C2	104.47(13)
C25-C24-H24A	113.0
C23-C24-H24A	113.0
C2-C24-H24A	113.0
C26-C25-C30	120.22(16)
C26-C25-C24	126.92(15)
C30-C25-C24	112.87(14)
C25-C26-C27	119.14(17)
C25-C26-H26A	120.4
C27-C26-H26A	120.4
C28-C27-C26	120.56(17)
C28-C27-H27A	119.7
C26-C27-H27A	119.7
C27-C28-C29	120.57(17)
C27-C28-H28A	119.7
C29-C28-H28A	119.7
C29-C30-C25	120.61(16)
C29-C30-C17	125.90(15)
C25-C30-C17	113.49(14)
C30-C29-C28	118.89(17)
C30-C29-H29A	120.6
C28-C29-H29A	120.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F1	48(1)	40(1)	65(1)	23(1)	13(1)	-8(1)
C1	22(1)	23(1)	23(1)	6(1)	0(1)	7(1)
F2	35(1)	61(1)	47(1)	25(1)	18(1)	22(1)
C2	22(1)	21(1)	20(1)	3(1)	-1(1)	7(1)
F3	60(1)	63(1)	55(1)	43(1)	25(1)	25(1)
C3	27(1)	25(1)	22(1)	2(1)	0(1)	10(1)
F4	48(1)	45(1)	39(1)	6(1)	8(1)	22(1)
C4	34(1)	22(1)	31(1)	0(1)	-4(1)	11(1)
F5	85(1)	47(1)	52(1)	3(1)	13(1)	46(1)
C5	30(1)	21(1)	40(1)	8(1)	-5(1)	3(1)
F6	34(1)	86(1)	56(1)	25(1)	11(1)	33(1)
C6	22(1)	26(1)	32(1)	10(1)	2(1)	5(1)
F7	53(1)	62(1)	31(1)	1(1)	11(1)	34(1)
C7	29(1)	30(1)	44(1)	17(1)	10(1)	5(1)
F8	28(1)	36(1)	65(1)	15(1)	12(1)	13(1)
C8	43(1)	37(1)	34(1)	20(1)	11(1)	14(1)
C9	38(1)	36(1)	29(1)	15(1)	2(1)	17(1)
C10	39(1)	29(1)	28(1)	7(1)	-3(1)	16(1)
C11	31(1)	30(1)	33(1)	8(1)	-4(1)	12(1)
C12	32(1)	34(1)	35(1)	8(1)	-1(1)	19(1)
C13	44(1)	28(1)	44(1)	8(1)	-4(1)	20(1)
C14	41(1)	30(1)	43(1)	17(1)	-1(1)	12(1)
C15	36(1)	39(1)	41(1)	4(1)	5(1)	23(1)
C16	32(1)	31(1)	28(1)	2(1)	7(1)	15(1)
C17	23(1)	24(1)	24(1)	6(1)	7(1)	9(1)
C18	25(1)	19(1)	25(1)	3(1)	2(1)	8(1)
C19	27(1)	26(1)	36(1)	2(1)	1(1)	10(1)
C20	32(1)	26(1)	41(1)	2(1)	-9(1)	13(1)
C21	41(1)	21(1)	32(1)	6(1)	-9(1)	7(1)
C22	32(1)	22(1)	26(1)	5(1)	0(1)	6(1)
C23	25(1)	17(1)	24(1)	2(1)	1(1)	6(1)

C24	23(1)	21(1)	23(1)	6(1)	5(1)	7(1)
C25	26(1)	17(1)	26(1)	6(1)	3(1)	9(1)
C26	27(1)	24(1)	35(1)	10(1)	2(1)	7(1)
C27	34(1)	25(1)	39(1)	6(1)	-9(1)	3(1)
C28	46(1)	24(1)	27(1)	3(1)	-4(1)	11(1)
C30	27(1)	19(1)	25(1)	6(1)	3(1)	10(1)
C29	38(1)	24(1)	25(1)	5(1)	5(1)	15(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **5**.

	x	y	z	U(eq)
H4A	3167	4598	4202	35
H5A	5222	4908	3220	37
H10A	1258	529	754	37
H11A	-636	728	1829	37
H13A	1383	5344	2492	44
H14A	3229	5150	1374	44
H17A	4918	-230	1764	28
H19A	6573	-1298	2796	36
H20A	6823	-2256	4160	40
H21A	4817	-2594	5183	38
H22A	2541	-1940	4882	33
H24A	989	-853	3812	26
H26A	-1098	-2622	2438	34
H27A	-1663	-3810	823	41
H28A	339	-3512	-206	39
H29A	2951	-2029	364	33

Table 1. Crystal data and structure refinement for *endo* furan adduct, **7a**.

Identification code	yz04	
Empirical formula	C ₂₀ H ₁₀ F ₈ O	
Formula weight	418.28	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P3(2)21	
Unit cell dimensions	a = 9.2358(4) Å	α = 90°.
	b = 9.2358(4) Å	β = 90°.
	c = 33.198(2) Å	γ = 120°.
Volume	2452.4(2) Å ³	
Z	6	
Density (calculated)	1.699 Mg/m ³	
Absorption coefficient	0.167 mm ⁻¹	
F(000)	1260	
Crystal size	0.19 x 0.11 x 0.08 mm ³	
Theta range for data collection	1.84 to 27.50°.	
Index ranges	-11 ≤ h ≤ 12, -11 ≤ k ≤ 12, -42 ≤ l ≤ 42	
Reflections collected	21640	
Independent reflections	3743 [R(int) = 0.0437]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9874 and 0.9725	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3743 / 0 / 265	
Goodness-of-fit on F ²	1.080	
Final R indices [I > 2σ(I)]	R1 = 0.0424, wR2 = 0.0929 [3036]	
R indices (all data)	R1 = 0.0583, wR2 = 0.1029	
Absolute structure parameter	0.3(7)	
Extinction coefficient	0.0082(8)	
Largest diff. peak and hole	0.345 and -0.372 e.Å ⁻³	
$R1 = \sum(F_o - F_c) / \sum F_o $		
$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$		
$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$		
$w = 1/[\sigma^2(F_o^2) + (0.0350 \cdot p)^2 + 1.31 \cdot p], p = [\max(F_o^2, 0) + 2 \cdot F_c^2] / 3$		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O1	6772(2)	8635(2)	636(1)	40(1)
F1	10034(3)	5370(3)	-23(1)	68(1)
F2	10844(2)	7761(2)	259(1)	72(1)
F3	11300(2)	4838(3)	548(1)	66(1)
F4	11416(2)	6858(3)	902(1)	73(1)
F5	2937(2)	347(2)	1009(1)	54(1)
F6	3134(2)	1746(2)	1555(1)	54(1)
F7	1874(2)	2138(2)	748(1)	53(1)
F8	3174(2)	4096(2)	1196(1)	45(1)
C1	7437(3)	6625(3)	526(1)	30(1)
C2	5805(3)	5859(3)	682(1)	29(1)
C3	4725(3)	4165(3)	631(1)	30(1)
C4	5168(3)	3343(3)	341(1)	34(1)
C5	6767(3)	4088(3)	190(1)	35(1)
C6	7994(3)	5695(3)	321(1)	31(1)
C7	9785(3)	6114(3)	305(1)	42(1)
C8	10361(3)	5476(4)	686(1)	43(1)
C9	8937(3)	4262(3)	945(1)	36(1)
C10	8354(3)	4900(3)	1245(1)	36(1)
C11	6716(3)	4000(3)	1373(1)	36(1)
C12	5641(3)	2459(3)	1196(1)	35(1)
C13	6319(4)	1691(3)	961(1)	39(1)
C14	7963(4)	2587(3)	835(1)	40(1)
C15	3809(3)	1894(3)	1181(1)	39(1)
C16	3387(3)	3109(3)	927(1)	36(1)
C17	8245(3)	8455(3)	668(1)	37(1)
C18	8435(4)	8497(3)	1128(1)	41(1)
C19	6893(3)	7780(3)	1274(1)	40(1)
C20	5743(3)	7285(3)	909(1)	36(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **7a**.

O1-C20	1.449(3)
O1-C17	1.455(3)
F1-C7	1.367(3)
F2-C7	1.344(3)
F3-C8	1.349(3)
F4-C8	1.359(3)
F5-C15	1.365(3)
F6-C15	1.365(3)
F7-C16	1.362(3)
F8-C16	1.360(3)
C1-C6	1.381(3)
C1-C2	1.406(3)
C1-C17	1.541(3)
C2-C3	1.383(3)
C2-C20	1.543(3)
C3-C4	1.408(3)
C3-C16	1.497(3)
C4-C5	1.373(4)
C4-H4A	0.9500
C5-C6	1.411(4)
C5-H5A	0.9500
C6-C7	1.500(4)
C7-C8	1.594(4)
C8-C9	1.502(4)
C9-C14	1.394(4)
C9-C10	1.395(3)
C10-C11	1.379(4)
C10-H10A	0.9500
C11-C12	1.393(4)
C11-H11A	0.9500
C12-C13	1.396(4)
C12-C15	1.501(4)
C13-C14	1.382(4)
C13-H13A	0.9500

C14-H14A	0.9500
C15-C16	1.600(4)
C17-C18	1.535(4)
C17-H17A	1.0000
C18-C19	1.326(4)
C18-H18A	0.9500
C19-C20	1.522(4)
C19-H19A	0.9500
C20-H20A	1.0000
C20-O1-C17	95.95(18)
C6-C1-C2	120.5(2)
C6-C1-C17	135.0(2)
C2-C1-C17	104.36(19)
C3-C2-C1	120.6(2)
C3-C2-C20	135.4(2)
C1-C2-C20	103.8(2)
C2-C3-C4	117.0(2)
C2-C3-C16	123.4(2)
C4-C3-C16	117.8(2)
C5-C4-C3	120.5(2)
C5-C4-H4A	119.7
C3-C4-H4A	119.7
C4-C5-C6	120.8(2)
C4-C5-H5A	119.6
C6-C5-H5A	119.6
C1-C6-C5	116.9(2)
C1-C6-C7	124.2(2)
C5-C6-C7	117.5(2)
F2-C7-F1	105.6(2)
F2-C7-C6	112.4(2)
F1-C7-C6	109.8(2)
F2-C7-C8	108.6(2)
F1-C7-C8	105.9(2)
C6-C7-C8	114.0(2)
F3-C8-F4	105.8(2)

F3-C8-C9	112.5(2)
F4-C8-C9	110.3(2)
F3-C8-C7	107.5(2)
F4-C8-C7	106.7(2)
C9-C8-C7	113.7(2)
C14-C9-C10	119.0(2)
C14-C9-C8	121.1(2)
C10-C9-C8	118.2(2)
C11-C10-C9	120.2(2)
C11-C10-H10A	119.9
C9-C10-H10A	119.9
C10-C11-C12	119.6(2)
C10-C11-H11A	120.2
C12-C11-H11A	120.2
C11-C12-C13	118.8(3)
C11-C12-C15	118.2(2)
C13-C12-C15	121.2(2)
C14-C13-C12	120.2(2)
C14-C13-H13A	119.9
C12-C13-H13A	119.9
C13-C14-C9	119.4(2)
C13-C14-H14A	120.3
C9-C14-H14A	120.3
F6-C15-F5	105.90(19)
F6-C15-C12	112.6(2)
F5-C15-C12	110.5(2)
F6-C15-C16	106.9(2)
F5-C15-C16	106.8(2)
C12-C15-C16	113.7(2)
F8-C16-F7	106.4(2)
F8-C16-C3	110.1(2)
F7-C16-C3	112.6(2)
F8-C16-C15	106.94(19)
F7-C16-C15	107.3(2)
C3-C16-C15	113.1(2)
O1-C17-C18	99.9(2)

O1-C17-C1	97.76(19)
C18-C17-C1	108.6(2)
O1-C17-H17A	116.0
C18-C17-H17A	116.0
C1-C17-H17A	116.0
C19-C18-C17	105.7(2)
C19-C18-H18A	127.2
C17-C18-H18A	127.2
C18-C19-C20	105.8(2)
C18-C19-H19A	127.1
C20-C19-H19A	127.1
O1-C20-C19	100.4(2)
O1-C20-C2	98.05(18)
C19-C20-C2	109.1(2)
O1-C20-H20A	115.6
C19-C20-H20A	115.6
C2-C20-H20A	115.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1	47(1)	31(1)	48(1)	4(1)	0(1)	23(1)
F1	71(1)	122(2)	42(1)	-2(1)	11(1)	70(1)
F2	40(1)	49(1)	119(2)	35(1)	16(1)	16(1)
F3	64(1)	92(2)	72(1)	21(1)	18(1)	61(1)
F4	58(1)	65(1)	55(1)	-7(1)	-7(1)	1(1)
F5	50(1)	25(1)	75(1)	-6(1)	9(1)	11(1)
F6	69(1)	45(1)	46(1)	13(1)	26(1)	27(1)
F7	33(1)	44(1)	67(1)	-4(1)	-6(1)	8(1)
F8	51(1)	43(1)	45(1)	-1(1)	13(1)	27(1)
C1	33(1)	29(1)	28(1)	4(1)	1(1)	16(1)
C2	30(1)	29(1)	31(1)	0(1)	-2(1)	15(1)
C3	31(1)	31(1)	28(1)	-3(1)	-2(1)	16(1)
C4	42(1)	30(1)	29(1)	-6(1)	-3(1)	17(1)
C5	46(2)	38(1)	27(1)	-1(1)	4(1)	25(1)
C6	35(1)	35(1)	26(1)	6(1)	6(1)	19(1)
C7	40(1)	45(2)	44(1)	8(1)	12(1)	24(1)
C8	38(2)	48(2)	45(2)	-3(1)	-1(1)	24(1)
C9	41(1)	40(1)	33(1)	1(1)	-4(1)	26(1)
C10	46(2)	36(1)	30(1)	-1(1)	-5(1)	23(1)
C11	49(2)	38(1)	26(1)	0(1)	-2(1)	25(1)
C12	48(2)	29(1)	30(1)	5(1)	5(1)	21(1)
C13	53(2)	29(1)	40(1)	1(1)	0(1)	24(1)
C14	49(2)	38(1)	41(1)	-2(1)	2(1)	28(1)
C15	47(2)	24(1)	38(1)	-1(1)	11(1)	12(1)
C16	33(1)	30(1)	40(1)	-8(1)	0(1)	13(1)
C17	36(1)	28(1)	44(1)	2(1)	3(1)	14(1)
C18	41(2)	31(1)	45(1)	-7(1)	-6(1)	14(1)
C19	49(2)	33(1)	38(1)	-8(1)	1(1)	19(1)
C20	34(1)	29(1)	45(1)	-1(1)	4(1)	16(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **7a**.

	x	y	z	U(eq)
H4A	4355	2265	248	41
H5A	7051	3515	-4	42
H10A	9088	5959	1362	43
H11A	6323	4428	1579	43
H13A	5648	549	888	47
H14A	8426	2066	675	48
H17A	9251	9285	514	44
H18A	9447	8943	1277	49
H19A	6572	7612	1549	48
H20A	4600	7109	961	43

Table 1. Crystal data and structure refinement for [2.2]paracyclophane adduct, **8**.

Identification code	yz02	
Empirical formula	C ₃₂ H ₂₂ F ₈	
Formula weight	558.50	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.4353(4) Å	α = 104.106(1)°.
	b = 11.4074(5) Å	β = 97.453(1)°.
	c = 15.4130(7) Å	γ = 104.071(1)°.
Volume	1204.8(1) Å ³	
Z	2	
Density (calculated)	1.540 Mg/m ³	
Absorption coefficient	0.132 mm ⁻¹	
F(000)	572	
Crystal size	0.32 x 0.19 x 0.12 mm ³	
Theta range for data collection	1.39 to 27.49°.	
Index ranges	-9 ≤ h ≤ 9, -14 ≤ k ≤ 14, -20 ≤ l ≤ 19	
Reflections collected	10991	
Independent reflections	5421 [R(int) = 0.0275]	
Completeness to theta = 27.49°	98.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9872 and 0.9563	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5421 / 0 / 361	
Goodness-of-fit on F ²	1.026	
Final R indices [I > 2σ(I)]	R1 = 0.0467, wR2 = 0.1173 [4305]	
R indices (all data)	R1 = 0.0600, wR2 = 0.1264	
Largest diff. peak and hole	0.308 and -0.246 e.Å ⁻³	

$$R1 = \sum(|F_o| - |F_c|) / \sum|F_o|$$

$$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$$

$$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$$

$$w = 1/[\sigma^2(F_o^2) + (0.0540 \cdot p)^2 + 0.61 \cdot p], p = [\max(F_o^2, 0) + 2 \cdot F_c^2] / 3$$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F1	6560(2)	7073(1)	505(1)	54(1)
F2	8461(2)	8640(1)	219(1)	49(1)
F3	8683(3)	5983(1)	-229(1)	72(1)
F4	11099(2)	7667(2)	155(1)	64(1)
F5	10537(2)	6486(1)	4441(1)	59(1)
F6	13484(2)	7491(2)	4577(1)	65(1)
F7	10136(2)	8558(1)	5055(1)	59(1)
F8	12862(2)	9524(1)	4847(1)	59(1)
C1	11111(2)	9747(2)	3143(1)	26(1)
C2	10399(2)	9521(2)	2208(1)	25(1)
C3	8778(2)	8530(2)	1766(1)	29(1)
C4	7685(2)	7950(2)	2306(1)	33(1)
C5	8396(3)	8158(2)	3214(1)	32(1)
C6	10221(2)	8949(2)	3617(1)	28(1)
C7	8365(3)	7854(2)	756(1)	36(1)
C8	9703(3)	6982(2)	480(1)	43(1)
C9	10556(3)	6604(2)	1274(1)	35(1)
C10	12360(3)	7309(2)	1764(1)	36(1)
C11	12849(3)	7405(2)	2680(1)	34(1)
C12	11531(3)	6791(2)	3103(1)	32(1)
C13	9891(3)	5888(2)	2567(1)	35(1)
C14	9403(3)	5789(2)	1651(1)	37(1)
C15	11707(3)	7314(2)	4115(1)	39(1)
C16	11216(3)	8640(2)	4413(1)	35(1)
C1'	14308(2)	10553(2)	2882(1)	28(1)
C2'	13700(2)	10369(2)	2001(1)	28(1)
C3'	11644(2)	10439(2)	1796(1)	28(1)
C4'	11650(2)	11737(2)	2379(1)	30(1)
C5'	12342(2)	11983(2)	3263(1)	29(1)
C6'	12915(2)	10861(2)	3490(1)	28(1)
C7'	14845(3)	10277(2)	1250(1)	36(1)

C8'	16866(3)	11223(2)	1528(1)	41(1)
C9'	16770(3)	12499(2)	2057(1)	36(1)
C10'	17408(2)	12927(2)	3005(1)	35(1)
C11'	16619(3)	13736(2)	3547(1)	36(1)
C12'	15152(3)	14129(2)	3160(1)	36(1)
C13'	14823(3)	13919(2)	2217(1)	40(1)
C14'	15624(3)	13116(2)	1673(1)	40(1)
C15'	13661(3)	14404(2)	3692(2)	42(1)
C16'	12744(3)	13230(2)	3992(1)	37(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **8**.

F1-C7	1.364(2)
F2-C7	1.357(2)
F3-C8	1.351(2)
F4-C8	1.366(2)
F5-C15	1.358(2)
F6-C15	1.360(2)
F7-C16	1.358(2)
F8-C16	1.349(2)
C1-C6	1.400(2)
C1-C2	1.406(2)
C1-C6'	1.534(2)
C2-C3	1.394(2)
C2-C3'	1.537(2)
C3-C4	1.405(2)
C3-C7	1.512(2)
C4-C5	1.371(3)
C4-H4A	0.9500
C5-C6	1.398(2)
C5-H5A	0.9500
C6-C16	1.509(2)
C7-C8	1.596(3)
C8-C9	1.509(3)
C9-C10	1.390(3)
C9-C14	1.393(3)
C10-C11	1.382(3)
C10-H10A	0.9500
C11-C12	1.390(3)
C11-H11A	0.9500
C12-C13	1.395(3)
C12-C15	1.504(3)
C13-C14	1.382(3)
C13-H13A	0.9500
C14-H14A	0.9500
C15-C16	1.615(3)

C1'-C2'	1.322(2)
C1'-C6'	1.530(2)
C1'-H1'A	0.9500
C2'-C7'	1.523(2)
C2'-C3'	1.546(2)
C3'-C4'	1.531(2)
C3'-H3'A	1.0000
C4'-C5'	1.327(2)
C4'-H4'A	0.9500
C5'-C16'	1.518(2)
C5'-C6'	1.545(2)
C6'-H6'A	1.0000
C7'-C8'	1.556(3)
C7'-H7'A	0.9900
C7'-H7'B	0.9900
C8'-C9'	1.508(3)
C8'-H8'A	0.9900
C8'-H8'B	0.9900
C9'-C14'	1.392(3)
C9'-C10'	1.400(3)
C10'-C11'	1.381(3)
C10'-H10B	0.9500
C11'-C12'	1.395(3)
C11'-H11B	0.9500
C12'-C13'	1.393(3)
C12'-C15'	1.511(3)
C13'-C14'	1.384(3)
C13'-H13B	0.9500
C14'-H14B	0.9500
C15'-C16'	1.553(3)
C15'-H15A	0.9900
C15'-H15B	0.9900
C16'-H16A	0.9900
C16'-H16B	0.9900
C6-C1-C2	119.67(15)

C6-C1-C6'	128.68(15)
C2-C1-C6'	111.57(14)
C3-C2-C1	119.97(15)
C3-C2-C3'	128.13(15)
C1-C2-C3'	111.86(14)
C2-C3-C4	118.02(16)
C2-C3-C7	123.58(16)
C4-C3-C7	116.93(15)
C5-C4-C3	120.51(16)
C5-C4-H4A	119.7
C3-C4-H4A	119.7
C4-C5-C6	120.61(16)
C4-C5-H5A	119.7
C6-C5-H5A	119.7
C5-C6-C1	117.92(16)
C5-C6-C16	115.62(15)
C1-C6-C16	124.80(16)
F2-C7-F1	105.72(14)
F2-C7-C3	113.61(15)
F1-C7-C3	109.51(15)
F2-C7-C8	107.85(16)
F1-C7-C8	106.07(15)
C3-C7-C8	113.53(15)
F3-C8-F4	106.81(16)
F3-C8-C9	112.93(17)
F4-C8-C9	110.20(18)
F3-C8-C7	107.64(17)
F4-C8-C7	106.30(16)
C9-C8-C7	112.59(15)
C10-C9-C14	119.33(18)
C10-C9-C8	118.75(17)
C14-C9-C8	119.90(18)
C11-C10-C9	119.88(17)
C11-C10-H10A	120.1
C9-C10-H10A	120.1
C10-C11-C12	119.58(17)

C10-C11-H11A	120.2
C12-C11-H11A	120.2
C11-C12-C13	119.20(17)
C11-C12-C15	118.44(17)
C13-C12-C15	121.01(17)
C14-C13-C12	119.95(17)
C14-C13-H13A	120.0
C12-C13-H13A	120.0
C13-C14-C9	119.35(18)
C13-C14-H14A	120.3
C9-C14-H14A	120.3
F5-C15-F6	105.82(16)
F5-C15-C12	110.55(16)
F6-C15-C12	111.39(17)
F5-C15-C16	107.17(16)
F6-C15-C16	107.16(16)
C12-C15-C16	114.30(14)
F8-C16-F7	106.04(15)
F8-C16-C6	112.85(14)
F7-C16-C6	111.35(16)
F8-C16-C15	106.64(16)
F7-C16-C15	106.78(14)
C6-C16-C15	112.74(14)
C2'-C1'-C6'	115.00(15)
C2'-C1'-H1'A	122.5
C6'-C1'-H1'A	122.5
C1'-C2'-C7'	127.67(16)
C1'-C2'-C3'	111.75(15)
C7'-C2'-C3'	120.06(15)
C4'-C3'-C2	103.34(13)
C4'-C3'-C2'	105.98(13)
C2-C3'-C2'	108.47(13)
C4'-C3'-H3'A	112.8
C2-C3'-H3'A	112.8
C2'-C3'-H3'A	112.8
C5'-C4'-C3'	114.52(15)

C5'-C4'-H4'A	122.7
C3'-C4'-H4'A	122.7
C4'-C5'-C16'	126.93(16)
C4'-C5'-C6'	112.04(15)
C16'-C5'-C6'	120.79(15)
C1'-C6'-C1	106.41(13)
C1'-C6'-C5'	106.32(13)
C1-C6'-C5'	105.04(13)
C1'-C6'-H6'A	112.8
C1-C6'-H6'A	112.8
C5'-C6'-H6'A	112.8
C2'-C7'-C8'	114.34(15)
C2'-C7'-H7'A	108.7
C8'-C7'-H7'A	108.7
C2'-C7'-H7'B	108.7
C8'-C7'-H7'B	108.7
H7'A-C7'-H7'B	107.6
C9'-C8'-C7'	109.37(15)
C9'-C8'-H8'A	109.8
C7'-C8'-H8'A	109.8
C9'-C8'-H8'B	109.8
C7'-C8'-H8'B	109.8
H8'A-C8'-H8'B	108.2
C14'-C9'-C10'	117.07(18)
C14'-C9'-C8'	120.75(17)
C10'-C9'-C8'	120.02(18)
C11'-C10'-C9'	120.75(17)
C11'-C10'-H10B	119.6
C9'-C10'-H10B	119.6
C10'-C11'-C12'	120.52(18)
C10'-C11'-H11B	119.7
C12'-C11'-H11B	119.7
C13'-C12'-C11'	117.30(19)
C13'-C12'-C15'	120.44(18)
C11'-C12'-C15'	119.90(18)
C14'-C13'-C12'	120.65(18)

C14'-C13'-H13B	119.7
C12'-C13'-H13B	119.7
C13'-C14'-C9'	120.74(18)
C13'-C14'-H14B	119.6
C9'-C14'-H14B	119.6
C12'-C15'-C16'	109.34(15)
C12'-C15'-H15A	109.8
C16'-C15'-H15A	109.8
C12'-C15'-H15B	109.8
C16'-C15'-H15B	109.8
H15A-C15'-H15B	108.3
C5'-C16'-C15'	114.22(16)
C5'-C16'-H16A	108.7
C15'-C16'-H16A	108.7
C5'-C16'-H16B	108.7
C15'-C16'-H16B	108.7
H16A-C16'-H16B	107.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F1	40(1)	54(1)	46(1)	8(1)	-9(1)	-10(1)
F2	60(1)	44(1)	38(1)	20(1)	-5(1)	4(1)
F3	109(1)	55(1)	35(1)	-10(1)	-8(1)	24(1)
F4	73(1)	86(1)	55(1)	41(1)	36(1)	28(1)
F5	97(1)	37(1)	49(1)	24(1)	27(1)	9(1)
F6	63(1)	76(1)	53(1)	14(1)	-11(1)	33(1)
F7	95(1)	62(1)	41(1)	27(1)	38(1)	33(1)
F8	69(1)	38(1)	50(1)	19(1)	-22(1)	-7(1)
C1	25(1)	22(1)	30(1)	7(1)	8(1)	8(1)
C2	25(1)	24(1)	29(1)	10(1)	6(1)	7(1)
C3	26(1)	27(1)	33(1)	10(1)	3(1)	7(1)
C4	24(1)	30(1)	44(1)	11(1)	8(1)	5(1)
C5	32(1)	29(1)	40(1)	12(1)	16(1)	7(1)
C6	31(1)	25(1)	29(1)	7(1)	11(1)	8(1)
C7	34(1)	34(1)	34(1)	12(1)	-3(1)	-2(1)
C8	57(1)	38(1)	30(1)	5(1)	12(1)	8(1)
C9	46(1)	28(1)	33(1)	6(1)	14(1)	13(1)
C10	38(1)	29(1)	46(1)	12(1)	22(1)	12(1)
C11	30(1)	29(1)	47(1)	12(1)	11(1)	11(1)
C12	37(1)	27(1)	40(1)	14(1)	9(1)	14(1)
C13	39(1)	26(1)	44(1)	15(1)	14(1)	7(1)
C14	41(1)	24(1)	42(1)	6(1)	9(1)	4(1)
C15	43(1)	36(1)	39(1)	19(1)	5(1)	10(1)
C16	44(1)	32(1)	28(1)	10(1)	8(1)	4(1)
C1'	23(1)	25(1)	37(1)	11(1)	5(1)	4(1)
C2'	27(1)	24(1)	33(1)	10(1)	8(1)	3(1)
C3'	28(1)	29(1)	28(1)	12(1)	4(1)	4(1)
C4'	26(1)	25(1)	38(1)	13(1)	4(1)	4(1)
C5'	27(1)	23(1)	36(1)	8(1)	6(1)	4(1)
C6'	28(1)	26(1)	27(1)	9(1)	2(1)	4(1)
C7'	35(1)	34(1)	37(1)	10(1)	13(1)	5(1)

C8'	33(1)	43(1)	45(1)	12(1)	15(1)	3(1)
C9'	29(1)	34(1)	40(1)	14(1)	8(1)	-3(1)
C10'	25(1)	35(1)	43(1)	19(1)	1(1)	-1(1)
C11'	33(1)	31(1)	35(1)	12(1)	-2(1)	-4(1)
C12'	38(1)	22(1)	44(1)	13(1)	1(1)	-2(1)
C13'	38(1)	30(1)	48(1)	21(1)	-3(1)	-1(1)
C14'	41(1)	37(1)	35(1)	17(1)	3(1)	-6(1)
C15'	46(1)	27(1)	49(1)	9(1)	3(1)	9(1)
C16'	37(1)	29(1)	41(1)	7(1)	7(1)	7(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**.

	x	y	z	U(eq)
H4A	6443	7410	2040	40
H5A	7641	7762	3572	39
H10A	13255	7724	1469	43
H11A	14079	7888	3018	41
H13A	9110	5340	2831	42
H14A	8291	5172	1281	45
H1'A	15520	10499	3120	34
H3'A	11155	10290	1131	34
H4'A	11196	12318	2128	36
H6'A	13446	11037	4154	33
H7'A	14142	10425	715	43
H7'B	14960	9409	1059	43
H8'A	17718	10916	1910	49
H8'B	17379	11289	975	49
H10B	18395	12659	3279	42
H11B	17079	14027	4189	43
H13B	14041	14332	1944	48
H14B	15389	12986	1031	48
H15A	12679	14612	3308	50
H15B	14244	15138	4237	50
H16A	13596	13216	4537	44
H16B	11541	13314	4173	44

Table 1. Crystal data and structure refinement for bis-naphthalene adduct, **12**.

Identification code	yz09	
Empirical formula	C ₃₆ H ₂₀ F ₈	
Formula weight	604.52	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.4437(7) Å	α = 87.693(2)°.
	b = 13.2605(7) Å	β = 78.725(2)°.
	c = 17.485(2) Å	γ = 64.870(2)°.
Volume	2558.8(2) Å ³	
Z	4	
Density (calculated)	1.569 Mg/m ³	
Absorption coefficient	0.131 mm ⁻¹	
F(000)	1232	
Crystal size	0.24 x 0.19 x 0.11 mm ³	
Theta range for data collection	1.19 to 27.50°.	
Index ranges	-8 ≤ h ≤ 16, -16 ≤ k ≤ 17, -21 ≤ l ≤ 22	
Reflections collected	17002	
Independent reflections	11267 [R(int) = 0.0266]	
Completeness to theta = 27.50°	95.9 %	
Absorption correction	Analytical	
Max. and min. transmission	0.9888 and 0.9607	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11267 / 0 / 793	
Goodness-of-fit on F ²	1.017	
Final R indices [I > 2σ(I)]	R1 = 0.0394, wR2 = 0.0963 [8161]	
R indices (all data)	R1 = 0.0617, wR2 = 0.1062	
Largest diff. peak and hole	0.304 and -0.223 e.Å ⁻³	

$$R1 = \sum(|F_o| - |F_c|) / \sum|F_o|$$

$$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$$

$$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$$

$$w = 1/[\sigma^2(F_o^2) + (0.522 * p)^2 + 0.4421 * p], p = [\max(F_o^2, 0) + 2 * F_c^2] / 3$$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **12**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
F1	7425(1)	3968(1)	4722(1)	44(1)
F2	5960(1)	5573(1)	4590(1)	38(1)
F3	6571(1)	4607(1)	568(1)	41(1)
F4	8471(1)	3846(1)	649(1)	40(1)
F5	7614(1)	6103(1)	4675(1)	52(1)
F6	9058(1)	4543(1)	4142(1)	47(1)
F7	8093(1)	5815(1)	330(1)	39(1)
F8	6227(1)	6512(1)	962(1)	35(1)
C1	4542(2)	5357(1)	3594(1)	30(1)
C2	5856(1)	4750(1)	3152(1)	26(1)
C3	6909(2)	4337(1)	3461(1)	26(1)
C4	7994(2)	3627(1)	2975(1)	28(1)
C5	8073(2)	3576(1)	2182(1)	27(1)
C6	7072(2)	4224(1)	1848(1)	26(1)
C7	5937(1)	4702(1)	2338(1)	25(1)
C8	4687(2)	5274(1)	2107(1)	30(1)
C9	4112(1)	6465(1)	2457(1)	27(1)
C10	3692(2)	7440(1)	2063(1)	33(1)
C11	3254(2)	8457(1)	2474(1)	37(1)
C12	3227(2)	8501(2)	3267(1)	38(1)
C13	3626(2)	7519(1)	3667(1)	33(1)
C14	4055(1)	6509(1)	3261(1)	26(1)
C15	3881(2)	4737(1)	3328(1)	37(1)
C16	3956(2)	4690(1)	2566(1)	38(1)
C17	7037(2)	4782(1)	4204(1)	32(1)
C18	7352(2)	4577(1)	1026(1)	29(1)
C19	10372(2)	4920(1)	2735(1)	29(1)
C20	9029(1)	5495(1)	2674(1)	25(1)
C21	8012(2)	5873(1)	3279(1)	26(1)
C22	6900(2)	6583(1)	3098(1)	26(1)
C23	6751(2)	6688(1)	2336(1)	25(1)

C24	7713(1)	6055(1)	1731(1)	24(1)
C25	8875(1)	5556(1)	1894(1)	24(1)
C26	10086(1)	4970(1)	1312(1)	27(1)
C27	10706(1)	3787(1)	1580(1)	27(1)
C28	11086(2)	2807(1)	1143(1)	33(1)
C29	11594(2)	1791(2)	1497(1)	38(1)
C30	11710(2)	1772(2)	2266(1)	41(1)
C31	11350(2)	2755(2)	2701(1)	36(1)
C32	10848(1)	3761(1)	2355(1)	28(1)
C33	10971(2)	5551(1)	2200(1)	34(1)
C34	10839(2)	5573(1)	1470(1)	34(1)
C35	7960(2)	5351(2)	4065(1)	33(1)
C36	7370(2)	5770(1)	1015(1)	27(1)
F1'	-5514(1)	12231(1)	4078(1)	49(1)
F2'	-4326(1)	10706(1)	4535(1)	42(1)
F3'	-766(1)	10462(1)	840(1)	40(1)
F4'	669(1)	9837(1)	1508(1)	41(1)
F5'	-5865(1)	11264(1)	3032(1)	49(1)
F6'	-5561(1)	10043(1)	3927(1)	52(1)
F7'	-61(1)	8387(1)	720(1)	41(1)
F8'	401(1)	8118(1)	1872(1)	37(1)
C1'	-1970(2)	10579(1)	4392(1)	28(1)
C2'	-2302(2)	10879(1)	3583(1)	24(1)
C3'	-3453(2)	11355(1)	3401(1)	25(1)
C4'	-3554(2)	11751(1)	2648(1)	26(1)
C5'	-2543(2)	11434(1)	2063(1)	26(1)
C6'	-1401(2)	10713(1)	2207(1)	24(1)
C7'	-1270(1)	10544(1)	2984(1)	24(1)
C8'	-84(2)	9944(1)	3287(1)	28(1)
C9'	-179(2)	8979(1)	3758(1)	27(1)
C10'	641(2)	7869(1)	3653(1)	31(1)
C11'	411(2)	7098(2)	4142(1)	38(1)
C12'	-629(2)	7432(2)	4713(1)	38(1)
C13'	-1452(2)	8555(2)	4822(1)	32(1)
C14'	-1213(2)	9323(1)	4348(1)	26(1)
C15'	-1109(2)	11107(1)	4454(1)	33(1)

C16'	-143(2)	10784(1)	3887(1)	34(1)
C17'	-4549(2)	11231(1)	3860(1)	32(1)
C18'	-489(2)	9987(1)	1519(1)	29(1)
C19'	-4882(2)	10186(1)	1527(1)	27(1)
C20'	-3866(1)	9677(1)	1997(1)	24(1)
C21'	-3973(1)	9661(1)	2808(1)	24(1)
C22'	-2955(2)	8954(1)	3104(1)	26(1)
C23'	-1827(2)	8515(1)	2630(1)	26(1)
C24'	-1680(1)	8778(1)	1844(1)	24(1)
C25'	-2707(1)	9251(1)	1514(1)	23(1)
C26'	-2763(2)	9447(1)	646(1)	28(1)
C27'	-3504(2)	10694(1)	582(1)	29(1)
C28'	-3139(2)	11407(2)	117(1)	40(1)
C29'	-3939(2)	12532(2)	145(1)	49(1)
C30'	-5072(2)	12932(2)	624(1)	50(1)
C31'	-5443(2)	12212(2)	1089(1)	39(1)
C32'	-4649(2)	11097(1)	1065(1)	29(1)
C33'	-4628(2)	9264(1)	930(1)	32(1)
C34'	-3548(2)	8884(1)	479(1)	31(1)
C35'	-4989(2)	10517(2)	3388(1)	31(1)
C36'	-471(2)	8784(1)	1476(1)	29(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **12**.

F1-C17	1.3665(18)
F2-C17	1.3637(19)
F3-C18	1.3618(19)
F4-C18	1.3642(19)
F5-C35	1.364(2)
F6-C35	1.3606(19)
F7-C36	1.3647(18)
F8-C36	1.3626(18)
C1-C14	1.523(2)
C1-C15	1.524(3)
C1-C2	1.535(2)
C1-H1A	1.0000
C2-C3	1.397(2)
C2-C7	1.411(2)
C3-C4	1.402(2)
C3-C17	1.511(2)
C4-C5	1.373(2)
C4-H4A	0.9500
C5-C6	1.402(2)
C5-H5A	0.9500
C6-C7	1.393(2)
C6-C18	1.515(2)
C7-C8	1.541(2)
C8-C9	1.525(2)
C8-C16	1.528(2)
C8-H8A	1.0000
C9-C10	1.383(2)
C9-C14	1.396(2)
C10-C11	1.390(3)
C10-H10A	0.9500
C11-C12	1.383(3)
C11-H11A	0.9500
C12-C13	1.396(2)
C12-H12A	0.9500

C13-C14	1.380(2)
C13-H13A	0.9500
C15-C16	1.318(3)
C15-H15A	0.9500
C16-H16A	0.9500
C17-C35	1.600(3)
C18-C36	1.591(2)
C19-C32	1.520(2)
C19-C33	1.525(2)
C19-C20	1.538(2)
C19-H19A	1.0000
C20-C21	1.397(2)
C20-C25	1.409(2)
C21-C22	1.394(2)
C21-C35	1.516(2)
C22-C23	1.375(2)
C22-H22A	0.9500
C23-C24	1.406(2)
C23-H23A	0.9500
C24-C25	1.394(2)
C24-C36	1.510(2)
C25-C26	1.543(2)
C26-C27	1.527(2)
C26-C34	1.533(2)
C26-H26A	1.0000
C27-C28	1.384(2)
C27-C32	1.398(2)
C28-C29	1.400(2)
C28-H28A	0.9500
C29-C30	1.380(3)
C29-H29A	0.9500
C30-C31	1.389(3)
C30-H30A	0.9500
C31-C32	1.382(2)
C31-H31A	0.9500
C33-C34	1.317(3)

C33-H33A	0.9500
C34-H34A	0.9500
F1'-C17'	1.3620(19)
F2'-C17'	1.3603(19)
F3'-C18'	1.3577(19)
F4'-C18'	1.3653(19)
F5'-C35'	1.3625(19)
F6'-C35'	1.363(2)
F7'-C36'	1.3599(18)
F8'-C36'	1.3652(19)
C1'-C14'	1.523(2)
C1'-C15'	1.528(2)
C1'-C2'	1.541(2)
C1'-H1'A	1.0000
C2'-C3'	1.395(2)
C2'-C7'	1.404(2)
C3'-C4'	1.406(2)
C3'-C17'	1.511(2)
C4'-C5'	1.374(2)
C4'-H4'A	0.9500
C5'-C6'	1.401(2)
C5'-H5'A	0.9500
C6'-C7'	1.398(2)
C6'-C18'	1.514(2)
C7'-C8'	1.538(2)
C8'-C9'	1.528(2)
C8'-C16'	1.531(2)
C8'-H8'A	1.0000
C9'-C10'	1.384(2)
C9'-C14'	1.396(2)
C10'-C11'	1.392(3)
C10'-H10B	0.9500
C11'-C12'	1.383(3)
C11'-H11B	0.9500
C12'-C13'	1.397(2)
C12'-H12B	0.9500

C13'-C14'	1.381(2)
C13'-H13B	0.9500
C15'-C16'	1.319(3)
C15'-H15B	0.9500
C16'-H16B	0.9500
C17'-C35'	1.600(3)
C18'-C36'	1.590(2)
C19'-C32'	1.525(2)
C19'-C33'	1.527(2)
C19'-C20'	1.538(2)
C19'-H19B	1.0000
C20'-C21'	1.398(2)
C20'-C25'	1.408(2)
C21'-C22'	1.400(2)
C21'-C35'	1.513(2)
C22'-C23'	1.373(2)
C22'-H22B	0.9500
C23'-C24'	1.401(2)
C23'-H23B	0.9500
C24'-C25'	1.392(2)
C24'-C36'	1.519(2)
C25'-C26'	1.540(2)
C26'-C27'	1.525(2)
C26'-C34'	1.532(2)
C26'-H26B	1.0000
C27'-C28'	1.385(2)
C27'-C32'	1.396(2)
C28'-C29'	1.395(3)
C28'-H28B	0.9500
C29'-C30'	1.382(3)
C29'-H29B	0.9500
C30'-C31'	1.398(3)
C30'-H30B	0.9500
C31'-C32'	1.382(2)
C31'-H31B	0.9500
C33'-C34'	1.313(2)

C33'-H33B	0.9500
C34'-H34B	0.9500
C14-C1-C15	106.78(14)
C14-C1-C2	105.53(13)
C15-C1-C2	104.83(14)
C14-C1-H1A	113.0
C15-C1-H1A	113.0
C2-C1-H1A	113.0
C3-C2-C7	119.98(14)
C3-C2-C1	127.81(15)
C7-C2-C1	112.07(14)
C2-C3-C4	117.74(15)
C2-C3-C17	125.00(14)
C4-C3-C17	115.83(15)
C5-C4-C3	120.19(15)
C5-C4-H4A	119.9
C3-C4-H4A	119.9
C4-C5-C6	120.68(15)
C4-C5-H5A	119.7
C6-C5-H5A	119.7
C7-C6-C5	118.09(15)
C7-C6-C18	123.95(15)
C5-C6-C18	116.18(14)
C6-C7-C2	119.44(15)
C6-C7-C8	128.12(15)
C2-C7-C8	112.35(14)
C9-C8-C16	106.05(14)
C9-C8-C7	106.20(13)
C16-C8-C7	104.41(13)
C9-C8-H8A	113.2
C16-C8-H8A	113.2
C7-C8-H8A	113.2
C10-C9-C14	120.15(15)
C10-C9-C8	127.12(15)
C14-C9-C8	112.72(14)

C9-C10-C11	119.14(17)
C9-C10-H10A	120.4
C11-C10-H10A	120.4
C12-C11-C10	120.76(16)
C12-C11-H11A	119.6
C10-C11-H11A	119.6
C11-C12-C13	120.11(16)
C11-C12-H12A	119.9
C13-C12-H12A	119.9
C14-C13-C12	119.14(17)
C14-C13-H13A	120.4
C12-C13-H13A	120.4
C13-C14-C9	120.63(15)
C13-C14-C1	126.63(15)
C9-C14-C1	112.71(14)
C16-C15-C1	114.47(16)
C16-C15-H15A	122.8
C1-C15-H15A	122.8
C15-C16-C8	114.11(17)
C15-C16-H16A	122.9
C8-C16-H16A	122.9
F2-C17-F1	105.66(12)
F2-C17-C3	111.93(14)
F1-C17-C3	112.24(14)
F2-C17-C35	106.07(14)
F1-C17-C35	106.84(14)
C3-C17-C35	113.55(13)
F3-C18-F4	105.72(13)
F3-C18-C6	114.13(14)
F4-C18-C6	110.38(13)
F3-C18-C36	107.39(13)
F4-C18-C36	106.37(13)
C6-C18-C36	112.36(13)
C32-C19-C33	106.79(13)
C32-C19-C20	105.35(13)
C33-C19-C20	104.87(13)

C32-C19-H19A	113.0
C33-C19-H19A	113.0
C20-C19-H19A	113.0
C21-C20-C25	119.52(14)
C21-C20-C19	128.25(14)
C25-C20-C19	112.09(14)
C22-C21-C20	117.98(15)
C22-C21-C35	115.91(14)
C20-C21-C35	124.21(14)
C23-C22-C21	120.53(15)
C23-C22-H22A	119.7
C21-C22-H22A	119.7
C22-C23-C24	120.22(15)
C22-C23-H23A	119.9
C24-C23-H23A	119.9
C25-C24-C23	117.98(14)
C25-C24-C36	124.27(14)
C23-C24-C36	116.39(14)
C24-C25-C20	119.76(14)
C24-C25-C26	127.78(14)
C20-C25-C26	112.36(14)
C27-C26-C34	105.89(13)
C27-C26-C25	106.79(13)
C34-C26-C25	103.86(13)
C27-C26-H26A	113.2
C34-C26-H26A	113.2
C25-C26-H26A	113.2
C28-C27-C32	120.57(15)
C28-C27-C26	126.48(16)
C32-C27-C26	112.93(14)
C27-C28-C29	118.63(17)
C27-C28-H28A	120.7
C29-C28-H28A	120.7
C30-C29-C28	120.48(17)
C30-C29-H29A	119.8
C28-C29-H29A	119.8

C29-C30-C31	120.90(17)
C29-C30-H30A	119.5
C31-C30-H30A	119.5
C32-C31-C30	118.91(18)
C32-C31-H31A	120.5
C30-C31-H31A	120.5
C31-C32-C27	120.48(16)
C31-C32-C19	126.93(16)
C27-C32-C19	112.57(14)
C34-C33-C19	114.98(16)
C34-C33-H33A	122.5
C19-C33-H33A	122.5
C33-C34-C26	113.64(16)
C33-C34-H34A	123.2
C26-C34-H34A	123.2
F6-C35-F5	105.79(14)
F6-C35-C21	111.89(14)
F5-C35-C21	112.73(15)
F6-C35-C17	106.65(14)
F5-C35-C17	106.73(13)
C21-C35-C17	112.57(14)
F8-C36-F7	105.66(12)
F8-C36-C24	110.14(13)
F7-C36-C24	113.81(14)
F8-C36-C18	105.46(13)
F7-C36-C18	107.67(13)
C24-C36-C18	113.49(13)
C14'-C1'-C15'	106.21(14)
C14'-C1'-C2'	106.10(12)
C15'-C1'-C2'	104.82(13)
C14'-C1'-H1'A	113.0
C15'-C1'-H1'A	113.0
C2'-C1'-H1'A	113.0
C3'-C2'-C7'	120.03(14)
C3'-C2'-C1'	127.95(15)
C7'-C2'-C1'	111.90(14)

C2'-C3'-C4'	117.73(15)
C2'-C3'-C17'	125.10(14)
C4'-C3'-C17'	115.39(15)
C5'-C4'-C3'	120.26(15)
C5'-C4'-H4'A	119.9
C3'-C4'-H4'A	119.9
C4'-C5'-C6'	120.62(14)
C4'-C5'-H5'A	119.7
C6'-C5'-H5'A	119.7
C7'-C6'-C5'	117.92(14)
C7'-C6'-C18'	124.09(14)
C5'-C6'-C18'	116.53(14)
C6'-C7'-C2'	119.75(14)
C6'-C7'-C8'	127.35(15)
C2'-C7'-C8'	112.77(13)
C9'-C8'-C16'	105.40(13)
C9'-C8'-C7'	107.11(13)
C16'-C8'-C7'	104.01(13)
C9'-C8'-H8'A	113.2
C16'-C8'-H8'A	113.2
C7'-C8'-H8'A	113.2
C10'-C9'-C14'	120.60(16)
C10'-C9'-C8'	126.63(16)
C14'-C9'-C8'	112.77(14)
C9'-C10'-C11'	118.85(17)
C9'-C10'-H10B	120.6
C11'-C10'-H10B	120.6
C12'-C11'-C10'	120.65(16)
C12'-C11'-H11B	119.7
C10'-C11'-H11B	119.7
C11'-C12'-C13'	120.44(17)
C11'-C12'-H12B	119.8
C13'-C12'-H12B	119.8
C14'-C13'-C12'	118.93(17)
C14'-C13'-H13B	120.5
C12'-C13'-H13B	120.5

C13'-C14'-C9'	120.50(15)
C13'-C14'-C1'	126.82(16)
C9'-C14'-C1'	112.68(14)
C16'-C15'-C1'	114.38(15)
C16'-C15'-H15B	122.8
C1'-C15'-H15B	122.8
C15'-C16'-C8'	114.08(16)
C15'-C16'-H16B	123.0
C8'-C16'-H16B	123.0
F2'-C17'-F1'	105.67(13)
F2'-C17'-C3'	111.88(14)
F1'-C17'-C3'	112.66(14)
F2'-C17'-C35'	106.22(14)
F1'-C17'-C35'	107.19(13)
C3'-C17'-C35'	112.74(13)
F3'-C18'-F4'	105.88(13)
F3'-C18'-C6'	110.17(13)
F4'-C18'-C6'	113.74(14)
F3'-C18'-C36'	106.44(13)
F4'-C18'-C36'	107.35(13)
C6'-C18'-C36'	112.78(13)
C32'-C19'-C33'	106.20(13)
C32'-C19'-C20'	105.79(13)
C33'-C19'-C20'	104.80(13)
C32'-C19'-H19B	113.1
C33'-C19'-H19B	113.1
C20'-C19'-H19B	113.1
C21'-C20'-C25'	119.45(14)
C21'-C20'-C19'	128.13(14)
C25'-C20'-C19'	112.30(13)
C20'-C21'-C22'	117.75(15)
C20'-C21'-C35'	125.11(14)
C22'-C21'-C35'	115.68(14)
C23'-C22'-C21'	120.62(15)
C23'-C22'-H22B	119.7
C21'-C22'-H22B	119.7

C22'-C23'-C24'	120.22(15)
C22'-C23'-H23B	119.9
C24'-C23'-H23B	119.9
C25'-C24'-C23'	118.07(15)
C25'-C24'-C36'	123.83(14)
C23'-C24'-C36'	116.42(14)
C24'-C25'-C20'	119.98(14)
C24'-C25'-C26'	127.69(14)
C20'-C25'-C26'	112.23(14)
C27'-C26'-C34'	105.84(14)
C27'-C26'-C25'	106.93(12)
C34'-C26'-C25'	103.94(13)
C27'-C26'-H26B	113.1
C34'-C26'-H26B	113.1
C25'-C26'-H26B	113.1
C28'-C27'-C32'	120.46(17)
C28'-C27'-C26'	126.69(17)
C32'-C27'-C26'	112.84(14)
C27'-C28'-C29'	118.6(2)
C27'-C28'-H28B	120.7
C29'-C28'-H28B	120.7
C30'-C29'-C28'	120.95(18)
C30'-C29'-H29B	119.5
C28'-C29'-H29B	119.5
C29'-C30'-C31'	120.51(19)
C29'-C30'-H30B	119.7
C31'-C30'-H30B	119.7
C32'-C31'-C30'	118.6(2)
C32'-C31'-H31B	120.7
C30'-C31'-H31B	120.7
C31'-C32'-C27'	120.91(17)
C31'-C32'-C19'	126.49(17)
C27'-C32'-C19'	112.60(14)
C34'-C33'-C19'	114.72(15)
C34'-C33'-H33B	122.6
C19'-C33'-H33B	122.6

C33'-C34'-C26'	114.01(15)
C33'-C34'-H34B	123.0
C26'-C34'-H34B	123.0
F5'-C35'-F6'	105.65(14)
F5'-C35'-C21'	111.74(13)
F6'-C35'-C21'	112.29(14)
F5'-C35'-C17'	106.36(14)
F6'-C35'-C17'	107.02(13)
C21'-C35'-C17'	113.27(13)
F7'-C36'-F8'	105.88(12)
F7'-C36'-C24'	113.88(13)
F8'-C36'-C24'	110.05(14)
F7'-C36'-C18'	108.16(13)
F8'-C36'-C18'	105.61(13)
C24'-C36'-C18'	112.72(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F1	44(1)	49(1)	32(1)	20(1)	-11(1)	-13(1)
F2	29(1)	45(1)	30(1)	0(1)	2(1)	-10(1)
F3	50(1)	48(1)	33(1)	-3(1)	-14(1)	-26(1)
F4	39(1)	35(1)	34(1)	-7(1)	6(1)	-8(1)
F5	58(1)	75(1)	28(1)	-14(1)	-2(1)	-35(1)
F6	28(1)	65(1)	41(1)	20(1)	-14(1)	-13(1)
F7	43(1)	50(1)	25(1)	9(1)	-2(1)	-24(1)
F8	34(1)	33(1)	36(1)	7(1)	-15(1)	-10(1)
C1	24(1)	32(1)	29(1)	6(1)	-1(1)	-9(1)
C2	23(1)	21(1)	31(1)	6(1)	-1(1)	-10(1)
C3	26(1)	23(1)	29(1)	9(1)	-4(1)	-11(1)
C4	23(1)	22(1)	37(1)	9(1)	-5(1)	-8(1)
C5	24(1)	17(1)	37(1)	-1(1)	1(1)	-8(1)
C6	28(1)	19(1)	30(1)	-2(1)	-2(1)	-12(1)
C7	25(1)	18(1)	31(1)	2(1)	-5(1)	-9(1)
C8	25(1)	29(1)	33(1)	-2(1)	-7(1)	-9(1)
C9	19(1)	27(1)	32(1)	1(1)	-5(1)	-7(1)
C10	25(1)	34(1)	33(1)	7(1)	-7(1)	-7(1)
C11	26(1)	26(1)	53(1)	7(1)	-6(1)	-6(1)
C12	25(1)	26(1)	56(1)	-8(1)	-4(1)	-7(1)
C13	22(1)	37(1)	35(1)	-6(1)	-3(1)	-8(1)
C14	16(1)	29(1)	29(1)	1(1)	-2(1)	-8(1)
C15	22(1)	31(1)	54(1)	8(1)	0(1)	-11(1)
C16	24(1)	29(1)	59(1)	-4(1)	-7(1)	-9(1)
C17	26(1)	34(1)	25(1)	9(1)	-3(1)	-6(1)
C18	29(1)	30(1)	27(1)	-4(1)	-4(1)	-10(1)
C19	24(1)	31(1)	32(1)	-1(1)	-6(1)	-10(1)
C20	23(1)	18(1)	32(1)	0(1)	-5(1)	-7(1)
C21	26(1)	25(1)	27(1)	-3(1)	-4(1)	-11(1)
C22	24(1)	21(1)	31(1)	-3(1)	-1(1)	-8(1)
C23	24(1)	18(1)	34(1)	4(1)	-6(1)	-9(1)

C24	26(1)	19(1)	28(1)	5(1)	-4(1)	-12(1)
C25	26(1)	19(1)	28(1)	2(1)	-2(1)	-12(1)
C26	24(1)	26(1)	27(1)	0(1)	0(1)	-10(1)
C27	19(1)	26(1)	33(1)	0(1)	1(1)	-9(1)
C28	25(1)	31(1)	37(1)	-4(1)	4(1)	-11(1)
C29	29(1)	26(1)	52(1)	-5(1)	7(1)	-9(1)
C30	30(1)	27(1)	53(1)	8(1)	2(1)	-6(1)
C31	25(1)	34(1)	38(1)	6(1)	-2(1)	-6(1)
C32	18(1)	28(1)	35(1)	0(1)	0(1)	-7(1)
C33	24(1)	31(1)	47(1)	-4(1)	-3(1)	-12(1)
C34	25(1)	28(1)	45(1)	2(1)	2(1)	-12(1)
C35	27(1)	41(1)	25(1)	-3(1)	-5(1)	-9(1)
C36	26(1)	29(1)	24(1)	6(1)	-3(1)	-11(1)
F1'	33(1)	44(1)	51(1)	-15(1)	3(1)	-1(1)
F2'	46(1)	62(1)	23(1)	8(1)	-8(1)	-28(1)
F3'	51(1)	48(1)	22(1)	5(1)	-3(1)	-24(1)
F4'	32(1)	55(1)	41(1)	-5(1)	1(1)	-28(1)
F5'	28(1)	61(1)	41(1)	-9(1)	-14(1)	1(1)
F6'	50(1)	85(1)	33(1)	-2(1)	7(1)	-46(1)
F7'	36(1)	51(1)	34(1)	-18(1)	5(1)	-17(1)
F8'	25(1)	33(1)	50(1)	-1(1)	-11(1)	-8(1)
C1'	31(1)	29(1)	21(1)	-1(1)	-7(1)	-9(1)
C2'	32(1)	18(1)	24(1)	-1(1)	-9(1)	-10(1)
C3'	29(1)	20(1)	24(1)	-3(1)	-5(1)	-7(1)
C4'	30(1)	20(1)	29(1)	1(1)	-11(1)	-8(1)
C5'	39(1)	22(1)	24(1)	4(1)	-12(1)	-16(1)
C6'	31(1)	22(1)	24(1)	2(1)	-5(1)	-16(1)
C7'	29(1)	20(1)	27(1)	1(1)	-9(1)	-12(1)
C8'	27(1)	31(1)	28(1)	2(1)	-9(1)	-14(1)
C9'	29(1)	29(1)	27(1)	3(1)	-14(1)	-13(1)
C10'	29(1)	32(1)	35(1)	-2(1)	-15(1)	-10(1)
C11'	42(1)	27(1)	47(1)	3(1)	-26(1)	-10(1)
C12'	47(1)	36(1)	40(1)	14(1)	-24(1)	-21(1)
C13'	36(1)	39(1)	27(1)	7(1)	-14(1)	-18(1)
C14'	29(1)	30(1)	24(1)	1(1)	-13(1)	-12(1)
C15'	45(1)	28(1)	30(1)	1(1)	-20(1)	-14(1)

C16'	41(1)	34(1)	36(1)	5(1)	-20(1)	-21(1)
C17'	28(1)	33(1)	25(1)	-3(1)	-4(1)	-5(1)
C18'	28(1)	38(1)	25(1)	2(1)	-2(1)	-18(1)
C19'	26(1)	33(1)	26(1)	3(1)	-10(1)	-13(1)
C20'	26(1)	22(1)	27(1)	4(1)	-10(1)	-13(1)
C21'	25(1)	28(1)	25(1)	4(1)	-7(1)	-15(1)
C22'	33(1)	26(1)	24(1)	6(1)	-10(1)	-17(1)
C23'	29(1)	20(1)	32(1)	2(1)	-13(1)	-11(1)
C24'	26(1)	19(1)	29(1)	-4(1)	-6(1)	-9(1)
C25'	28(1)	21(1)	24(1)	0(1)	-6(1)	-13(1)
C26'	32(1)	35(1)	21(1)	-1(1)	-5(1)	-17(1)
C27'	42(1)	33(1)	21(1)	4(1)	-15(1)	-22(1)
C28'	65(1)	51(1)	21(1)	8(1)	-16(1)	-39(1)
C29'	94(2)	44(1)	30(1)	15(1)	-29(1)	-44(1)
C30'	87(2)	29(1)	41(1)	9(1)	-36(1)	-22(1)
C31'	51(1)	33(1)	34(1)	3(1)	-23(1)	-13(1)
C32'	38(1)	32(1)	24(1)	4(1)	-17(1)	-17(1)
C33'	39(1)	34(1)	32(1)	6(1)	-18(1)	-21(1)
C34'	42(1)	32(1)	25(1)	0(1)	-13(1)	-18(1)
C35'	25(1)	43(1)	25(1)	3(1)	-4(1)	-14(1)
C36'	25(1)	30(1)	29(1)	-7(1)	-4(1)	-9(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **12**.

	x	y	z	U(eq)
H1A	4468	5384	4173	36
H4A	8676	3180	3195	34
H5A	8813	3098	1857	32
H8A	4731	5237	1531	35
H10A	3703	7414	1520	39
H11A	2969	9130	2207	45
H12A	2938	9201	3539	45
H13A	3602	7545	4213	40
H15A	3450	4410	3681	44
H16A	3588	4326	2324	45
H19A	10498	4909	3284	35
H22A	6239	6997	3505	32
H23A	5996	7189	2217	30
H26A	9988	4993	757	33
H28A	11003	2823	613	39
H29A	11860	1110	1205	46
H30A	12041	1077	2502	49
H31A	11447	2736	3228	43
H33A	11406	5902	2381	41
H34A	11179	5929	1077	40
H1'A	-2693	10833	4828	33
H4'A	-4323	12240	2544	32
H5'A	-2620	11705	1556	32
H8'A	655	9704	2863	33
H10B	1349	7636	3255	38
H11B	975	6336	4083	45
H12B	-786	6895	5033	45
H13B	-2165	8786	5216	39
H15B	-1257	11624	4865	40
H16B	463	11049	3855	40

H19B	-5711	10463	1862	33
H22B	-3045	8777	3637	31
H23B	-1144	8031	2836	31
H26B	-1946	9152	295	34
H28B	-2361	11135	-213	48
H29B	-3702	13031	-171	58
H30B	-5602	13702	638	60
H31B	-6225	12482	1415	47
H33B	-5205	8987	888	38
H34B	-3278	8310	84	37