

Supramolecular stabilization of α,ω -diphenylpolyynes by complexation to the tridentate Lewis acid [*o*-C₆F₄Hg]₃

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- ◆ Additional spectroscopic and thermal analysis data (2 pages)
- ◆ Crystal data and structure refinement for **2** (5 pages)
- ◆ Crystal data and structure refinement for **3** (4 pages)
- ◆ Crystal data and structure refinement for **4** (5 pages)
- ◆ Crystal data and structure refinement for **5** (5 pages)

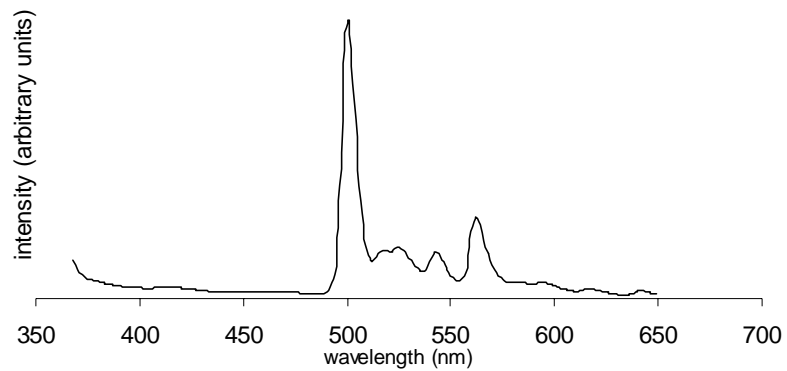


Figure S1: Emission scan of **2** at 77 K, $\lambda_{\text{ex}} = 348$ nm.

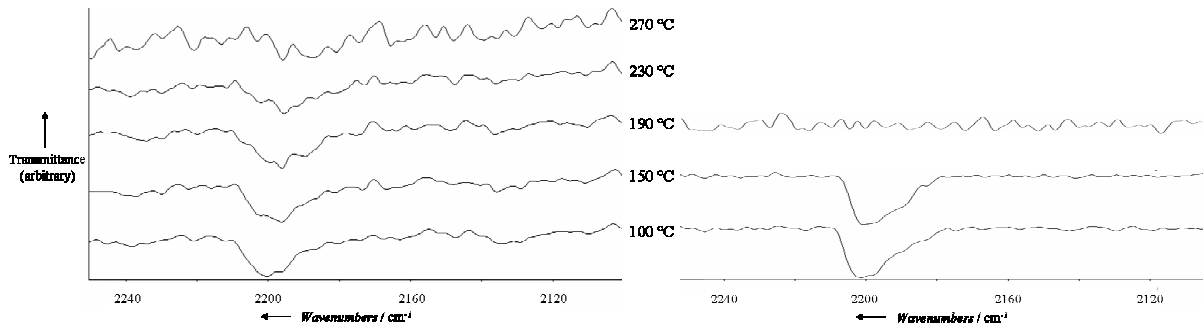


Fig S2: IR measurements taken at increasing temperatures on KBr samples of **4** (left) and $\text{Ph}(\text{C}\equiv\text{C})_4\text{Ph}$ (right).

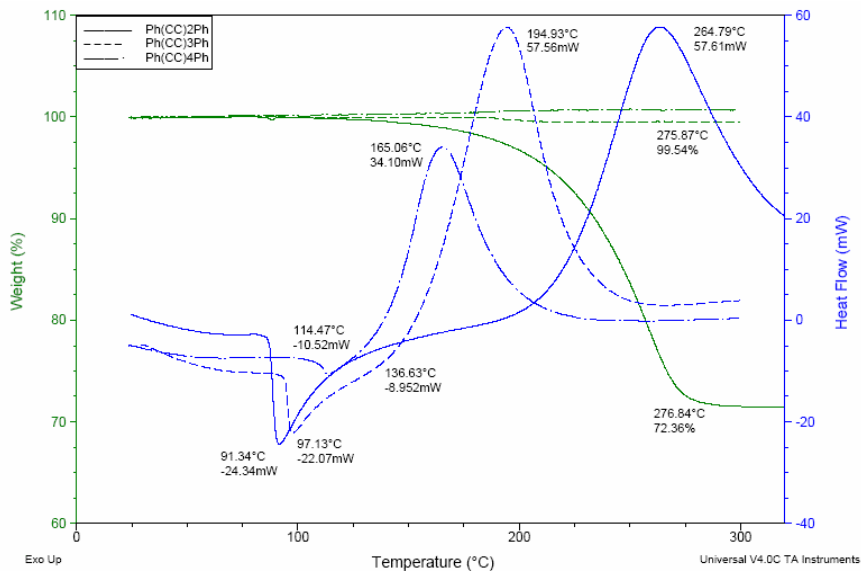


Figure S3: DSC and TGA data traces for Ph(C≡C)₂Ph, Ph(C≡C)₃Ph, and Ph(C≡C)₄Ph. Heating rate = 20 °C/minute.

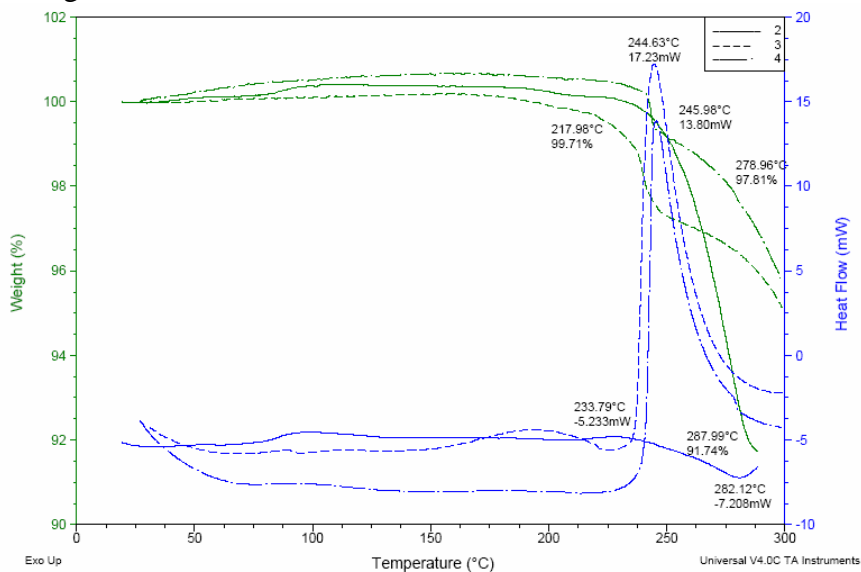


Figure S4: DSC and TGA data traces for **2**, **3**, and **4**. Heating rate = 20 °C/minute.

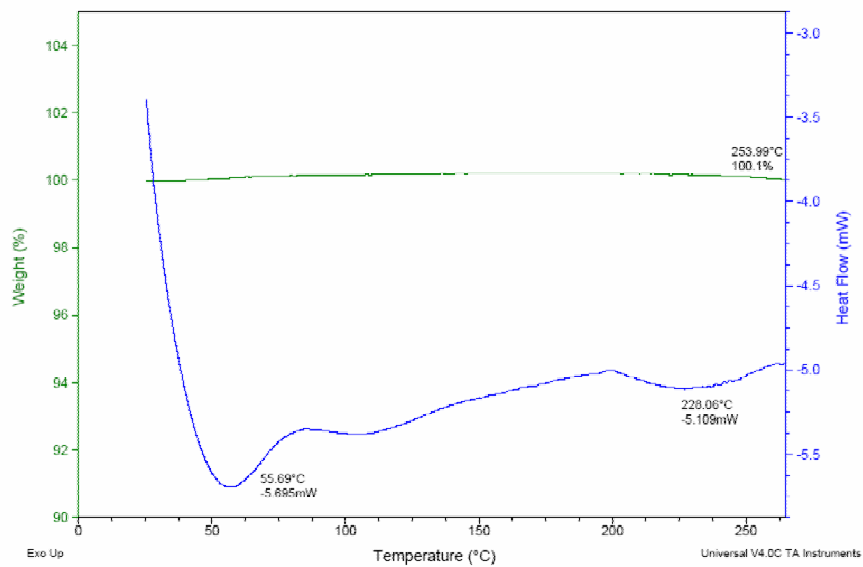


Figure S5: DSC and TGA data traces for **1**. Heating rate = 20 °C/minute.

Crystal structure data for 2:1 trimeric perfluoro-*o*-phenylene mercury 1,4-diphenylbutadiyne adduct, **2**.

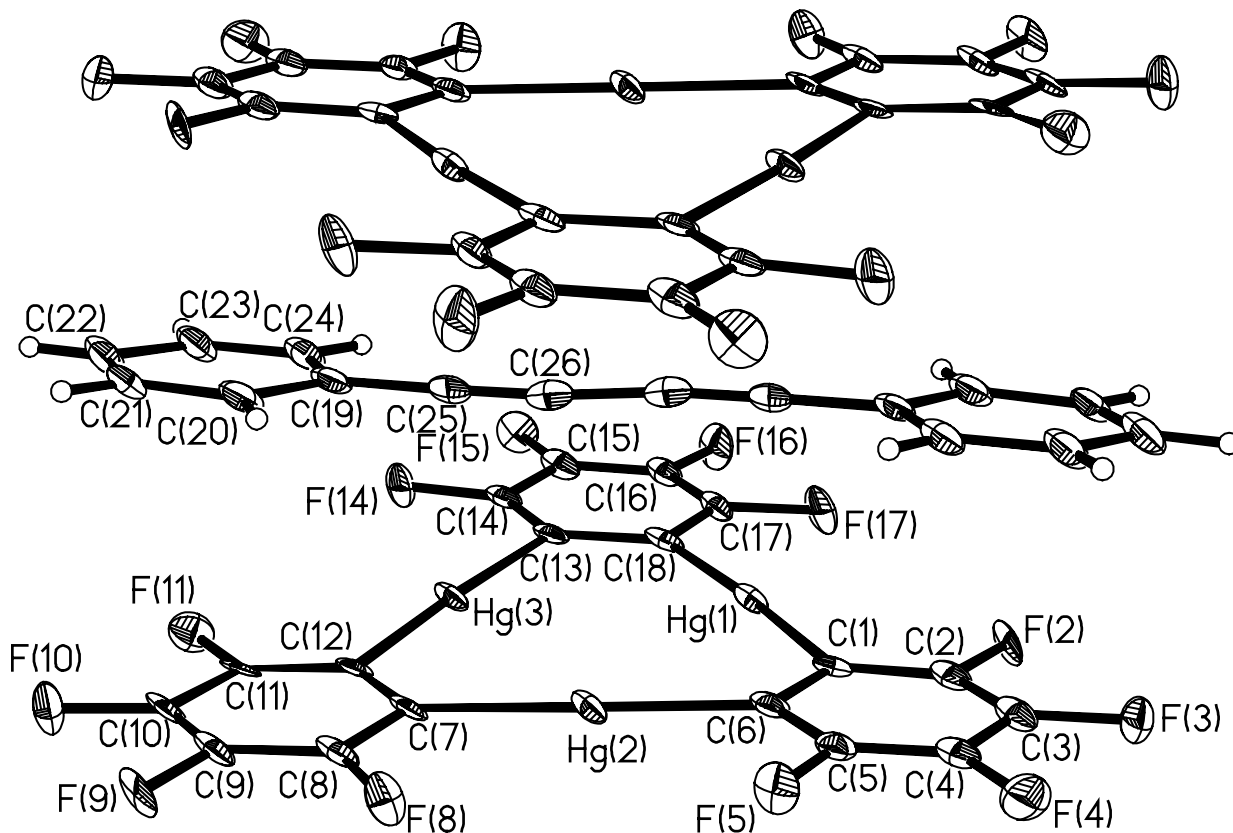


Table 1. Crystal data and structure refinement for **2**.

Identification code	2	
Empirical formula	C ₅₂ H ₁₀ F ₂₄ Hg ₆	
Formula weight	2294.14	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.0887(18) Å	α = 68.33(3)°
	b = 10.574(2) Å	β = 78.31(3)°
	c = 13.650(3) Å	γ = 83.00(3)°
Volume	1192.2(4) Å ³	
Z	1	
Density (calculated)	3.195 Mg/m ³	
Absorption coefficient	19.380 mm ⁻¹	
F(000)	1018	
Crystal size	0.08 x 0.07 x 0.065 mm ³	
Theta range for data collection	1.63 to 23.34°	
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -15 ≤ l ≤ 15	

Reflections collected	6872
Independent reflections	3346 [R(int) = 0.0475]
Completeness to theta = 23.34°	96.6 %
Absorption correction	SADABS
T _{min} /T _{max}	0.342430
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3346 / 144 / 370
Goodness-of-fit on F ²	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0599, wR2 = 0.1583
R indices (all data)	R1 = 0.0646, wR2 = 0.1649
Largest diff. peak and hole	4.300 and -4.879 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Hg(1)	3869(1)	8766(1)	9477(1)	16(1)
Hg(2)	7614(1)	7393(1)	9862(1)	17(1)
Hg(3)	6515(1)	8046(1)	7337(1)	16(1)
F(2)	2317(10)	9332(9)	11581(7)	22(2)
F(3)	3167(11)	8698(9)	13500(8)	29(2)
F(4)	5953(11)	7471(10)	13820(7)	32(2)
F(5)	7825(9)	6913(9)	12243(7)	24(2)
F(8)	10969(10)	6223(9)	9719(7)	26(2)
F(9)	12898(9)	5643(9)	8161(8)	26(2)
F(10)	12150(10)	6213(10)	6218(7)	27(2)
F(11)	9403(10)	7332(9)	5846(7)	27(2)
F(14)	4743(9)	8602(9)	5479(7)	25(2)
F(15)	1972(10)	9800(9)	5123(7)	28(2)
F(16)	97(10)	10512(10)	6652(8)	29(2)
F(17)	896(10)	9990(10)	8569(8)	29(2)
C(1)	4612(16)	8414(14)	10888(12)	15(2)
C(2)	3727(17)	8694(15)	11734(13)	19(2)
C(3)	4110(17)	8396(15)	12698(13)	21(2)
C(4)	5526(17)	7787(15)	12859(13)	20(2)
C(5)	6450(17)	7494(15)	12056(13)	18(2)
C(6)	6064(17)	7805(15)	11045(13)	18(2)
C(7)	9083(17)	7064(15)	8596(13)	18(2)
C(8)	10512(16)	6510(15)	8773(13)	20(2)
C(9)	11503(16)	6210(15)	7974(13)	20(2)
C(10)	11141(16)	6502(15)	6988(13)	20(2)
C(11)	9713(16)	7081(15)	6815(13)	17(2)
C(12)	8714(16)	7352(15)	7586(13)	17(2)
C(13)	4297(16)	8736(14)	7203(12)	17(2)
C(14)	3854(17)	8981(15)	6248(12)	18(2)
C(15)	2412(17)	9557(15)	6043(13)	22(2)
C(16)	1459(16)	9910(14)	6833(13)	19(2)
C(17)	1901(17)	9633(14)	7827(12)	18(2)
C(18)	3313(17)	9060(15)	8045(13)	18(2)
C(19)	6949(17)	4601(16)	7793(12)	21(2)
C(20)	8352(18)	3922(17)	7784(13)	24(2)
C(21)	9082(18)	3696(17)	6854(13)	24(2)

C(22)	8477(17)	4160(16)	5930(14)	28(3)
C(23)	7077(18)	4875(16)	5950(14)	27(2)
C(24)	6301(18)	5102(16)	6836(13)	25(2)
C(25)	6150(17)	4788(16)	8756(13)	20(4)
C(26)	5441(19)	4955(17)	9532(14)	24(4)

Table 3. Bond lengths [Å] and angles [°] for 2.

Hg(1)-C(18)	2.023(15)	C(18)-Hg(1)-C(1)	175.2(7)
Hg(1)-C(1)	2.059(14)	C(6)-Hg(2)-C(7)	176.1(7)
Hg(2)-C(6)	2.057(16)	C(13)-Hg(3)-C(12)	175.8(6)
Hg(2)-C(7)	2.070(16)	C(2)-C(1)-C(6)	116.5(14)
Hg(3)-C(13)	2.080(15)	C(2)-C(1)-Hg(1)	122.7(11)
Hg(3)-C(12)	2.093(15)	C(6)-C(1)-Hg(1)	120.7(12)
F(2)-C(2)	1.391(18)	C(3)-C(2)-C(1)	125.3(14)
F(3)-C(3)	1.359(19)	C(3)-C(2)-F(2)	117.4(14)
F(4)-C(4)	1.355(18)	C(1)-C(2)-F(2)	117.3(13)
F(5)-C(5)	1.354(17)	C(2)-C(3)-F(3)	121.9(14)
F(8)-C(8)	1.354(18)	C(2)-C(3)-C(4)	118.3(16)
F(9)-C(9)	1.365(18)	F(3)-C(3)-C(4)	119.8(14)
F(10)-C(10)	1.347(19)	C(5)-C(4)-F(4)	120.8(14)
F(11)-C(11)	1.331(18)	C(5)-C(4)-C(3)	119.2(15)
F(14)-C(14)	1.343(18)	F(4)-C(4)-C(3)	120.0(15)
F(15)-C(15)	1.320(18)	C(4)-C(5)-F(5)	117.3(14)
F(16)-C(16)	1.347(17)	C(4)-C(5)-C(6)	123.0(15)
F(17)-C(17)	1.351(19)	F(5)-C(5)-C(6)	119.6(14)
C(1)-C(2)	1.37(2)	C(5)-C(6)-C(1)	117.6(15)
C(1)-C(6)	1.42(2)	C(5)-C(6)-Hg(2)	119.3(11)
C(2)-C(3)	1.34(2)	C(1)-C(6)-Hg(2)	123.1(12)
C(3)-C(4)	1.39(2)	C(8)-C(7)-C(12)	118.5(15)
C(4)-C(5)	1.35(2)	C(8)-C(7)-Hg(2)	117.5(12)
C(5)-C(6)	1.40(2)	C(12)-C(7)-Hg(2)	124.0(11)
C(7)-C(8)	1.39(2)	F(8)-C(8)-C(9)	118.0(13)
C(7)-C(12)	1.40(2)	F(8)-C(8)-C(7)	122.3(15)
C(8)-C(9)	1.37(2)	C(9)-C(8)-C(7)	119.7(15)
C(9)-C(10)	1.37(2)	F(9)-C(9)-C(10)	119.2(14)
C(10)-C(11)	1.39(2)	F(9)-C(9)-C(8)	119.3(14)
C(11)-C(12)	1.34(2)	C(10)-C(9)-C(8)	121.5(14)
C(13)-C(14)	1.37(2)	F(10)-C(10)-C(9)	119.9(13)
C(13)-C(18)	1.43(2)	F(10)-C(10)-C(11)	121.9(15)
C(14)-C(15)	1.41(2)	C(9)-C(10)-C(11)	118.2(16)
C(15)-C(16)	1.38(2)	F(11)-C(11)-C(12)	122.4(14)
C(16)-C(17)	1.41(2)	F(11)-C(11)-C(10)	116.2(15)
C(17)-C(18)	1.39(2)	C(12)-C(11)-C(10)	121.5(15)
C(19)-C(20)	1.39(2)	C(11)-C(12)-C(7)	120.6(14)
C(19)-C(24)	1.43(2)	C(11)-C(12)-Hg(3)	120.1(11)
C(19)-C(25)	1.44(2)	C(7)-C(12)-Hg(3)	119.2(11)
C(20)-C(21)	1.40(2)	C(14)-C(13)-C(18)	121.1(14)
C(21)-C(22)	1.38(2)	C(14)-C(13)-Hg(3)	117.6(12)
C(22)-C(23)	1.40(2)	C(18)-C(13)-Hg(3)	121.0(11)
C(23)-C(24)	1.36(2)	F(14)-C(14)-C(13)	121.2(13)
C(25)-C(26)	1.19(2)	F(14)-C(14)-C(15)	116.5(13)
C(26)-C(26)#1	1.39(4)	C(13)-C(14)-C(15)	122.1(15)
		F(15)-C(15)-C(16)	119.5(14)

F(15)-C(15)-C(14)	122.7(15)	C(20)-C(19)-C(24)	119.3(15)
C(16)-C(15)-C(14)	117.8(15)	C(20)-C(19)-C(25)	120.1(14)
F(16)-C(16)-C(15)	119.5(14)	C(24)-C(19)-C(25)	120.6(15)
F(16)-C(16)-C(17)	120.3(14)	C(19)-C(20)-C(21)	119.3(16)
C(15)-C(16)-C(17)	120.2(14)	C(22)-C(21)-C(20)	122.3(16)
F(17)-C(17)-C(18)	120.4(14)	C(21)-C(22)-C(23)	117.3(17)
F(17)-C(17)-C(16)	116.8(13)	C(24)-C(23)-C(22)	123.0(17)
C(18)-C(17)-C(16)	122.8(15)	C(23)-C(24)-C(19)	118.7(16)
C(17)-C(18)-C(13)	116.0(14)	C(26)-C(25)-C(19)	177.4(17)
C(17)-C(18)-Hg(1)	119.8(12)	C(25)-C(26)-C(26)#1	175(2)
C(13)-C(18)-Hg(1)	124.2(11)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2. 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
Hg(1)	9(1)	18(1)	19(1)	-3(1)	1(1)	-4(1)
Hg(2)	8(1)	19(1)	21(1)	-5(1)	2(1)	-4(1)
Hg(3)	7(1)	17(1)	23(1)	-4(1)	1(1)	-4(1)
F(2)	9(4)	23(5)	27(5)	-7(4)	8(4)	4(4)
F(3)	30(6)	28(5)	30(6)	-19(5)	8(4)	-2(4)
F(4)	37(6)	40(6)	23(5)	-12(5)	-7(4)	-11(5)
F(5)	13(5)	34(5)	28(5)	-12(4)	-11(4)	10(4)
F(8)	17(5)	34(5)	21(5)	-7(4)	-2(4)	3(4)
F(9)	2(4)	33(5)	39(6)	-11(5)	0(4)	4(4)
F(10)	16(5)	42(6)	23(5)	-16(5)	1(4)	5(4)
F(11)	27(5)	27(5)	25(5)	-5(4)	-5(4)	-5(4)
F(14)	12(5)	34(5)	29(5)	-14(5)	1(4)	5(4)
F(15)	23(5)	30(5)	29(6)	-7(4)	-10(4)	3(4)
F(16)	15(5)	37(6)	37(6)	-19(5)	-5(4)	12(4)
F(17)	9(5)	43(6)	32(6)	-13(5)	3(4)	4(4)
C(1)	13(4)	12(4)	19(5)	-2(4)	-3(4)	-8(4)
C(2)	16(5)	12(4)	23(5)	0(4)	0(4)	-6(4)
C(3)	16(4)	14(4)	26(5)	-1(4)	2(4)	-5(4)
C(4)	16(5)	15(4)	26(5)	-3(4)	-2(4)	-7(4)
C(5)	17(5)	13(4)	23(5)	-4(4)	1(4)	-8(4)
C(6)	16(4)	14(4)	21(5)	-3(4)	1(4)	-9(4)
C(7)	8(4)	13(4)	27(5)	-4(4)	3(4)	-8(4)
C(8)	10(4)	16(4)	27(5)	-1(4)	1(4)	-7(4)
C(9)	9(4)	14(4)	28(5)	1(4)	3(4)	-5(4)
C(10)	9(4)	14(4)	30(5)	-1(4)	4(4)	-7(4)
C(11)	9(4)	13(4)	29(5)	-4(4)	-1(4)	-9(4)
C(12)	10(4)	13(4)	27(5)	-6(4)	2(4)	-9(4)
C(13)	13(4)	12(4)	23(5)	-3(4)	1(4)	-8(4)
C(14)	13(4)	13(4)	24(5)	-3(4)	0(4)	-7(4)
C(15)	17(4)	17(4)	26(5)	-1(4)	-2(4)	-5(4)
C(16)	14(4)	13(4)	25(5)	-1(4)	0(4)	-3(4)
C(17)	12(4)	13(4)	22(5)	-1(4)	3(4)	-3(4)
C(18)	12(4)	14(4)	23(5)	0(4)	-1(4)	-8(4)
C(19)	16(4)	27(5)	22(5)	-9(4)	2(4)	-14(4)

C(20)	17(5)	28(5)	26(5)	-7(4)	1(4)	-13(4)
C(21)	14(5)	26(5)	28(5)	-8(4)	5(4)	-10(4)
C(22)	17(5)	27(5)	31(5)	-5(4)	8(4)	-8(4)
C(23)	17(5)	27(5)	30(5)	-6(4)	6(4)	-10(4)
C(24)	17(5)	28(5)	26(5)	-7(4)	3(4)	-12(4)
C(25)	12(8)	27(9)	27(10)	-13(8)	-6(8)	-8(7)
C(26)	25(10)	19(8)	31(10)	-10(8)	-7(8)	-7(7)

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

	x	y	z	U(eq)
H(20)	8813	3614	8403	29
H(21)	10029	3204	6860	29
H(22)	8989	4002	5303	33
H(23)	6650	5217	5316	32
H(24)	5348	5584	6822	30

Crystal structure data for 1:1 trimeric perfluoro-*o*-phenylene mercury 1,6-diphenylhexatriyne adduct, **3**.

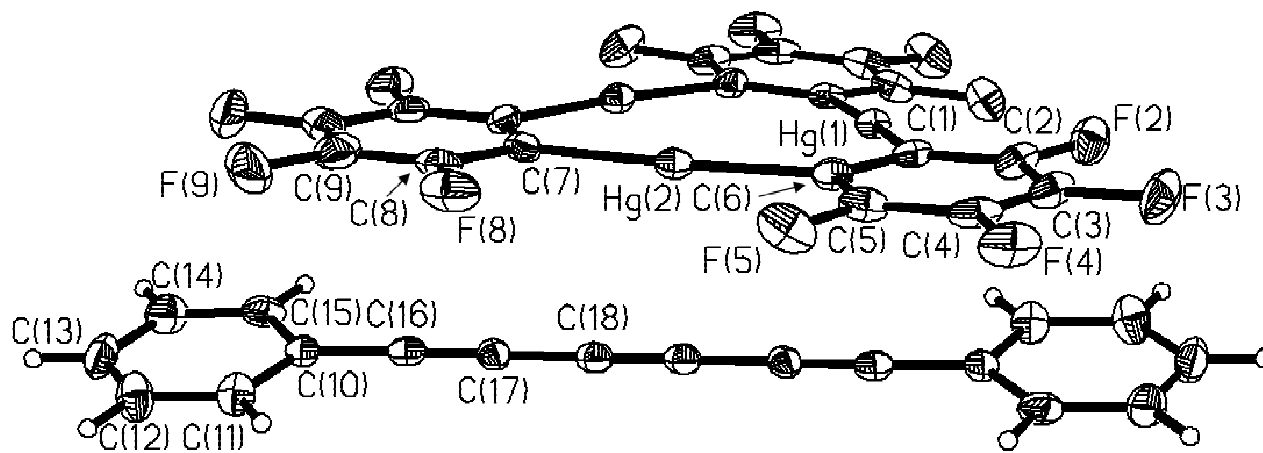


Table 1. Crystal data and structure refinement for **3**.

Identification code	3	
Empirical formula	C ₃₆ H ₁₀ F ₁₂ Hg ₃	
Formula weight	1272.21	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 12.360(3) Å	α = 90°.
	b = 30.321(6) Å	β = 108.43(3)°.
	c = 9.0688(18) Å	γ = 90°.
Volume	3224.4(11) Å ³	
Z	4	
Density (calculated)	2.621 Mg/m ³	
Absorption coefficient	14.345 mm ⁻¹	
F(000)	2296	
Crystal size	0.13 x 0.10 x 0.08 mm ³	
Theta range for data collection	1.34 to 27.55°.	
Index ranges	-16 ≤ h ≤ 15, -39 ≤ k ≤ 39, -11 ≤ l ≤ 11	
Reflections collected	13487	
Independent reflections	3716 [R(int) = 0.0488]	
Completeness to theta = 27.55°	99.4 %	
Absorption correction	SADABS	
T _{min} /T _{max}	0.257089	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3716 / 0 / 231	
Goodness-of-fit on F ²	1.008	
Final R indices [I > 2σ(I)]	R1 = 0.0336, wR2 = 0.0853	

R indices (all data)
Largest diff. peak and hole

R1 = 0.0403, wR2 = 0.0881
2.056 and -2.540 e.Å⁻³

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

	x	y	z	U(eq)
Hg(1)	5000	3531(1)	2500	17(1)
Hg(2)	5592(1)	2497(1)	933(1)	19(1)
C(1)	5598(5)	3507(2)	595(7)	20(1)
C(2)	5791(5)	3892(2)	-80(7)	25(1)
C(3)	6261(5)	3889(3)	-1282(7)	28(2)
C(4)	6535(5)	3498(2)	-1809(7)	26(2)
C(5)	6342(5)	3107(2)	-1162(7)	25(1)
C(6)	5866(5)	3101(2)	53(7)	21(1)
C(7)	5244(5)	1917(2)	1881(7)	21(1)
C(8)	5462(5)	1523(2)	1340(8)	29(2)
C(9)	5233(6)	1123(3)	1888(9)	36(2)
C(10)	7837(5)	3945(2)	-6356(7)	22(1)
C(11)	7313(6)	4271(2)	-5718(7)	27(1)
C(12)	7354(6)	4705(2)	-6120(8)	34(2)
C(13)	7923(6)	4827(2)	-7152(8)	35(2)
C(14)	8456(6)	4509(3)	-7779(8)	33(2)
C(15)	8415(5)	4074(2)	-7402(8)	28(2)
C(16)	7760(5)	3490(2)	-5972(7)	22(1)
C(17)	7656(5)	3115(2)	-5646(7)	21(1)
C(18)	7546(5)	2685(2)	-5211(7)	23(1)
F(2)	5526(3)	4283(1)	410(5)	33(1)
F(3)	6440(4)	4271(2)	-1926(5)	39(1)
F(4)	6995(3)	3498(2)	-2973(5)	36(1)
F(5)	6626(3)	2729(2)	-1722(4)	35(1)
F(8)	5917(3)	1502(2)	151(5)	39(1)
F(9)	5466(4)	732(2)	1332(6)	54(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for 3.

Hg(1)-C(1)	2.084(6)	C(4)-C(5)	1.378(10)
Hg(1)-C(1)#1	2.084(6)	C(5)-F(5)	1.346(8)
Hg(1)-C(17)	9.071(7)	C(5)-C(6)	1.403(8)
Hg(1)-C(16)	9.342(7)	C(7)-C(8)	1.352(9)
Hg(2)-C(7)	2.061(6)	C(7)-C(7)#1	1.432(12)
Hg(2)-C(6)	2.068(7)	C(8)-F(8)	1.366(9)
Hg(2)-C(18)	6.761(7)	C(8)-C(9)	1.373(11)
C(1)-C(2)	1.373(9)	C(9)-F(9)	1.356(8)
C(1)-C(6)	1.404(9)	C(9)-C(9)#1	1.404(16)
C(2)-F(2)	1.343(8)	C(10)-C(11)	1.404(9)
C(2)-C(3)	1.388(9)	C(10)-C(15)	1.411(9)
C(3)-F(3)	1.347(8)	C(10)-C(16)	1.435(9)
C(3)-C(4)	1.359(10)	C(11)-C(12)	1.369(10)
C(4)-F(4)	1.348(7)	C(12)-C(13)	1.387(10)

C(13)-C(14)	1.386(11)	C(5)-C(6)-C(1)	117.9(6)
C(14)-C(15)	1.368(10)	C(5)-C(6)-Hg(2)	118.3(5)
C(16)-C(17)	1.191(9)	C(1)-C(6)-Hg(2)	123.8(4)
C(17)-C(18)	1.381(9)	C(8)-C(7)-C(7)#1	117.8(4)
C(18)-C(18)#2	1.202(14)	C(8)-C(7)-Hg(2)	120.7(5)
		C(7)#1-C(7)-Hg(2)	121.49(16)
C(1)-Hg(1)-C(1)#1	176.0(4)	C(7)-C(8)-F(8)	120.4(7)
C(1)-Hg(1)-C(17)	6.0(2)	C(7)-C(8)-C(9)	124.2(7)
C(1)#1-Hg(1)-C(17)	170.0(2)	F(8)-C(8)-C(9)	115.4(6)
C(1)-Hg(1)-C(16)	1.37(19)	F(9)-C(9)-C(8)	123.1(7)
C(1)#1-Hg(1)-C(16)	177.16(19)	F(9)-C(9)-C(9)#1	118.9(4)
C(17)-Hg(1)-C(16)	7.22(5)	C(8)-C(9)-C(9)#1	118.0(4)
C(7)-Hg(2)-C(6)	175.9(2)	C(11)-C(10)-C(15)	118.7(6)
C(7)-Hg(2)-C(18)	126.31(17)	C(11)-C(10)-C(16)	120.3(6)
C(6)-Hg(2)-C(18)	57.50(18)	C(15)-C(10)-C(16)	121.0(6)
C(2)-C(1)-C(6)	119.7(6)	C(12)-C(11)-C(10)	120.4(7)
C(2)-C(1)-Hg(1)	119.8(5)	C(11)-C(12)-C(13)	120.4(7)
C(6)-C(1)-Hg(1)	120.4(5)	C(14)-C(13)-C(12)	119.9(7)
F(2)-C(2)-C(1)	120.6(6)	C(15)-C(14)-C(13)	120.6(7)
F(2)-C(2)-C(3)	118.2(6)	C(14)-C(15)-C(10)	120.1(6)
C(1)-C(2)-C(3)	121.2(7)	C(17)-C(16)-C(10)	177.4(7)
F(3)-C(3)-C(4)	120.3(6)	C(17)-C(16)-Hg(1)	73.3(4)
F(3)-C(3)-C(2)	120.0(7)	C(10)-C(16)-Hg(1)	104.8(4)
C(4)-C(3)-C(2)	119.7(6)	C(16)-C(17)-C(18)	177.9(7)
F(4)-C(4)-C(3)	119.3(6)	C(16)-C(17)-Hg(1)	99.5(4)
F(4)-C(4)-C(5)	120.4(6)	C(18)-C(17)-Hg(1)	78.7(4)
C(3)-C(4)-C(5)	120.3(6)	C(18)#2-C(18)-C(17)	178.1(9)
F(5)-C(5)-C(4)	118.2(6)	C(18)#2-C(18)-Hg(2)	64.2(6)
F(5)-C(5)-C(6)	120.7(6)	C(17)-C(18)-Hg(2)	114.1(4)
C(4)-C(5)-C(6)	121.2(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x+3/2,-y+1/2,-z-1

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3. 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
Hg(1)	17(1)	23(1)	13(1)	0	5(1)	0
Hg(2)	16(1)	25(1)	17(1)	-1(1)	7(1)	1(1)
C(1)	13(3)	31(4)	16(3)	0(2)	4(2)	-2(2)
C(2)	22(3)	38(4)	16(3)	-1(3)	6(2)	-10(3)
C(3)	22(3)	46(5)	14(3)	7(3)	5(2)	-11(3)
C(4)	13(3)	54(5)	14(3)	3(3)	7(2)	-1(3)
C(5)	19(3)	41(4)	17(3)	1(3)	7(2)	5(3)
C(6)	17(3)	27(4)	20(3)	-2(2)	8(2)	1(2)
C(7)	15(3)	23(3)	23(3)	-1(2)	5(2)	4(2)
C(8)	14(3)	36(4)	29(3)	-5(3)	-2(2)	3(3)
C(9)	24(3)	37(4)	41(4)	-13(3)	0(3)	-2(3)
C(10)	20(3)	22(3)	20(3)	0(2)	3(2)	0(2)
C(11)	35(4)	27(4)	19(3)	-3(2)	8(3)	-2(3)
C(12)	49(4)	25(4)	26(3)	-3(3)	10(3)	1(3)
C(13)	40(4)	24(4)	34(4)	5(3)	5(3)	-11(3)

C(14)	31(3)	38(4)	31(4)	10(3)	13(3)	-2(3)
C(15)	18(3)	40(4)	27(3)	3(3)	10(2)	3(3)
C(16)	17(3)	29(4)	18(3)	-2(2)	3(2)	0(3)
C(17)	20(3)	21(3)	19(3)	-1(2)	1(2)	1(2)
C(18)	18(3)	24(4)	23(3)	-5(3)	4(2)	1(3)
F(2)	42(2)	30(2)	26(2)	0(2)	11(2)	-7(2)
F(3)	47(2)	39(3)	32(2)	9(2)	15(2)	-16(2)
F(4)	26(2)	66(3)	23(2)	7(2)	18(2)	-1(2)
F(5)	36(2)	49(3)	27(2)	1(2)	20(2)	15(2)
F(8)	28(2)	51(3)	36(2)	-18(2)	10(2)	8(2)
F(9)	48(3)	30(3)	69(3)	-15(2)	-4(2)	12(2)

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

	x	y	z	U(eq)
H(11)	6927	4191	-5003	32
H(12)	6992	4923	-5689	40
H(13)	7948	5128	-7429	41
H(14)	8852	4594	-8476	39
H(15)	8776	3858	-7845	33

Crystal structure data for 2:1 trimeric perfluoro-*o*-phenylene mercury 1,8-diphenyloctatetrayne adduct, **4**.

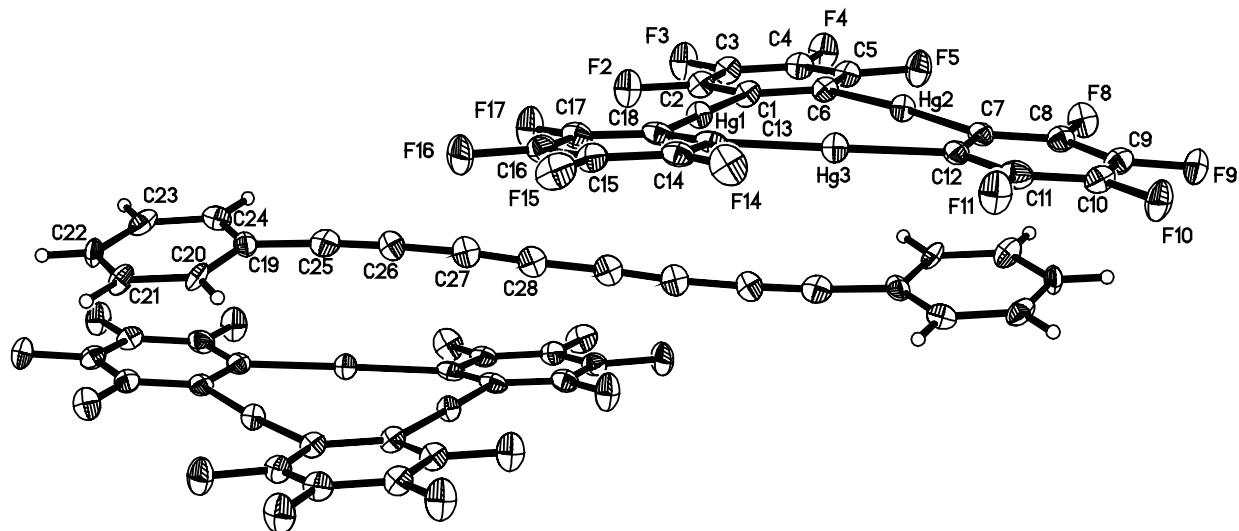


Table 1. Crystal data and structure refinement for **4**.

Identification code	4	
Empirical formula	C ₂₈ H ₅ F ₁₂ Hg ₃	
Formula weight	1171.09	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.9766(14) Å	α = 95.01(3)°
	b = 10.317(2) Å	β = 93.27(3)°
	c = 18.189(4) Å	γ = 102.36(3)°
Volume	1270.1(4) Å ³	
Z	2	
Density (calculated)	3.062 Mg/m ³	
Absorption coefficient	18.194 mm ⁻¹	
F(000)	1042	
Crystal size	0.37 x 0.10 x 0.06 mm ³	
Theta range for data collection	1.13 to 23.29°	
Index ranges	-7 ≤ h ≤ 7, -11 ≤ k ≤ 11, -20 ≤ l ≤ 20	
Reflections collected	8031	
Independent reflections	3641 [R(int) = 0.0509]	
Completeness to theta = 23.29°	99.2 %	
Absorption correction	SADABS	
T _{min} /T _{max}	0.230142	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3641 / 96 / 388	
Goodness-of-fit on F ²	1.013	
Final R indices [I > 2σ(I)]	R1 = 0.0377, wR2 = 0.0907	

R indices (all data)
Largest diff. peak and hole

R1 = 0.0435, wR2 = 0.1056
2.265 and -1.968 e.Å⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Hg(1)	2594(1)	8494(1)	6505(1)	19(1)
Hg(2)	982(1)	8086(1)	8334(1)	19(1)
Hg(3)	693(1)	5187(1)	7042(1)	21(1)
C(1)	2712(16)	10090(11)	7288(6)	18(2)
C(2)	3389(17)	11367(11)	7093(7)	19(2)
C(3)	3538(17)	12487(12)	7589(7)	23(2)
C(4)	2978(17)	12320(12)	8291(7)	23(2)
C(5)	2317(17)	11054(12)	8496(6)	21(2)
C(6)	2126(17)	9940(11)	8019(6)	18(2)
C(7)	-263(16)	6190(12)	8582(6)	19(2)
C(8)	-1064(17)	6018(12)	9260(7)	21(2)
C(9)	-2005(17)	4780(12)	9433(7)	22(2)
C(10)	-2163(17)	3648(12)	8946(7)	22(2)
C(11)	-1369(18)	3819(13)	8266(7)	25(3)
C(12)	-433(16)	5039(12)	8065(6)	20(2)
C(13)	1839(17)	5503(12)	6045(7)	21(2)
C(14)	1843(17)	4390(12)	5544(7)	21(2)
C(15)	2452(17)	4524(12)	4832(7)	23(2)
C(16)	3072(17)	5779(13)	4610(7)	23(2)
C(17)	3120(17)	6913(12)	5106(7)	23(2)
C(18)	2484(17)	6771(12)	5804(7)	22(2)
C(19)	-3462(17)	8518(13)	7764(6)	23(3)
C(20)	-3060(16)	9464(13)	8385(7)	22(3)
C(21)	-3664(17)	9116(12)	9055(7)	24(3)
C(22)	-4623(17)	7814(14)	9129(7)	27(3)
C(23)	-4995(17)	6872(13)	8514(7)	26(3)
C(24)	-4424(17)	7200(14)	7830(7)	28(3)
C(25)	-2773(18)	8895(12)	7060(7)	23(3)
C(26)	-2108(18)	9239(12)	6491(7)	22(3)
C(27)	-1286(18)	9585(11)	5866(7)	22(3)
C(28)	-448(19)	9861(12)	5320(7)	24(3)
F(2)	3955(11)	11567(7)	6406(4)	31(2)
F(3)	4217(11)	13739(7)	7395(4)	34(2)
F(4)	3165(11)	13420(7)	8787(4)	33(2)
F(5)	1797(11)	10945(7)	9195(4)	32(2)
F(8)	-868(10)	7072(7)	9766(4)	28(2)
F(9)	-2789(10)	4651(7)	10087(4)	28(2)
F(10)	-3023(10)	2449(7)	9118(4)	31(2)
F(11)	-1514(11)	2696(7)	7797(4)	34(2)
F(14)	1216(11)	3128(7)	5725(4)	32(2)
F(15)	2424(10)	3453(7)	4347(4)	31(2)
F(16)	3599(11)	5916(7)	3917(4)	32(2)
F(17)	3722(11)	8122(7)	4881(4)	33(2)

Table 3. Bond lengths [Å] and angles [°] for 4.

Hg(1)-C(1)	2.066(11)	C(6)-C(1)-Hg(1)	123.1(8)
Hg(1)-C(18)	2.080(12)	F(2)-C(2)-C(3)	117.1(10)
Hg(2)-C(6)	2.053(12)	F(2)-C(2)-C(1)	120.9(10)
Hg(2)-C(7)	2.063(12)	C(3)-C(2)-C(1)	122.0(11)
Hg(3)-C(13)	2.047(13)	F(3)-C(3)-C(4)	119.7(11)
Hg(3)-C(12)	2.066(12)	F(3)-C(3)-C(2)	121.8(11)
C(1)-C(2)	1.385(17)	C(4)-C(3)-C(2)	118.6(11)
C(1)-C(6)	1.424(16)	F(4)-C(4)-C(3)	118.8(11)
C(2)-F(2)	1.352(14)	F(4)-C(4)-C(5)	121.0(11)
C(2)-C(3)	1.383(16)	C(3)-C(4)-C(5)	120.1(11)
C(3)-F(3)	1.362(14)	F(5)-C(5)-C(6)	119.7(11)
C(3)-C(4)	1.371(17)	F(5)-C(5)-C(4)	117.7(10)
C(4)-F(4)	1.366(14)	C(6)-C(5)-C(4)	122.6(12)
C(4)-C(5)	1.380(18)	C(5)-C(6)-C(1)	118.2(11)
C(5)-F(5)	1.351(14)	C(5)-C(6)-Hg(2)	121.0(9)
C(5)-C(6)	1.355(16)	C(1)-C(6)-Hg(2)	120.7(8)
C(7)-C(8)	1.392(17)	C(8)-C(7)-C(12)	118.1(11)
C(7)-C(12)	1.429(17)	C(8)-C(7)-Hg(2)	119.5(9)
C(8)-F(8)	1.340(14)	C(12)-C(7)-Hg(2)	122.2(9)
C(8)-C(9)	1.377(17)	F(8)-C(8)-C(9)	119.0(11)
C(9)-F(9)	1.343(14)	F(8)-C(8)-C(7)	119.4(11)
C(9)-C(10)	1.384(17)	C(9)-C(8)-C(7)	121.5(12)
C(10)-F(10)	1.326(14)	F(9)-C(9)-C(8)	120.0(11)
C(10)-C(11)	1.393(18)	F(9)-C(9)-C(10)	118.6(11)
C(11)-F(11)	1.360(14)	C(8)-C(9)-C(10)	121.4(12)
C(11)-C(12)	1.379(17)	F(10)-C(10)-C(9)	121.6(11)
C(13)-C(14)	1.402(16)	F(10)-C(10)-C(11)	121.3(11)
C(13)-C(18)	1.405(18)	C(9)-C(10)-C(11)	117.1(11)
C(14)-F(14)	1.357(14)	F(11)-C(11)-C(12)	120.0(11)
C(14)-C(15)	1.396(17)	F(11)-C(11)-C(10)	116.5(11)
C(15)-F(15)	1.348(13)	C(12)-C(11)-C(10)	123.5(11)
C(15)-C(16)	1.377(18)	C(11)-C(12)-C(7)	118.2(11)
C(16)-F(16)	1.342(14)	C(11)-C(12)-Hg(3)	120.5(9)
C(16)-C(17)	1.407(17)	C(7)-C(12)-Hg(3)	121.2(8)
C(17)-F(17)	1.335(14)	C(14)-C(13)-C(18)	117.5(11)
C(17)-C(18)	1.380(17)	C(14)-C(13)-Hg(3)	118.3(9)
C(19)-C(20)	1.401(17)	C(18)-C(13)-Hg(3)	124.0(9)
C(19)-C(24)	1.401(18)	F(14)-C(14)-C(15)	116.8(10)
C(19)-C(25)	1.449(18)	F(14)-C(14)-C(13)	121.5(11)
C(20)-C(21)	1.364(17)	C(15)-C(14)-C(13)	121.7(12)
C(21)-C(22)	1.388(18)	F(15)-C(15)-C(16)	118.7(11)
C(22)-C(23)	1.391(18)	F(15)-C(15)-C(14)	121.7(11)
C(23)-C(24)	1.376(18)	C(16)-C(15)-C(14)	119.6(11)
C(25)-C(26)	1.208(17)	F(16)-C(16)-C(15)	119.9(11)
C(26)-C(27)	1.345(18)	F(16)-C(16)-C(17)	120.2(11)
C(27)-C(28)	1.205(18)	C(15)-C(16)-C(17)	119.9(12)
C(28)-C(28)#1	1.38(3)	F(17)-C(17)-C(18)	120.7(11)
		F(17)-C(17)-C(16)	119.1(11)
C(1)-Hg(1)-C(18)	174.3(5)	C(18)-C(17)-C(16)	120.1(12)
C(6)-Hg(2)-C(7)	176.2(5)	C(17)-C(18)-C(13)	121.2(11)
C(13)-Hg(3)-C(12)	175.2(5)	C(17)-C(18)-Hg(1)	117.9(9)
C(2)-C(1)-C(6)	118.4(10)	C(13)-C(18)-Hg(1)	120.9(9)
C(2)-C(1)-Hg(1)	118.5(9)	C(20)-C(19)-C(24)	120.4(11)

C(20)-C(19)-C(25)	119.4(12)	C(23)-C(24)-C(19)	118.3(12)
C(24)-C(19)-C(25)	120.1(11)	C(26)-C(25)-C(19)	176.7(13)
C(21)-C(20)-C(19)	120.0(12)	C(25)-C(26)-C(27)	176.8(13)
C(20)-C(21)-C(22)	120.2(12)	C(28)-C(27)-C(26)	175.7(13)
C(21)-C(22)-C(23)	119.7(12)	C(27)-C(28)-C(28)#1	177.7(18)
C(24)-C(23)-C(22)	121.3(13)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. 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
Hg(1)	22(1)	15(1)	19(1)	-2(1)	2(1)	6(1)
Hg(2)	22(1)	15(1)	21(1)	2(1)	3(1)	6(1)
Hg(3)	24(1)	17(1)	21(1)	1(1)	4(1)	6(1)
C(1)	21(4)	12(4)	22(4)	-6(3)	5(3)	5(3)
C(2)	23(4)	11(4)	24(4)	-3(3)	4(3)	8(3)
C(3)	26(4)	17(4)	26(4)	-1(3)	4(4)	6(3)
C(4)	26(4)	19(4)	26(4)	-3(4)	2(4)	9(3)
C(5)	23(4)	19(4)	22(4)	-4(3)	3(3)	10(3)
C(6)	20(4)	13(4)	23(4)	0(3)	3(3)	7(3)
C(7)	18(4)	20(4)	22(4)	7(3)	-1(3)	6(3)
C(8)	20(4)	20(4)	24(4)	3(3)	1(3)	7(3)
C(9)	19(4)	19(4)	27(4)	2(4)	3(4)	5(3)
C(10)	19(5)	17(5)	30(5)	2(4)	3(4)	4(4)
C(11)	24(7)	26(8)	23(7)	-6(6)	-3(5)	5(6)
C(12)	17(5)	21(5)	22(5)	9(4)	0(4)	6(4)
C(13)	19(4)	21(4)	24(4)	-3(3)	-6(3)	9(3)
C(14)	20(4)	20(4)	24(4)	-3(3)	-4(3)	10(3)
C(15)	22(4)	23(4)	24(4)	-5(4)	2(3)	7(3)
C(16)	21(4)	24(4)	22(4)	-4(3)	0(3)	4(4)
C(17)	23(4)	22(4)	23(4)	-2(3)	-4(4)	4(3)
C(18)	20(4)	21(4)	21(4)	-5(3)	-7(3)	6(3)
C(19)	22(6)	34(8)	18(6)	6(6)	3(5)	16(6)
C(20)	16(6)	24(7)	26(7)	4(5)	12(5)	4(5)
C(21)	24(7)	22(7)	29(7)	-3(6)	12(5)	11(5)
C(22)	24(7)	44(9)	17(7)	14(6)	9(5)	11(6)
C(23)	17(6)	26(8)	38(8)	11(6)	9(6)	8(5)
C(24)	22(7)	36(9)	26(7)	5(6)	-3(6)	6(6)
C(25)	25(7)	19(7)	30(8)	-1(6)	3(6)	15(5)
C(26)	30(7)	17(7)	20(7)	-3(6)	3(6)	11(5)
C(27)	32(7)	9(6)	25(8)	0(5)	4(6)	9(5)
C(28)	32(7)	13(7)	26(7)	0(5)	2(6)	5(5)
F(2)	46(5)	18(4)	29(4)	2(3)	11(3)	5(3)
F(3)	51(5)	17(4)	34(4)	4(3)	13(4)	6(3)
F(4)	47(5)	20(4)	28(4)	-9(3)	8(3)	5(3)
F(5)	43(4)	27(4)	26(4)	-1(3)	12(3)	5(3)
F(8)	38(4)	20(4)	27(4)	0(3)	5(3)	12(3)
F(9)	32(4)	29(4)	25(4)	8(3)	12(3)	6(3)
F(10)	39(4)	18(4)	32(4)	7(3)	12(3)	-4(3)
F(11)	46(5)	21(4)	30(4)	-1(3)	9(4)	1(3)

F(14)	46(5)	19(4)	32(4)	-3(3)	2(3)	13(3)
F(15)	31(4)	24(4)	37(4)	-15(3)	5(3)	9(3)
F(16)	42(4)	37(5)	18(4)	-4(3)	11(3)	10(4)
F(17)	50(5)	20(4)	28(4)	1(3)	15(3)	2(3)

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

	x	y	z	U(eq)
H(20)	-2366	10349	8340	26
H(21)	-3427	9766	9472	28
H(22)	-5025	7569	9597	32
H(23)	-5656	5983	8567	31
H(24)	-4677	6549	7413	34

Crystal structure data for 2:1 trimeric perfluoro-*o*-phenylene mercury 1,12-diphenyldodecahexayne adduct, **5**.

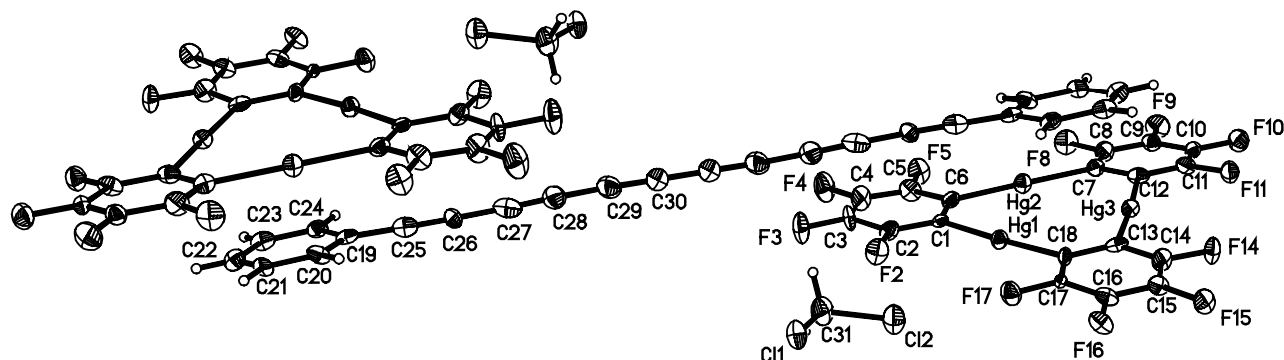


Table 1. Crystal data and structure refinement for **5**.

Identification code	5	
Empirical formula	C ₃₁ H ₇ Cl ₂ F ₁₂ Hg ₃	
Formula weight	1280.04	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/c	
Unit cell dimensions	a = 9.6848(19) Å	α = 90°.
	b = 7.1522(14) Å	β = 95.49(3)°.
	c = 43.542(9) Å	γ = 90°.
Volume	3002.3(10) Å ³	
Z	4	
Density (calculated)	2.832 Mg/m ³	
Absorption coefficient	15.580 mm ⁻¹	
F(000)	2300	
Crystal size	0.10 x 0.035 x 0.025 mm ³	
Theta range for data collection	0.94 to 27.57°.	
Index ranges	-12 ≤ h ≤ 12, -8 ≤ k ≤ 9, -56 ≤ l ≤ 56	
Reflections collected	23337	
Independent reflections	6954 [R(int) = 0.0718]	
Completeness to theta = 27.57°	99.8 %	
Absorption correction	SADABS	
T _{min} /T _{max}	0.442009	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6954 / 0 / 433	
Goodness-of-fit on F ²	1.009	
Final R indices [I > 2σ(I)]	R1 = 0.0528, wR2 = 0.0956	
R indices (all data)	R1 = 0.0849, wR2 = 0.1100	
Largest diff. peak and hole	1.750 and -2.320 e.Å ⁻³	

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

	x	y	z	U(eq)
Hg(1)	2825(1)	3486(1)	1219(1)	21(1)
Hg(2)	-747(1)	5028(1)	1047(1)	24(1)
Hg(3)	927(1)	5558(1)	1811(1)	20(1)
F(2)	3726(7)	1731(11)	609(2)	35(2)
F(3)	2433(8)	1206(12)	45(2)	44(2)
F(4)	-257(8)	2392(14)	-86(2)	47(2)
F(5)	-1577(7)	4122(12)	349(2)	37(2)
F(8)	-3752(7)	6749(11)	1047(2)	37(2)
F(9)	-5080(7)	8464(12)	1486(2)	40(2)
F(10)	-3836(7)	8773(11)	2069(2)	35(2)
F(11)	-1271(7)	7387(11)	2219(2)	30(2)
F(14)	2987(7)	6016(11)	2392(2)	31(2)
F(15)	5674(7)	5066(11)	2532(2)	34(2)
F(16)	7099(7)	3325(10)	2106(2)	28(2)
F(17)	5860(7)	2600(11)	1540(2)	31(2)
C(1)	1749(12)	3157(16)	786(3)	20(3)
C(2)	2407(12)	2338(18)	552(3)	25(3)
C(3)	1733(14)	2023(19)	259(3)	29(3)
C(4)	398(14)	2660(20)	195(3)	34(3)
C(5)	-241(12)	3525(19)	425(3)	28(3)
C(6)	368(12)	3786(17)	721(3)	23(3)
C(7)	-1762(12)	6202(17)	1395(3)	20(3)
C(8)	-3076(13)	6930(20)	1333(3)	31(3)
C(9)	-3773(12)	7788(18)	1555(3)	25(3)
C(10)	-3151(13)	7953(18)	1853(3)	26(3)
C(11)	-1842(12)	7214(19)	1920(3)	25(3)
C(12)	-1114(12)	6370(17)	1701(3)	23(3)
C(13)	2987(12)	4766(16)	1884(3)	23(3)
C(14)	3664(13)	5137(19)	2175(3)	27(3)
C(15)	5045(12)	4650(18)	2256(3)	23(3)
C(16)	5771(12)	3797(17)	2038(3)	23(3)
C(17)	5111(11)	3418(15)	1746(2)	15(2)
C(18)	3734(12)	3920(16)	1660(2)	20(3)
C(19)	1275(12)	-212(17)	1495(3)	24(3)
C(20)	1997(12)	-240(17)	1790(3)	22(3)
C(21)	1387(12)	451(17)	2042(3)	26(3)
C(22)	58(13)	1245(17)	1998(3)	27(3)
C(23)	-632(11)	1314(17)	1702(3)	21(3)
C(24)	-26(12)	619(18)	1456(3)	25(3)
C(25)	1875(13)	-1034(18)	1235(3)	27(3)
C(26)	2361(12)	-1676(18)	1016(3)	27(3)
C(27)	2943(14)	-2410(20)	769(3)	35(3)
C(28)	3482(15)	-3020(20)	559(3)	37(3)
C(29)	4127(14)	-3830(20)	320(3)	38(4)
C(30)	4681(15)	-4580(20)	112(3)	37(3)
C(31)	7004(15)	180(20)	606(3)	39(4)
Cl(1)	8657(4)	-908(5)	654(1)	38(1)
Cl(2)	6742(3)	1568(6)	934(1)	42(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

Hg(1)-C(18)	2.059(11)	C(13)-Hg(3)-C(12)	175.5(5)
Hg(1)-C(1)	2.079(11)	C(2)-C(1)-C(6)	118.8(11)
Hg(2)-C(7)	2.062(12)	C(2)-C(1)-Hg(1)	119.4(9)
Hg(2)-C(6)	2.065(12)	C(6)-C(1)-Hg(1)	121.8(8)
Hg(3)-C(13)	2.069(12)	F(2)-C(2)-C(1)	119.7(11)
Hg(3)-C(12)	2.072(12)	F(2)-C(2)-C(3)	117.9(10)
F(2)-C(2)	1.349(13)	C(1)-C(2)-C(3)	122.3(11)
F(3)-C(3)	1.338(13)	F(3)-C(3)-C(4)	122.1(11)
F(4)-C(4)	1.338(14)	F(3)-C(3)-C(2)	119.0(11)
F(5)-C(5)	1.372(13)	C(4)-C(3)-C(2)	118.8(11)
F(8)-C(8)	1.360(14)	F(4)-C(4)-C(5)	121.5(12)
F(9)-C(9)	1.361(14)	F(4)-C(4)-C(3)	119.7(11)
F(10)-C(10)	1.337(13)	C(5)-C(4)-C(3)	118.8(11)
F(11)-C(11)	1.370(13)	C(4)-C(5)-F(5)	116.6(11)
F(14)-C(14)	1.357(14)	C(4)-C(5)-C(6)	124.1(11)
F(15)-C(15)	1.331(13)	F(5)-C(5)-C(6)	119.3(11)
F(16)-C(16)	1.336(13)	C(5)-C(6)-C(1)	117.1(11)
F(17)-C(17)	1.340(12)	C(5)-C(6)-Hg(2)	119.8(9)
C(1)-C(2)	1.382(16)	C(1)-C(6)-Hg(2)	123.1(8)
C(1)-C(6)	1.414(17)	C(8)-C(7)-C(12)	117.9(11)
C(2)-C(3)	1.394(17)	C(8)-C(7)-Hg(2)	120.4(9)
C(3)-C(4)	1.373(18)	C(12)-C(7)-Hg(2)	121.6(9)
C(4)-C(5)	1.374(18)	F(8)-C(8)-C(9)	117.5(11)
C(5)-C(6)	1.381(16)	F(8)-C(8)-C(7)	119.9(11)
C(7)-C(8)	1.377(17)	C(9)-C(8)-C(7)	122.6(12)
C(7)-C(12)	1.421(16)	F(9)-C(9)-C(8)	120.8(11)
C(8)-C(9)	1.374(17)	F(9)-C(9)-C(10)	119.3(11)
C(9)-C(10)	1.384(17)	C(8)-C(9)-C(10)	119.9(12)
C(10)-C(11)	1.379(17)	F(10)-C(10)-C(11)	122.0(11)
C(11)-C(12)	1.378(17)	F(10)-C(10)-C(9)	119.8(11)
C(13)-C(18)	1.403(16)	C(11)-C(10)-C(9)	118.2(11)
C(13)-C(14)	1.397(16)	F(11)-C(11)-C(12)	120.7(11)
C(14)-C(15)	1.394(16)	F(11)-C(11)-C(10)	116.3(11)
C(15)-C(16)	1.376(17)	C(12)-C(11)-C(10)	123.0(11)
C(16)-C(17)	1.393(16)	C(11)-C(12)-C(7)	118.4(11)
C(17)-C(18)	1.396(16)	C(11)-C(12)-Hg(3)	120.2(9)
C(19)-C(24)	1.389(17)	C(7)-C(12)-Hg(3)	121.2(9)
C(19)-C(20)	1.403(17)	C(18)-C(13)-C(14)	118.8(11)
C(19)-C(25)	1.445(18)	C(18)-C(13)-Hg(3)	124.4(9)
C(20)-C(21)	1.385(17)	C(14)-C(13)-Hg(3)	116.7(9)
C(21)-C(22)	1.403(16)	F(14)-C(14)-C(15)	117.2(10)
C(22)-C(23)	1.395(17)	F(14)-C(14)-C(13)	120.4(11)
C(23)-C(24)	1.363(16)	C(15)-C(14)-C(13)	122.5(11)
C(25)-C(26)	1.196(17)	F(15)-C(15)-C(16)	120.2(11)
C(26)-C(27)	1.364(18)	F(15)-C(15)-C(14)	121.1(11)
C(27)-C(28)	1.180(19)	C(16)-C(15)-C(14)	118.6(11)
C(28)-C(29)	1.390(19)	F(16)-C(16)-C(15)	120.2(11)
C(29)-C(30)	1.223(18)	F(16)-C(16)-C(17)	120.2(10)
C(30)-C(30)#1	1.34(3)	C(15)-C(16)-C(17)	119.7(11)
C(31)-Cl(1)	1.774(14)	F(17)-C(17)-C(16)	117.7(10)
C(31)-Cl(2)	1.779(14)	F(17)-C(17)-C(18)	119.9(9)
		C(16)-C(17)-C(18)	122.4(10)
C(18)-Hg(1)-C(1)	174.9(5)	C(13)-C(18)-C(17)	118.0(10)
C(7)-Hg(2)-C(6)	176.2(5)	C(13)-C(18)-Hg(1)	120.5(9)

C(17)-C(18)-Hg(1)	121.5(8)	C(23)-C(24)-C(19)	120.9(11)
C(24)-C(19)-C(20)	119.0(11)	C(26)-C(25)-C(19)	178.3(14)
C(24)-C(19)-C(25)	120.4(11)	C(25)-C(26)-C(27)	178.7(15)
C(20)-C(19)-C(25)	120.6(11)	C(28)-C(27)-C(26)	178.1(16)
C(21)-C(20)-C(19)	120.4(11)	C(27)-C(28)-C(29)	176.9(17)
C(20)-C(21)-C(22)	119.4(12)	C(30)-C(29)-C(28)	178.3(17)
C(23)-C(22)-C(21)	119.5(11)	C(29)-C(30)-C(30)#1	179(2)
C(24)-C(23)-C(22)	120.6(11)	Cl(1)-C(31)-Cl(2)	110.2(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y-1,-z

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
Hg(1)	22(1)	25(1)	17(1)	-2(1)	-1(1)	0(1)
Hg(2)	21(1)	28(1)	22(1)	-2(1)	-1(1)	2(1)
Hg(3)	19(1)	21(1)	21(1)	1(1)	-1(1)	1(1)
F(2)	23(4)	44(5)	36(4)	-7(4)	-6(3)	8(3)
F(3)	43(5)	67(6)	21(4)	-14(4)	2(3)	12(4)
F(4)	36(5)	81(7)	24(4)	-9(4)	-4(3)	6(4)
F(5)	27(4)	55(5)	27(4)	0(4)	-6(3)	7(4)
F(8)	20(4)	49(5)	38(4)	-1(4)	-8(3)	8(3)
F(9)	21(4)	48(5)	52(5)	-4(4)	4(4)	5(4)
F(10)	26(4)	41(5)	39(4)	-9(4)	8(3)	2(3)
F(11)	27(4)	40(5)	25(4)	-6(3)	3(3)	0(3)
F(14)	28(4)	42(5)	22(4)	-13(3)	0(3)	8(3)
F(15)	22(4)	57(5)	21(4)	-3(4)	-7(3)	-4(4)
F(16)	18(4)	40(5)	26(4)	10(3)	2(3)	5(3)
F(17)	25(4)	39(5)	30(4)	-3(3)	7(3)	5(3)
C(1)	22(6)	20(7)	17(5)	-3(5)	1(5)	-11(5)
C(2)	22(7)	24(7)	27(7)	-4(5)	-3(5)	2(5)
C(3)	38(8)	38(8)	14(6)	-5(6)	9(5)	9(6)
C(4)	32(8)	54(10)	12(6)	-1(6)	-11(5)	-1(7)
C(5)	19(6)	35(8)	27(7)	7(6)	-4(5)	8(6)
C(6)	25(7)	22(7)	21(6)	-2(5)	-2(5)	-5(5)
C(7)	23(6)	21(6)	17(6)	4(5)	-3(5)	-1(5)
C(8)	26(7)	41(9)	24(6)	-3(6)	-3(5)	-6(6)
C(9)	21(6)	23(7)	30(7)	2(5)	6(5)	2(5)
C(10)	22(6)	26(7)	30(7)	-12(6)	11(5)	-6(5)
C(11)	19(6)	35(8)	20(6)	6(5)	-3(5)	-6(5)
C(12)	16(6)	20(7)	33(7)	5(5)	1(5)	1(5)
C(13)	18(6)	16(6)	33(7)	2(5)	-2(5)	-4(5)
C(14)	24(7)	36(8)	21(6)	0(6)	-7(5)	0(6)
C(15)	18(6)	31(8)	19(6)	7(5)	-4(5)	-1(5)
C(16)	20(6)	26(7)	22(6)	13(5)	0(5)	1(5)
C(17)	21(6)	14(6)	12(5)	-4(4)	5(4)	-6(5)
C(18)	30(7)	18(6)	12(5)	-2(5)	4(5)	-2(5)
C(19)	24(6)	16(6)	31(7)	1(5)	0(5)	-7(5)
C(20)	16(6)	22(7)	29(6)	-1(5)	-2(5)	-1(5)
C(21)	21(6)	23(7)	33(7)	5(6)	-6(5)	-1(5)
C(22)	25(7)	22(7)	32(7)	-1(6)	-1(5)	5(5)

C(23)	6(5)	25(7)	33(7)	1(5)	2(5)	5(5)
C(24)	18(6)	34(8)	23(6)	7(6)	1(5)	-5(5)
C(25)	21(6)	24(7)	36(7)	8(6)	-4(5)	1(5)
C(26)	18(6)	31(8)	33(7)	-7(6)	11(5)	-1(5)
C(27)	26(7)	32(8)	47(9)	11(7)	3(6)	-3(6)
C(28)	40(9)	39(9)	30(7)	0(7)	4(6)	-7(7)
C(29)	27(7)	48(10)	39(8)	-5(7)	6(6)	-8(7)
C(30)	42(9)	33(8)	39(8)	-5(7)	12(7)	-5(7)
C(31)	39(8)	54(10)	21(6)	-1(7)	-4(6)	4(7)
Cl(1)	45(2)	44(2)	24(2)	-4(2)	7(1)	6(2)
Cl(2)	24(2)	65(3)	36(2)	-16(2)	-1(1)	7(2)

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

	x	y	z	U(eq)
H(20)	2910	-735	1818	27
H(21)	1864	388	2243	31
H(22)	-369	1732	2168	32
H(23)	-1532	1851	1671	25
H(24)	-500	703	1255	30
H(31A)	6272	-786	577	46
H(31B)	6940	979	419	46