Crystallization of 4-6: In a vial, approximately 50 mg of flavins **4**-**6** were dissolved in 5 mL of formic acid. Gentle heating may be required to completely dissolve the flavins. The open vial was securely placed in a jar containing water. The jar was sealed and wrapped in aluminum foil and allowed to stand undisturbed. Crystallization of the flavins occurred over several weeks.

Table 1. Crystal data and structure refinement for 9,10-Dimethylflavin (**4**).

Identification code	9,10-Dimethylflavin (**4**)	
Empirical formula	C12.50 H12 N4 O3.50	
Formula weight	274.26	
Temperature	110(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.430(12) ≈	α= 90∞.
	b = 18.341(12) ≈	β= 102.044(9)∞.
	c = 7.691(5) ≈	γ = 90∞.
Volume	2543(3) $≈^3$	
Z	8	
Density (calculated)	1.433 Mg/m^3	
Absorption coefficient	0.108 mm^{-1}	
F(000)	1144	
Crystal size	0.109 x 0.157 x 0.401 mm^3	
Theta range for data collection	1.58 to 24.99∞.	
Index ranges	-21<=h<=21, -21<=k<=20, -9<=l<=7	
Reflections collected	11443	
Independent reflections	4423 [R(int) = 0.0565]	
Completeness to theta = 24.99∞	98.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4423 / 0 / 361	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2sigma(I)]	R1 = 0.0596, wR2 = 0.1526	
R indices (all data)	R1 = 0.0983, wR2 = 0.1718	
Largest diff. peak and hole	0.328 and -0.466 $e.≈^{-3}$	

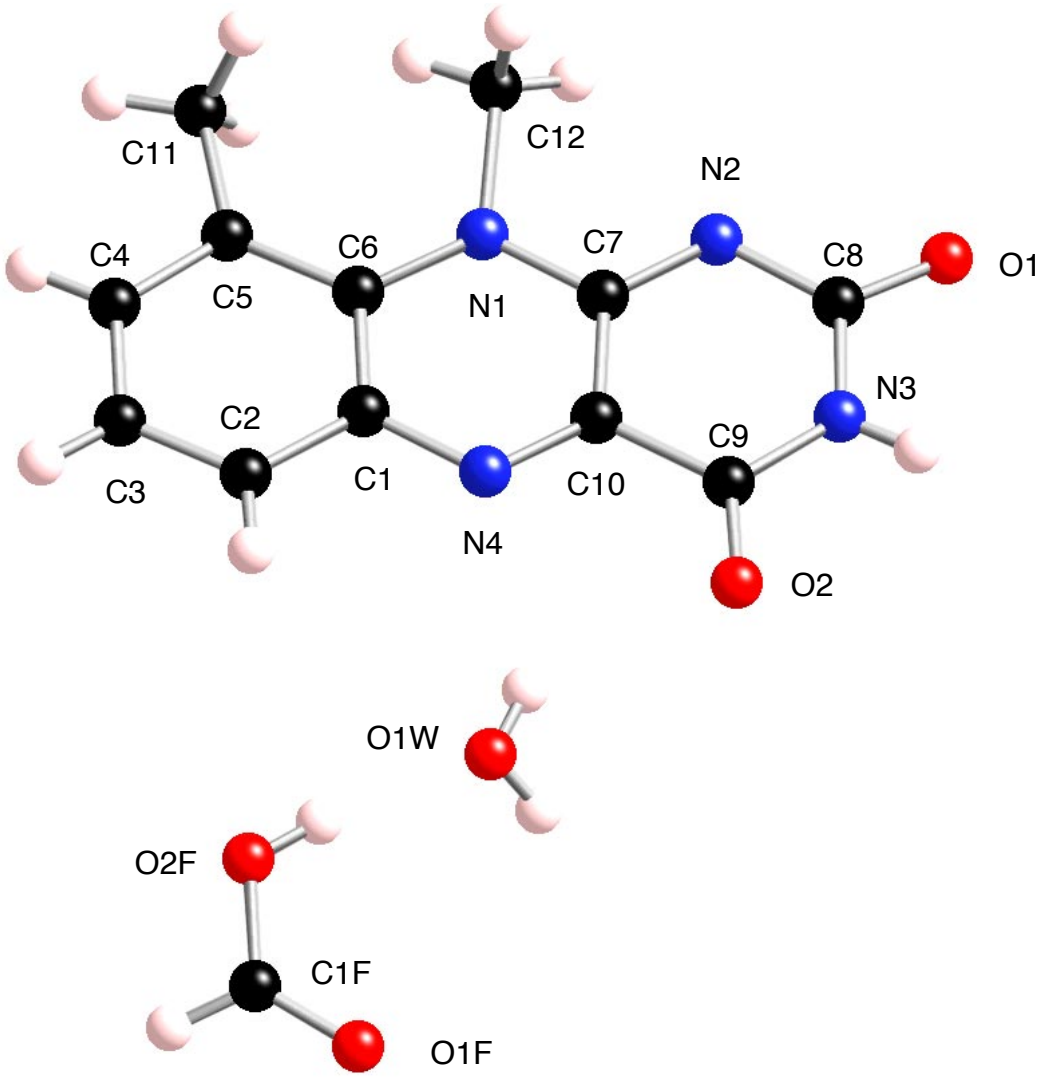
C11
C12
N2
C4
C6
C7
C8
O1
C5
N1
N3
C2
C9
C3
C1
C10
N4
O2
O1W
O2F
C1F
O1F

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for 9,10-Dimethylflavin (**4**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	3516(1)	7976(1)	3383(3)	30(1)
O(2A)	2661(1)	5589(1)	2977(3)	30(1)
N(1A)	5063(1)	6228(1)	6800(3)	31(1)
N(2A)	4316(1)	7125(1)	5050(3)	27(1)
N(3A)	3110(1)	6778(1)	3162(3)	27(1)
N(4A)	3952(1)	5147(1)	5523(3)	25(1)
C(1A)	4608(2)	4962(2)	6778(4)	27(1)
C(2A)	4684(2)	4212(2)	7325(4)	30(1)
C(3A)	5316(2)	3984(2)	8583(4)	32(1)
C(4A)	5877(2)	4514(2)	9294(4)	32(1)
C(5A)	5841(2)	5262(2)	8790(4)	29(1)
C(6A)	5183(2)	5498(2)	7480(4)	26(1)
C(7A)	4405(2)	6427(2)	5608(4)	25(1)
C(8A)	3646(2)	7325(2)	3861(4)	26(1)
C(9A)	3153(2)	6040(2)	3621(4)	25(1)
C(10A)	3857(2)	5837(2)	4998(4)	25(1)
C(11A)	6501(2)	5749(2)	9712(5)	50(1)
C(12A)	5500(5)	6854(4)	7848(14)	33(3)
C(12')	5709(3)	6807(2)	6958(8)	25(2)
O(1B)	1811(1)	7255(1)	10732(3)	38(1)
O(2B)	2392(1)	9690(1)	11952(3)	30(1)
N(1B)	70(1)	8972(1)	7901(4)	32(1)
N(2B)	920(1)	8085(1)	9351(3)	29(1)
N(3B)	2082(1)	8473(1)	11352(3)	27(1)
N(4B)	1092(1)	10103(1)	9372(3)	27(1)
C(1B)	415(2)	10275(2)	8168(4)	28(1)
C(2B)	274(2)	11029(2)	7760(4)	32(1)
C(3B)	-388(2)	11247(2)	6605(4)	36(1)
C(4B)	-919(2)	10697(2)	5841(4)	32(1)
C(5B)	-821(2)	9937(2)	6197(4)	28(1)

C(6B)	-125(2)	9711(2)	7400(4)	28(1)
C(7B)	754(2)	8792(2)	9018(4)	24(1)
C(8B)	1602(2)	7904(2)	10469(4)	28(1)
C(9B)	1956(2)	9221(2)	11126(4)	25(1)
C(10B)	1242(2)	9409(2)	9767(4)	24(1)
C(11B)	-1469(2)	9438(2)	5297(5)	39(1)
C(12B)	-522(3)	8374(3)	7671(11)	21(2)
C(12")	-357(4)	8286(3)	6873(12)	32(2)
O(1F)	1669(2)	2611(1)	5449(4)	65(1)
O(2F)	2878(1)	2880(1)	6704(4)	58(1)
C(1F)	2270(2)	2470(2)	6471(6)	49(1)
O(1W)	2620(1)	4037(1)	4551(3)	45(1)

Table 3. Bond lengths [≈] and angles [∞] for 9,10-Dimethylflavin (**4**).

O(1A)-C(8A)	1.258(3)
O(2A)-C(9A)	1.253(3)
N(1A)-C(7A)	1.408(4)
N(1A)-C(6A)	1.437(4)
N(1A)-C(12A)	1.531(8)
N(1A)-C(12')	1.581(5)
N(2A)-C(7A)	1.349(4)
N(2A)-C(8A)	1.422(4)
N(3A)-C(9A)	1.396(4)
N(3A)-C(8A)	1.432(4)
N(4A)-C(10A)	1.329(4)
N(4A)-C(1A)	1.421(4)
C(1A)-C(2A)	1.435(4)
C(1A)-C(6A)	1.465(4)
C(2A)-C(3A)	1.414(4)
C(3A)-C(4A)	1.440(4)
C(4A)-C(5A)	1.423(4)
C(5A)-C(6A)	1.471(4)
C(5A)-C(11A)	1.557(4)
C(7A)-C(10A)	1.488(4)
C(9A)-C(10A)	1.540(4)
O(1B)-C(8B)	1.255(3)
O(2B)-C(9B)	1.256(3)
N(1B)-C(7B)	1.409(4)
N(1B)-C(6B)	1.434(4)
N(1B)-C(12B)	1.532(6)
N(1B)-C(12")	1.602(7)
N(2B)-C(7B)	1.344(4)
N(2B)-C(8B)	1.407(4)
N(3B)-C(9B)	1.396(4)
N(3B)-C(8B)	1.443(4)
N(4B)-C(10B)	1.324(4)
N(4B)-C(1B)	1.426(4)
C(1B)-C(2B)	1.430(4)

C(1B)-C(6B)	1.470(4)
C(2B)-C(3B)	1.409(4)
C(3B)-C(4B)	1.442(4)
C(4B)-C(5B)	1.425(4)
C(5B)-C(6B)	1.476(4)
C(5B)-C(11B)	1.549(4)
C(7B)-C(10B)	1.485(4)
C(9B)-C(10B)	1.540(4)
O(1F)-C(1F)	1.245(4)
O(2F)-C(1F)	1.331(4)

C(7A)-N(1A)-C(6A)	121.7(2)
C(7A)-N(1A)-C(12A)	115.8(4)
C(6A)-N(1A)-C(12A)	118.9(4)
C(7A)-N(1A)-C(12')	114.1(3)
C(6A)-N(1A)-C(12')	122.8(3)
C(12A)-N(1A)-C(12')	31.9(4)
C(7A)-N(2A)-C(8A)	118.7(2)
C(9A)-N(3A)-C(8A)	125.8(2)
C(10A)-N(4A)-C(1A)	118.3(2)
N(4A)-C(1A)-C(2A)	116.4(3)
N(4A)-C(1A)-C(6A)	122.5(2)
C(2A)-C(1A)-C(6A)	121.1(3)
C(3A)-C(2A)-C(1A)	120.0(3)
C(2A)-C(3A)-C(4A)	119.0(3)
C(5A)-C(4A)-C(3A)	123.9(3)
C(4A)-C(5A)-C(6A)	117.1(3)
C(4A)-C(5A)-C(11A)	116.2(3)
C(6A)-C(5A)-C(11A)	126.7(3)
N(1A)-C(6A)-C(1A)	116.5(2)
N(1A)-C(6A)-C(5A)	124.5(3)
C(1A)-C(6A)-C(5A)	119.0(3)
N(2A)-C(7A)-N(1A)	119.0(2)
N(2A)-C(7A)-C(10A)	124.1(3)
N(1A)-C(7A)-C(10A)	116.9(2)
O(1A)-C(8A)-N(2A)	121.3(2)

O(1A)-C(8A)-N(3A)	118.7(2)
N(2A)-C(8A)-N(3A)	120.0(2)
O(2A)-C(9A)-N(3A)	122.8(3)
O(2A)-C(9A)-C(10A)	123.3(3)
N(3A)-C(9A)-C(10A)	113.9(2)
N(4A)-C(10A)-C(7A)	124.0(3)
N(4A)-C(10A)-C(9A)	118.6(2)
C(7A)-C(10A)-C(9A)	117.3(2)
C(7B)-N(1B)-C(6B)	121.8(2)
C(7B)-N(1B)-C(12B)	115.3(3)
C(6B)-N(1B)-C(12B)	121.0(3)
C(7B)-N(1B)-C(12")	113.7(3)
C(6B)-N(1B)-C(12")	122.7(3)
C(12B)-N(1B)-C(12")	27.9(3)
C(7B)-N(2B)-C(8B)	118.9(2)
C(9B)-N(3B)-C(8B)	125.6(2)
C(10B)-N(4B)-C(1B)	118.3(2)
N(4B)-C(1B)-C(2B)	116.8(3)
N(4B)-C(1B)-C(6B)	122.2(3)
C(2B)-C(1B)-C(6B)	121.0(3)
C(3B)-C(2B)-C(1B)	120.5(3)
C(2B)-C(3B)-C(4B)	118.9(3)
C(5B)-C(4B)-C(3B)	123.9(3)
C(4B)-C(5B)-C(6B)	117.0(3)
C(4B)-C(5B)-C(11B)	115.9(3)
C(6B)-C(5B)-C(11B)	127.1(3)
N(1B)-C(6B)-C(1B)	116.5(2)
N(1B)-C(6B)-C(5B)	124.7(2)
C(1B)-C(6B)-C(5B)	118.7(3)
N(2B)-C(7B)-N(1B)	118.8(2)
N(2B)-C(7B)-C(10B)	124.5(2)
N(1B)-C(7B)-C(10B)	116.7(2)
O(1B)-C(8B)-N(2B)	121.9(2)
O(1B)-C(8B)-N(3B)	118.2(3)
N(2B)-C(8B)-N(3B)	119.9(2)
O(2B)-C(9B)-N(3B)	122.6(2)

O(2B)-C(9B)-C(10B)	123.8(2)
N(3B)-C(9B)-C(10B)	113.6(2)
N(4B)-C(10B)-C(7B)	124.3(3)
N(4B)-C(10B)-C(9B)	118.6(2)
C(7B)-C(10B)-C(9B)	117.1(2)
O(1F)-C(1F)-O(2F)	125.5(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3) for 9,10-Dimethylflavin (**4**). The anisotropic displacement factor exponent takes the form: -2_^{2}[h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	28(1)	20(1)	38(1)	-1(1)	-5(1)	2(1)
O(2A)	27(1)	28(1)	33(1)	0(1)	-1(1)	-4(1)
N(1A)	25(1)	25(1)	37(2)	-4(1)	-9(1)	2(1)
N(2A)	22(1)	26(1)	31(2)	-3(1)	-2(1)	1(1)
N(3A)	22(1)	25(1)	29(1)	-1(1)	-4(1)	2(1)
N(4A)	26(1)	25(1)	24(1)	-2(1)	1(1)	2(1)
C(1A)	30(2)	28(2)	21(2)	-2(1)	2(1)	5(1)
C(2A)	34(2)	27(2)	27(2)	-2(1)	6(1)	3(1)
C(3A)	41(2)	33(2)	23(2)	6(1)	6(2)	13(1)
C(4A)	30(2)	40(2)	27(2)	6(1)	6(1)	14(1)
C(5A)	23(2)	41(2)	23(2)	1(1)	7(1)	7(1)
C(6A)	28(2)	25(2)	25(2)	-2(1)	2(1)	7(1)
C(7A)	23(2)	26(2)	23(2)	-2(1)	0(1)	5(1)
C(8A)	22(2)	29(2)	25(2)	-3(1)	1(1)	3(1)
C(9A)	22(2)	25(2)	27(2)	-1(1)	3(1)	1(1)
C(10A)	23(2)	25(2)	25(2)	-3(1)	2(1)	2(1)
C(11A)	26(2)	55(2)	61(3)	30(2)	-9(2)	-2(2)
O(1B)	33(1)	23(1)	48(2)	-3(1)	-13(1)	3(1)
O(2B)	26(1)	27(1)	34(1)	-3(1)	-2(1)	-1(1)
N(1B)	24(1)	27(1)	39(2)	5(1)	-7(1)	-1(1)
N(2B)	24(1)	27(1)	33(2)	-1(1)	-3(1)	3(1)
N(3B)	19(1)	26(1)	32(2)	1(1)	-5(1)	3(1)
N(4B)	24(1)	27(1)	29(1)	0(1)	3(1)	2(1)
C(1B)	23(2)	29(2)	31(2)	2(1)	2(1)	4(1)
C(2B)	29(2)	28(2)	37(2)	1(1)	3(2)	3(1)
C(3B)	33(2)	30(2)	42(2)	9(1)	4(2)	7(1)
C(4B)	25(2)	39(2)	32(2)	6(1)	3(1)	9(1)
C(5B)	21(2)	36(2)	27(2)	1(1)	2(1)	4(1)
C(6B)	24(2)	30(2)	29(2)	1(1)	2(1)	3(1)
C(7B)	19(2)	29(2)	24(2)	-1(1)	3(1)	0(1)

C(8B)	25(2)	26(2)	30(2)	-2(1)	1(1)	-1(1)
C(9B)	21(2)	26(2)	27(2)	0(1)	2(1)	0(1)
C(10B)	21(2)	25(2)	26(2)	-1(1)	4(1)	2(1)
C(11B)	28(2)	41(2)	42(2)	5(2)	-8(2)	4(1)
O(1F)	49(2)	64(2)	74(2)	12(2)	-7(2)	-9(1)
O(2F)	46(2)	48(2)	74(2)	7(1)	-5(1)	-2(1)
C(1F)	49(2)	44(2)	50(2)	1(2)	5(2)	0(2)
O(1W)	46(1)	27(1)	62(2)	-3(1)	10(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (≈^{2}x 10 ^{3}) for 9,10-Dimethylflavin (**4**).

	x	y	z	U(eq)
H(3AA)	2718	6919	2373	32
H(2AB)	4309	3870	6841	36
H(3AB)	5370	3490	8953	39
H(4AB)	6296	4355	10151	39
H(11A)	6863	5450	10525	75
H(11B)	6318	6137	10383	75
H(11C)	6740	5965	8809	75
H(12A)	5302	6954	8912	50
H(12B)	5452	7292	7102	50
H(12C)	6024	6717	8200	50
H(12D)	5950	6756	5943	37
H(12E)	6074	6725	8064	37
H(12F)	5503	7299	6967	37
H(3BB)	2489	8337	12097	32
H(2BA)	629	11385	8273	38
H(3BA)	-482	11748	6332	43
H(4BA)	-1360	10851	5055	39
H(11D)	-1860	9735	4568	59
H(11E)	-1671	9183	6212	59
H(11F)	-1288	9080	4542	59
H(12G)	-793	8405	8638	32
H(12H)	-283	7895	7701	32
H(12I)	-869	8437	6528	32
H(12J)	-150	8175	5828	48
H(12K)	-885	8401	6493	48
H(12L)	-296	7863	7668	48
H(1F)	2839	3316	6323	70
H(2F)	2340	2051	7237	58
H(1W)	2210	4183	4606	54
H(2W)	2817	4458	4612	54

Table 6. Crystal data and structure refinement for 8,9,10-Trimethylflavin (**5**).

Identification code	8,9,10-Trimethylflavin (**5**)	
Empirical formula	C13 H14 N4 O3	
Formula weight	274.28	
Temperature	110(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	C	
Unit cell dimensions	a = 23.503(5) ≈	α= 90∞.
	b = 6.7106(10) ≈	β= 117.677(3)∞.
	c = 17.435(3) ≈	γ = 90∞.
Volume	2435.2(7) $≈^3$	
Z	8	
Density (calculated)	1.496 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	1152	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.96 to 25.00∞.	
Index ranges	-21<=h<=27, -7<=k<=7, -20<=l<=17	
Reflections collected	5901	
Independent reflections	2093 [R(int) = 0.0376]	
Completeness to theta = 25.00∞	97.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2093 / 0 / 181	
Goodness-of-fit on F^2	1.010	
Final R indices [I>2sigma(I)]	R1 = 0.0689, wR2 = 0.1552	
R indices (all data)	R1 = 0.1253, wR2 = 0.1838	
Largest diff. peak and hole	0.531 and -0.280 $e.≈^{-3}$	

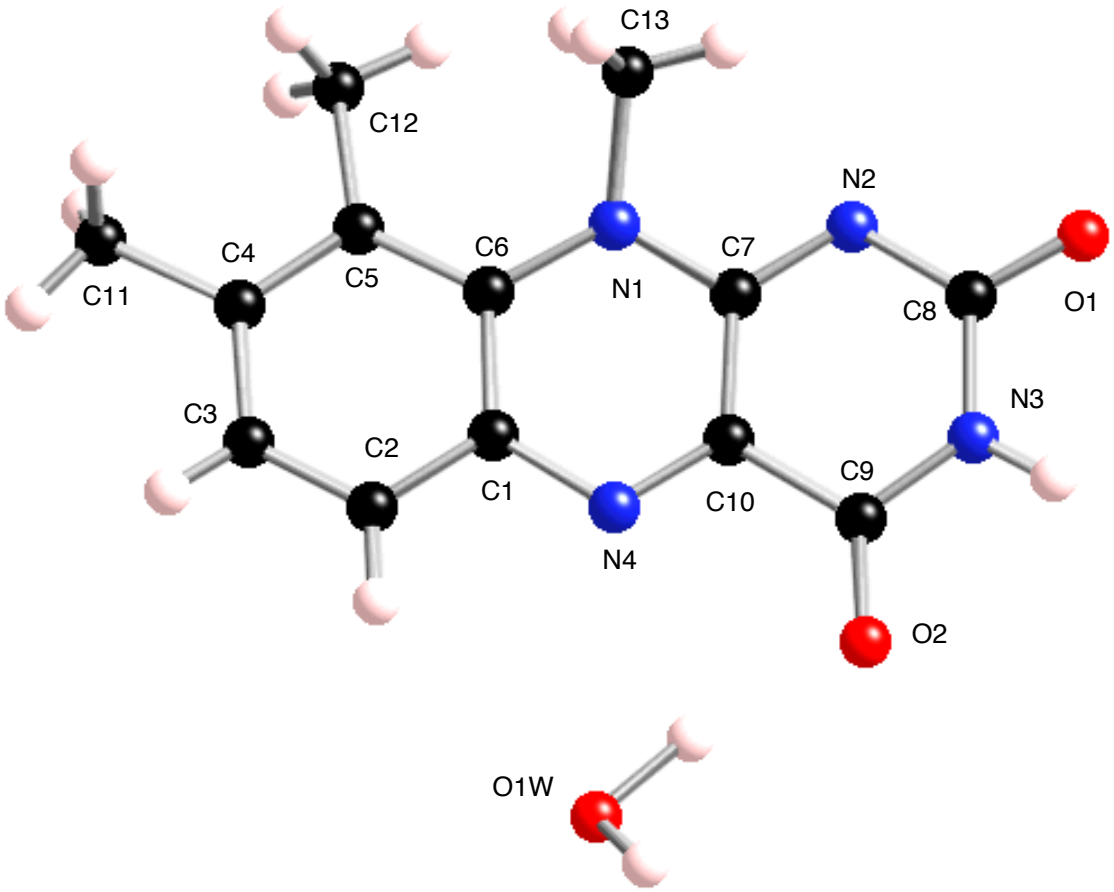
C13
C12
N2
C4
C6
C7
C5
N1
C8
O1
C11
C3
N3
C2
C9
C1
C10
N4
O2
O1W

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for 8,9,10-Trimethylflavin (**5**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9338(1)	8468(4)	6518(2)	42(1)
O(2)	9301(1)	7943(4)	9085(1)	38(1)
N(1)	7368(1)	8462(4)	6425(2)	28(1)
N(2)	8355(1)	8356(4)	6440(2)	30(1)
N(3)	9312(1)	8157(4)	7793(2)	32(1)
N(4)	7974(1)	8219(4)	8232(2)	30(1)
C(1)	7316(2)	8291(5)	7766(2)	29(1)
C(2)	6972(2)	8341(5)	8240(2)	33(1)
C(3)	6317(2)	8329(5)	7815(2)	36(1)
C(4)	5982(2)	8199(5)	6909(2)	35(1)
C(5)	6303(2)	8120(5)	6406(2)	32(1)
C(6)	6988(2)	8284(5)	6845(2)	28(1)
C(7)	8022(2)	8300(5)	6875(2)	27(1)
C(8)	9007(2)	8333(5)	6893(2)	31(1)
C(9)	9013(2)	8074(5)	8299(2)	28(1)
C(10)	8301(2)	8157(5)	7796(2)	26(1)
C(11)	5257(2)	8154(6)	6479(2)	46(1)
C(12)	5913(2)	7748(6)	5451(2)	44(1)
C(13)	7110(2)	9126(6)	5512(2)	42(1)
O(1W)	8568(2)	1705(4)	5254(2)	77(1)

Table 8. Bond lengths [≈] and angles [∞] for 8,9,10-Trimethylflavin (**5**).

O(1)-C(8)	1.230(4)
O(2)-C(9)	1.216(3)
N(1)-C(7)	1.368(4)
N(1)-C(6)	1.398(4)
N(1)-C(13)	1.484(4)
N(2)-C(7)	1.320(4)
N(2)-C(8)	1.359(4)
N(3)-C(9)	1.361(4)
N(3)-C(8)	1.395(4)
N(4)-C(10)	1.310(4)
N(4)-C(1)	1.373(4)
C(1)-C(2)	1.400(5)
C(1)-C(6)	1.422(4)
C(2)-C(3)	1.362(5)
C(3)-C(4)	1.403(5)
C(4)-C(5)	1.398(5)
C(4)-C(11)	1.510(5)
C(5)-C(6)	1.430(5)
C(5)-C(12)	1.503(5)
C(7)-C(10)	1.428(4)
C(9)-C(10)	1.487(4)
C(7)-N(1)-C(6)	120.9(3)
C(7)-N(1)-C(13)	115.4(3)
C(6)-N(1)-C(13)	123.0(3)
C(7)-N(2)-C(8)	118.4(3)
C(9)-N(3)-C(8)	125.6(3)
C(10)-N(4)-C(1)	117.4(3)
N(4)-C(1)-C(2)	116.8(3)
N(4)-C(1)-C(6)	122.6(3)
C(2)-C(1)-C(6)	120.6(3)
C(3)-C(2)-C(1)	119.6(3)
C(2)-C(3)-C(4)	121.0(3)
C(5)-C(4)-C(3)	121.6(3)

C(5)-C(4)-C(11)	120.1(3)
C(3)-C(4)-C(11)	118.3(3)
C(4)-C(5)-C(6)	117.6(3)
C(4)-C(5)-C(12)	118.2(3)
C(6)-C(5)-C(12)	124.1(3)
N(1)-C(6)-C(1)	116.6(3)
N(1)-C(6)-C(5)	124.1(3)
C(1)-C(6)-C(5)	119.3(3)
N(2)-C(7)-N(1)	118.5(3)
N(2)-C(7)-C(10)	124.3(3)
N(1)-C(7)-C(10)	117.2(3)
O(1)-C(8)-N(2)	120.7(3)
O(1)-C(8)-N(3)	118.8(3)
N(2)-C(8)-N(3)	120.5(3)
O(2)-C(9)-N(3)	123.2(3)
O(2)-C(9)-C(10)	123.5(3)
N(3)-C(9)-C(10)	113.3(3)
N(4)-C(10)-C(7)	124.3(3)
N(4)-C(10)-C(9)	117.6(3)
C(7)-C(10)-C(9)	118.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($\approx^2$x 10^3) for 8,9,10-Trimethylflavin (**5**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	62(2)	33(1)	2(1)	16(1)	-3(1)
O(2)	31(1)	52(2)	26(1)	-1(1)	8(1)	-1(1)
N(1)	28(2)	26(2)	23(2)	-1(1)	6(1)	1(1)
N(2)	29(2)	32(2)	25(2)	0(1)	9(1)	1(1)
N(3)	23(2)	38(2)	28(2)	0(1)	8(1)	-1(1)
N(4)	30(2)	24(2)	31(2)	-1(1)	11(1)	-2(1)
C(1)	27(2)	23(2)	31(2)	1(2)	8(2)	1(2)
C(2)	34(2)	30(2)	33(2)	1(2)	13(2)	0(2)
C(3)	33(2)	32(2)	42(2)	5(2)	18(2)	6(2)
C(4)	29(2)	29(2)	41(2)	2(2)	11(2)	5(2)
C(5)	28(2)	22(2)	38(2)	1(2)	9(2)	1(2)
C(6)	31(2)	20(2)	30(2)	2(1)	12(2)	5(2)
C(7)	26(2)	23(2)	27(2)	0(1)	8(2)	-1(2)
C(8)	34(2)	29(2)	27(2)	1(2)	12(2)	-3(2)
C(9)	29(2)	26(2)	28(2)	-1(2)	12(2)	-1(2)
C(10)	28(2)	21(2)	25(2)	-1(1)	9(2)	1(1)
C(11)	30(2)	53(3)	49(2)	5(2)	12(2)	4(2)
C(12)	33(2)	51(3)	38(2)	0(2)	7(2)	2(2)
C(13)	38(2)	49(2)	30(2)	5(2)	7(2)	4(2)
O(1W)	118(3)	63(2)	56(2)	14(2)	46(2)	30(2)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($\approx^2$x 10^3) for 8,9,10-Trimethylflavin (**5**).

	x	y	z	U(eq)
H(3AB)	9735	8095	8056	38
H(2AA)	7193	8382	8855	40
H(3AA)	6084	8410	8137	43
H(11A)	5112	8247	6921	70
H(11B)	5103	6904	6157	70
H(11C)	5086	9282	6079	70
H(12A)	6199	7697	5183	66
H(12B)	5601	8828	5188	66
H(12C)	5685	6477	5357	66
H(13A)	7456	9126	5347	64
H(13B)	6935	10476	5453	64
H(13C)	6768	8216	5134	64
H(1W1)	8786	1808	4728	115
H(2W1)	8899	531	5686	115

Table 11. Crystal data and structure refinement for 9,10-Propanoflavin (**6**).

Identification code	9,10-Propanoflavin (**6**)	
Empirical formula	C14 H12 N4 O4	
Formula weight	300.28	
Temperature	296(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.0378(5) ≈	α= 105.792(2)∞.
	b = 9.4623(10) ≈	β= 98.797(2)∞.
	c = 14.2196(15) ≈	γ = 92.324(2)∞.
Volume	642.17(12) $≈^3$	
Z	2	
Density (calculated)	1.553 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	312	
Crystal size	0.156 x 0.301 x 0.762 mm^3	
Theta range for data collection	2.33 to 24.99∞.	
Index ranges	-5<=h<=5, -9<=k<=11, -16<=l<=15	
Reflections collected	3283	
Independent reflections	2164 [R(int) = 0.0331]	
Completeness to theta = 24.99∞	96.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2164 / 0 / 199	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1439	
R indices (all data)	R1 = 0.0639, wR2 = 0.1549	
Largest diff. peak and hole	0.446 and -0.240 $e.≈^{-3}$	

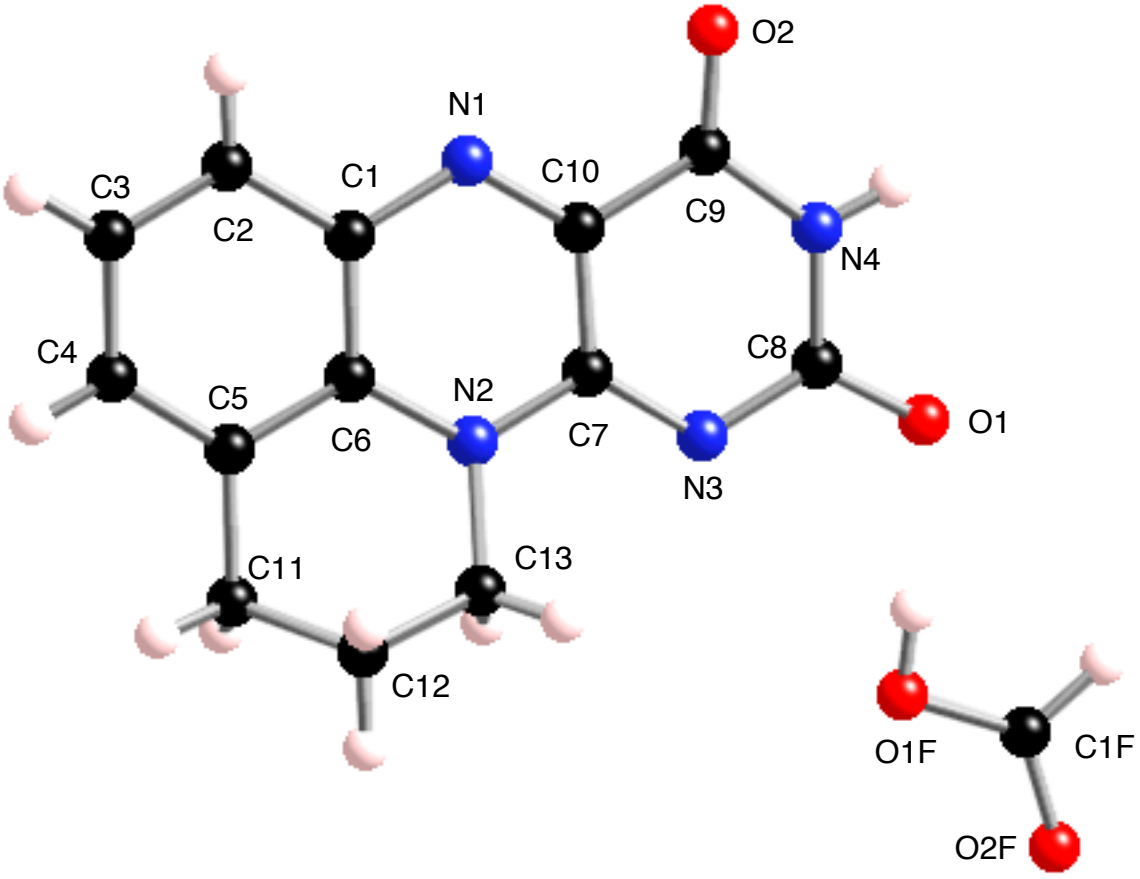
O2
N1
C3
C1
C10
C9
C2
N4
C4
C8
C5
N2
O1
C6
C7
N3
C11
C13
C12
O1F
C1F
O2F

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for 9,10-Propanoflavin (**6**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1F)	8726(3)	6038(2)	3151(1)	72(1)
C(1F)	6846(4)	6915(2)	3057(1)	62(1)
O(2F)	5774(3)	7536(2)	3728(1)	85(1)
O(1)	-128(2)	5110(1)	1271(1)	59(1)
O(2)	5310(3)	2535(2)	-688(1)	67(1)
N(1)	7456(3)	1347(2)	832(1)	48(1)
N(2)	5955(3)	2519(1)	2679(1)	43(1)
N(3)	2865(3)	3858(2)	2004(1)	49(1)
N(4)	2573(3)	3782(2)	304(1)	52(1)
C(1)	8505(3)	871(2)	1628(1)	45(1)
C(2)	10354(3)	-199(2)	1496(1)	53(1)
C(3)	11435(4)	-693(2)	2282(1)	58(1)
C(4)	10681(4)	-114(2)	3212(1)	54(1)
C(5)	8886(3)	944(2)	3381(1)	48(1)
C(6)	7770(3)	1451(2)	2573(1)	43(1)
C(7)	4752(3)	2932(2)	1886(1)	42(1)
C(8)	1722(3)	4274(2)	1209(1)	48(1)
C(9)	4557(3)	2862(2)	107(1)	49(1)
C(10)	5678(3)	2314(2)	960(1)	44(1)
C(11)	8167(4)	1602(2)	4387(1)	60(1)
C(12)	7478(4)	3174(2)	4488(1)	59(1)
C(13)	5252(4)	3235(2)	3669(1)	53(1)

Table 13. Bond lengths [≈] and angles [∞] for 9,10-Propanoflavin (**6**).

O(1F)-C(1F)	1.300(2)
C(1F)-O(2F)	1.194(2)
O(1)-C(8)	1.2442(19)
O(2)-C(9)	1.2107(19)
N(1)-C(10)	1.303(2)
N(1)-C(1)	1.370(2)
N(2)-C(7)	1.357(2)
N(2)-C(6)	1.383(2)
N(2)-C(13)	1.490(2)
N(3)-C(7)	1.318(2)
N(3)-C(8)	1.351(2)
N(4)-C(9)	1.363(2)
N(4)-C(8)	1.384(2)
C(1)-C(2)	1.398(2)
C(1)-C(6)	1.418(2)
C(2)-C(3)	1.372(2)
C(3)-C(4)	1.402(3)
C(4)-C(5)	1.374(2)
C(5)-C(6)	1.412(2)
C(5)-C(11)	1.502(2)
C(7)-C(10)	1.444(2)
C(9)-C(10)	1.489(2)
C(11)-C(12)	1.515(2)
C(12)-C(13)	1.502(2)
O(2F)-C(1F)-O(1F)	122.94(18)
C(10)-N(1)-C(1)	117.85(14)
C(7)-N(2)-C(6)	121.06(14)
C(7)-N(2)-C(13)	118.32(14)
C(6)-N(2)-C(13)	120.62(13)
C(7)-N(3)-C(8)	118.14(14)
C(9)-N(4)-C(8)	125.79(14)
N(1)-C(1)-C(2)	118.63(15)
N(1)-C(1)-C(6)	121.34(15)

C(2)-C(1)-C(6)	120.03(15)
C(3)-C(2)-C(1)	119.75(16)
C(2)-C(3)-C(4)	119.62(16)
C(5)-C(4)-C(3)	122.94(16)
C(4)-C(5)-C(6)	117.48(15)
C(4)-C(5)-C(11)	122.69(15)
C(6)-C(5)-C(11)	119.79(15)
N(2)-C(6)-C(5)	121.31(14)
N(2)-C(6)-C(1)	118.51(14)
C(5)-C(6)-C(1)	120.18(15)
N(3)-C(7)-N(2)	119.05(14)
N(3)-C(7)-C(10)	124.57(15)
N(2)-C(7)-C(10)	116.38(14)
O(1)-C(8)-N(3)	120.87(15)
O(1)-C(8)-N(4)	118.14(14)
N(3)-C(8)-N(4)	120.98(14)
O(2)-C(9)-N(4)	122.61(15)
O(2)-C(9)-C(10)	124.08(15)
N(4)-C(9)-C(10)	113.31(14)
N(1)-C(10)-C(7)	124.58(15)
N(1)-C(10)-C(9)	118.49(14)
C(7)-C(10)-C(9)	116.90(14)
C(5)-C(11)-C(12)	109.70(14)
C(13)-C(12)-C(11)	110.79(15)
N(2)-C(13)-C(12)	110.95(14)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($\approx^2$x 10^3) for 9,10-Propanoflavin (**6**). The anisotropic displacement factor exponent takes the form: -2_^{2}[h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1F)	73(1)	88(1)	59(1)	21(1)	18(1)	22(1)
C(1F)	67(1)	63(1)	57(1)	18(1)	12(1)	8(1)
O(2F)	91(1)	94(1)	76(1)	18(1)	36(1)	24(1)
O(1)	63(1)	65(1)	53(1)	19(1)	15(1)	28(1)
O(2)	81(1)	85(1)	44(1)	23(1)	21(1)	38(1)
N(1)	54(1)	49(1)	42(1)	12(1)	9(1)	14(1)
N(2)	48(1)	46(1)	37(1)	11(1)	10(1)	9(1)
N(3)	52(1)	50(1)	45(1)	12(1)	11(1)	14(1)
N(4)	59(1)	60(1)	44(1)	20(1)	11(1)	22(1)
C(1)	49(1)	46(1)	41(1)	12(1)	7(1)	7(1)
C(2)	61(1)	54(1)	47(1)	13(1)	12(1)	16(1)
C(3)	62(1)	55(1)	60(1)	21(1)	11(1)	21(1)
C(4)	58(1)	57(1)	50(1)	23(1)	4(1)	10(1)
C(5)	51(1)	48(1)	45(1)	15(1)	7(1)	5(1)
C(6)	44(1)	40(1)	43(1)	11(1)	7(1)	3(1)
C(7)	45(1)	40(1)	41(1)	9(1)	8(1)	6(1)
C(8)	49(1)	48(1)	48(1)	14(1)	9(1)	13(1)
C(9)	53(1)	53(1)	43(1)	14(1)	9(1)	14(1)
C(10)	47(1)	45(1)	39(1)	9(1)	8(1)	9(1)
C(11)	69(1)	70(1)	46(1)	24(1)	11(1)	16(1)
C(12)	73(1)	65(1)	39(1)	11(1)	12(1)	13(1)
C(13)	62(1)	57(1)	43(1)	13(1)	18(1)	15(1)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($\approx^2$x 10^3) for 9,10-Propanoflavin (**6**).

	x	y	z	U(eq)
H(1F)	9068	5787	2564	86
H(2F)	6272	7157	2392	75
H(4B)	1780	4083	-176	63
H(2A)	10849	-575	878	64
H(3A)	12661	-1407	2199	69
H(4A)	11430	-462	3736	64
H(11A)	9674	1588	4898	72
H(11B)	6635	1023	4473	72
H(12A)	6921	3578	5124	71
H(12B)	9065	3771	4465	71
H(13A)	3604	2738	3741	64
H(13B)	4935	4255	3718	64