Supporting Information

Synthesis and fluorescence studies of novel bisarylmethylidene derivatives of 2-methoxy-2-methyl-1,3-dioxan-5-one

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

Identification code	3a.	
Empirical formula	C ₂₂ H ₂₂ O ₄	
Formula weight	350.22	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.307 Å b = 10.36 Å c = 10.951 Å	α = 110.68°. β = 91.83°. γ = 104.7°.
Volume	946.9 Å ³	
Z	2	
Density (calculated)	1.228 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	372	
Crystal size	0.8 x 0.2 x 0.1 mm ³	
Theta range for data collection	3.025 to 24.999°.	
Index ranges	-10 ≤ h ≤ 11, -11 ≤ k ≤ 12, -13 ≤ l ≤ 13	
Reflections collected	6510	
Independent reflections	3227 [R(int) = 0.1516]	
Completeness to theta = 25°	96.7 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3227 / 0 / 239	
Goodness-of-fit on F2	0.751	
Final R indices	R1 = 0.0594, wR ² =	
[I > 2σ(I)]	0.1141	
R indices (all data)	R1 = 0.1541, wR ² =	
	0.1449	
Largest diff. peak and hole	0.135 and -0.154 e.Å ⁻³	

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

x	y	z	U(eq)
C(1)	2935(4)	1513(4)	4690(3) 54(1)
C(2)	2164(4)	2964(4)	3729(3) 58(1)
C(3)	1522(4)	1662(4)	2546(3) 60(1)
C(4)	1973(4)	353(4)	2417(3) 57(1)
C(5)	1567(4)	-829(4)	1346(3) 56(1)
C(6)	1898(4)	-2186(4)	1040(3) 56(1)
C(7)	2569(4)	-2601(4)	1965(3) 69(1)
C(8)	2864(4)	-3891(4)	1601(3) 71(1)
C(9)	2520(5)	-4888(4)	315(3) 72(1)
C(10)	1839(5)	-4485(5)	-583(3) 92(2)
C(11)	1538(5)	-3194(4)	-238(3) 77(1)
C(12)	2821(6)	-6326(5)	-32(4) 102(2)
C(13)	1872(4)	4229(4)	3943(3) 58(1)
C(14)	2341(4)	5562(4)	5034(3) 58(1)
C(15)	3433(4)	5933(4)	6118(3) 71(1)
C(16)	3784(5)	7227(4)	7122(4) 73(1)
C(17)	3093(5)	8280(4)	7154(3) 71(1)
C(18)	2027(5)	7944(4)	6095(4) 76(1)
C(19)	1682(4)	6657(4)	5066(4) 70(1)
C(20)	3474(6)	9708(5)	8288(4) 99(1)
C(21)	1180(4)	1902(4)	6227(3) 74(1)
C(22)	4199(4)	1569(4)	5631(3) 70(1)
O(1)	2971(2)	461(2)	3461(2) 61(1)
O(2)	3188(2)	2867(2)	4638(2) 58(1)
O(3)	603(3)	1648(3)	1706(2) 85(1)
O(4)	1489(3)	1030(2)	4994(2) 59(1)

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

C(1)-O(2)	1.384(4)	C(16)-H(14)	0.93
C(1)-O(1)	1.409(4)	C(17)-C(18)	1.385(5)
C(1)-O(4)	1.406(4)	C(17)-C(20)	1.505(5)
C(1)-C(22)	1.515(4)	C(18)-C(19)	1.360(5)
C(2)-C(13)	1.347(4)	C(18)-H(10)	0.93
C(2)-O(2)	1.403(3)	C(19)-H(9)	0.93
C(2)-C(3)	1.471(5)	C(20)-H(11)	0.96
C(3)-O(3)	1.230(3)	C(20)-H(12)	0.96
C(3)-C(4)	1.480(5)	C(20)-H(13)	0.96
C(4)-C(5)	1.319(5)	C(21)-O(4)	1.420(4)
C(4)-O(1)	1.404(3)	C(21)-H(17)	0.96
C(5)-C(6)	1.442(4)	C(21)-H(18)	0.96
C(5)-H(8)	0.93	C(21)-H(19)	0.96
C(6)-C(11)	1.386(4)	C(22)-H(20)	0.96
C(6)-C(7)	1.415(4)	C(22)-H(21)	0.96
C(7)-C(8)	1.356(4)	C(22)-H(22)	0.96
C(7)-H(7)	0.93	O(2)-C(1)-O(1)	112.2(3)
C(8)-C(9)	1.389(5)	O(2)-C(1)-O(4)	111.4(3)
C(8)-H(6)	0.93	O(1)-C(1)-O(4)	104.1(3)
C(9)-C(10)	1.388(4)	O(2)-C(1)-C(22)	107.7(3)
C(9)-C(12)	1.504(5)	O(1)-C(1)-C(22)	106.7(3)
C(10)-C(11)	1.360(5)	O(4)-C(1)-C(22)	114.8(3)
C(10)-H(2)	0.93	C(13)-C(2)-O(2)	119.6(3)
C(11)-H(1)	0.93	C(13)-C(2)-C(3)	123.7(3)
C(12)-H(3)	0.96	O(2)-C(2)-C(3)	116.7(3)
C(12)-H(4)	0.96	O(3)-C(3)-C(4)	120.9(3)
C(12)-H(5)	0.96	O(3)-C(3)-C(2)	120.9(3)
C(13)-C(14)	1.422(5)	C(4)-C(3)-C(2)	118.1(3)
C(13)-H(16)	0.93	C(5)-C(4)-O(1)	120.5(3)
C(14)-C(19)	1.411(5)	C(5)-C(4)-C(3)	122.9(3)
C(14)-C(15)	1.411(4)	O(1)-C(4)-C(3)	116.4(3)
C(15)-C(16)	1.352(5)	C(4)-C(5)-C(6)	130.7(3)
C(15)-H(15)	0.93	C(4)-C(5)-H(8)	114.7
C(16)-C(17)	1.391(5)	C(6)-C(5)-H(8)	114.7

C(11)-C(6)-C(7)	115.7(3)	C(18)-C(17)-C(16)	116.6(4)
C(11)-C(6)-C(5)	119.6(3)	C(18)-C(17)-C(20)	121.6(4)
C(7)-C(6)-C(5)	124.7(3)	C(16)-C(17)-C(20)	121.8(4)
C(8)-C(7)-C(6)	121.4(3)	C(19)-C(18)-C(17)	121.8(4)
C(8)-C(7)-H(7)	119.3	C(19)-C(18)-H(10)	119.1
C(6)-C(7)-H(7)	119.3	C(17)-C(18)-H(10)	119.1
C(7)-C(8)-C(9)	122.6(3)	C(18)-C(19)-C(14)	122.3(3)
C(7)-C(8)-H(6)	118.7	C(18)-C(19)-H(9)	118.9
C(9)-C(8)-H(6)	118.7	C(14)-C(19)-H(9)	118.9
C(8)-C(9)-C(10)	115.7(4)	C(17)-C(20)-H(11)	109.5
C(8)-C(9)-C(12)	120.6(3)	C(17)-C(20)-H(12)	109.5
C(10)-C(9)-C(12)	123.6(3)	H(11)-C(20)-H(12)	109.5
C(11)-C(10)-C(9)	122.6(3)	C(17)-C(20)-H(13)	109.5
C(11)-C(10)-H(2)	118.7	H(11)-C(20)-H(13)	109.5
C(9)-C(10)-H(2)	118.7	H(12)-C(20)-H(13)	109.5
C(10)-C(11)-C(6)	122.0(3)	O(4)-C(21)-H(17)	109.5
C(10)-C(11)-H(1)	119	O(4)-C(21)-H(18)	109.5
C(6)-C(11)-H(1)	119	H(17)-C(21)-H(18)	109.5
C(9)-C(12)-H(3)	109.5	O(4)-C(21)-H(19)	109.5
C(9)-C(12)-H(4)	109.5	H(17)-C(21)-H(19)	109.5
H(3)-C(12)-H(4)	109.5	H(18)-C(21)-H(19)	109.5
C(9)-C(12)-H(5)	109.5	C(1)-C(22)-H(20)	109.5
H(3)-C(12)-H(5)	109.5	C(1)-C(22)-H(21)	109.5
H(4)-C(12)-H(5)	109.5	H(20)-C(22)-H(21)	109.5
C(2)-C(13)-C(14)	131.2(3)	C(1)-C(22)-H(22)	109.5
C(2)-C(13)-H(16)	114.4	H(20)-C(22)-H(22)	109.5
C(14)-C(13)-H(16)	114.4	H(21)-C(22)-H(22)	109.5
C(19)-C(14)-C(15)	114.9(3)	C(4)-O(1)-C(1)	115.2(2)
C(19)-C(14)-C(13)	118.5(3)	C(1)-O(2)-C(2)	114.5(2)
C(15)-C(14)-C(13)	126.6(3)	C(1)-O(4)-C(21)	115.2(3)
C(16)-C(15)-C(14)	122.2(3)		
C(16)-C(15)-H(15)	118.9		
C(14)-C(15)-H(15)	118.9		
C(15)-C(16)-C(17)	122.2(3)		
C(15)-C(16)-H(14)	118.9		
C(17)-C(16)-H(14)	118.9		

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

U11	U22	U33	U23	U13	U12	
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C(1)	58(2)	56(2)	47(2)	16(2)	-7(2)	20(2)
C(2)	61(2)	69(2)	51(2)	27(2)	3(2)	25(2)
C(3)	67(2)	70(3)	51(2)	26(2)	7(2)	27(2)
C(4)	57(2)	72(2)	43(2)	25(2)	-1(2)	18(2)
C(5)	68(2)	64(2)	39(2)	20(2)	2(2)	24(2)
C(6)	71(2)	61(2)	39(2)	20(2)	3(2)	21(2)
C(7)	90(3)	68(3)	46(2)	13(2)	-5(2)	30(2)
C(8)	94(3)	60(2)	56(2)	17(2)	-8(2)	28(2)
C(9)	94(3)	70(3)	60(2)	24(2)	8(2)	34(2)
C(10)	149(4)	82(3)	44(2)	13(2)	3(2)	47(3)
C(11)	114(3)	66(3)	46(2)	13(2)	-4(2)	34(2)
C(12)	147(4)	83(3)	77(3)	20(2)	13(3)	52(3)
C(13)	65(2)	63(2)	56(2)	30(2)	4(2)	23(2)
C(14)	60(2)	62(2)	56(2)	27(2)	9(2)	19(2)
C(15)	73(3)	75(3)	71(2)	31(2)	2(2)	29(2)
C(16)	86(3)	68(3)	62(2)	24(2)	-2(2)	17(2)
C(17)	86(3)	61(2)	61(2)	21(2)	17(2)	17(2)
C(18)	81(3)	71(3)	87(3)	34(2)	17(2)	32(2)
C(19)	78(3)	67(3)	70(2)	27(2)	5(2)	31(2)
C(20)	125(4)	93(3)	72(3)	26(2)	10(3)	27(3)
C(21)	86(3)	85(3)	54(2)	22(2)	18(2)	36(2)
C(22)	73(3)	78(3)	57(2)	19(2)	-13(2)	31(2)
O(1)	71(2)	68(2)	42(1)	12(1)	-3(1)	32(1)
O(2)	57(1)	61(2)	58(1)	22(1)	-4(1)	21(1)
O(3)	110(2)	94(2)	57(1)	26(1)	-17(2)	48(2)
O(4)	64(2)	64(2)	47(1)	19(1)	5(1)	17(1)