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Supporting information for article:

Crystal structure of (2*E*)-1-(5-chlorothiophen-2-yl)-3-[4-(dimethyl amino) phenyl]prop-2-en-1-one

Rafael E. Rodríguez-Lugo, Neudo Urdaneta, Bruno Pribanic and Vanessa R. Landaeta

Solid-state emissive chalcone: X-ray single-crystal determination

Rafael R. Rodríguez-Lugo, Neudo Urdaneta, Bruno Pribanic and Vanessa R. Landaeta.

Abstract Orange rectangular blocks suitable for x-ray diffraction analysis were obtained for the previously reported chalcone (2*E*)-1-(5-chlorothiophen-2-yl)-3-[4-(dimethyl amino) phenyl]prop-2-en-1-one, **1**. This solid-emissive chalcone exhibits a planar structure and the bond parameters are compared with related compounds already described in the literature. The determination of the structure of this chalcone is quite relevant because it will play an important role in theoretical calculations to investigate potential two-photon absorption processes and could also be useful to study the interaction of such compound with a biological target.

S1. Computing Details

Data collection: *Xcalibur, Sapphire3* (Oxford Diffraction Limited); cell refinement: *SAINT* (Bruker, 2012); data reduction: S*AINT* (Bruker, 2012); program(s) used to solve structure: *Olex2.solve* (Bourhis, 2013); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Olex2* (Dolomanov, 2009).

S2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table S1. Most of the H atoms present were found in a difference Fourier map and were refined freely. Those H atoms which after the refinement did not refine properly were placed in idealized positions and refined using a riding model with appropriate displacement parameters of Uiso(H) = 1.2Ueq(parent). Default effective C—H distances for T = 100 K were 0.93 (aromatics/HC=CH) and 0.96 Å (NCH_3).

Table S1 Crystal data and structure refinement.

Crystal data	
Empirical formula	$C_{15}H_{14}ClNOS$
Formula weight	291.78
Temperature /K	100
Crystal system, space group	Monoclinic, $P2_1/n$
a, *b*, *c*/Å	7.4534(3), 17.4357(5), 10.7079(4)
β/°	101.479(4)
Volume/Å^3	1363.71(8)
Z	4
Radiation type	Mo *Kα*
μ/mm^{-1}	0.423
Crystal size/mm^3	0.3 × 0.28 × 0.25
Data collection and refinement	
Diffractometer	Xcalibur, Sapphire3
Absortion correction	Empirical, using spherical harmonics (SCALE3 ABSPACK)
T_{min}, T_{max}	0.621, 1.000
2Θ range for data collection	6.04 to 61°
Index ranges	$-10 \le h \le 10$, $-24 \le k \le 23$, $-15 \le l \le 15$
Reflections collected	14824
Independent reflections	4168[R(int) = 0.0444]
Data/restraints/parameters	4168/0/174
Goodness-of-fit on F^2	1.038
Final R indexes [I>2σ (I)]	R_1 = 0.0502, wR_2 = 0.1391
Final R indexes [all data]	R_1 = 0.0619, wR_2 = 0.1480
Largest diff. peak/hole / e Å^{-3}	0.48/-0.33

S3. Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of *F*2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on *F*2,conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative *F*2. The threshold expression of $F2 > \sigma(F2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on *F*2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$).

Atom	*x*	*y*	*z*	U(eq)
S1	4003.1(6)	9132.4(2)	6277.6(4)	20.64(13)
Cl2	4636.6(6)	10640.6(2)	7578.5(5)	29.39(14)
O3	3535.4(19)	7588.3(7)	5246.9(11)	26.0(3)
C4	5721(2)	3930.0(9)	8161.6(16)	19.9(3)
C5	4997(2)	5420.9(9)	7079.7(16)	18.7(3)
C6	4697(2)	8292.3(9)	7094.4(15)	17.3(3)
C7	5490(2)	8433.9(9)	8344.6(16)	20.3(3)
C8	5534(2)	9224.9(10)	8653.5(16)	21.3(3)
C9	4997(2)	6860.8(9)	7050.4(15)	18.7(3)
C10	4374(2)	4751.8(9)	6393.7(16)	21.1(3)
C11	4791(2)	9659.9(9)	7623.1(16)	20.6(3)
N12	6077(2)	3216.8(8)	8687.0(15)	25.4(3)
C13	6983(3)	3135.9(10)	10016.0(17)	27.3(4)
C14	4727(2)	4027.7(9)	6905.6(17)	21.1(3)
C15	5437(3)	2536.6(10)	7962.8(19)	28.3(4)
C16	6337(2)	4600.9(9)	8867.0(16)	20.0(3)
C17	5988(2)	5317.8(9)	8330.0(16)	20.0(3)

C18	4360(2)	7570.1(9)	6372.7(15)	18.7(3)
C19	4564(2)	6166.4(9)	6509.7(16)	19.4(3)

Table S3 Atomic displacement parameters (Å^2).

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	24.1(2)	13.6(2)	22.4(2)	1.54(13)	0.20(15)	0.19(14)
Cl2	31.8(3)	11.7(2)	44.0(3)	-2.24(15)	5.7(2)	1.16(15)
O3	34.9(7)	18.6(6)	21.1(6)	-0.7(4)	-2.3(5)	-3.3(5)
C4	19.1(7)	14.5(7)	26.9(8)	-0.5(6)	6.7(6)	-0.8(6)
C5	17.9(7)	14.9(7)	23.2(7)	-1.8(6)	4.1(6)	0.3(6)
C6	17.2(7)	13.4(7)	20.4(7)	0.8(5)	1.6(5)	-0.7(5)
C7	20.9(8)	15.0(7)	23.1(7)	-0.3(6)	-0.3(6)	1.2(6)
C8	19.8(8)	16.6(7)	24.9(8)	-4.7(6)	-1.4(6)	0.7(6)
C9	20.2(8)	15.1(7)	20.9(7)	-0.4(5)	4.1(6)	-1.1(6)
C10	19.8(7)	17.9(8)	24.5(8)	-2.4(6)	2.0(6)	-1.4(6)
C11	18.9(7)	11.9(7)	30.4(8)	-3.2(6)	3.8(6)	-0.4(6)
N12	31.7(8)	11.6(6)	31.8(8)	1.3(5)	3.8(6)	-3.0(5)
C13	37.7(10)	19.5(8)	26.2(8)	4.1(6)	9.7(7)	2.3(7)
C14	22.5(8)	13.6(7)	26.8(8)	-2.8(6)	3.7(6)	-1.9(6)
C15	29.7(9)	13.0(7)	40.8(10)	-2.2(7)	3.6(8)	-2.8(7)
C16	23.0(8)	15.8(7)	21.4(7)	-1.6(6)	4.8(6)	1.1(6)
C17	22.3(8)	14.1(7)	23.4(7)	-4.7(6)	4.1(6)	0.0(6)
C18	19.5(7)	14.0(7)	22.1(7)	-0.9(5)	3.0(6)	-2.0(6)
C19	18.2(7)	16.7(7)	23.0(7)	-0.9(6)	3.0(6)	-0.7(6)

Table S4 Geometric parameters (Å, °).

S1-C6	1.7315(16)	C6-C7	1.374(2)
S1-C11	1.7118(17)	C6-C18	1.473(2)
Cl-C11	1.7139(17)	C7-C8	1.417(2)
O3-C18	1.2399(19)	C8-C11	1.362(2)
C4-N12	1.369(2)	C9-C18	1.464(2)
C4-C14	1.411(2)	C9-C19	1.353(2)
C4-C16	1.418(2)	C10-C14	1.381(2)
C5-C10	1.407(2)	N12-C13	1.455(2)
C5-C17	1.406(2)	N12-C15	1.445(2)
C5-C19	1.445(2)	C16-C17	1.379(2)
C11-S1-C6	90.65(8)	S1-C11-Cl2	120.18(10)
N12-C4-C14	121.57(15)	C8-C11-S1	113.49(12)
N12-C4-C16	120.97(16)	C8-C11-Cl2	126.32(13)
C14-C4-C16	117.46(14)	C4-N12-C13	120.27(15)
C10-C5-C19	120.17(15)	C4-N12-C15	120.57(15)
C17-C5-C10	116.57(15)	C15-N12-C13	118.98(15)
C17-C5-C19	123.24(15)	C10-C14-C4	120.76(15)
C7-C6-S1	111.56(12)	C17-C16-C4	120.75(15)
C7-C6-C18	131.33(15)	C16-C17-C5	122.20(15)
C18-C6-S1	117.11(12)	O3-C18-C6	119.21(14)
C6-C7-C8	112.83(14)	O3-C18-C9	123.54(15)
C11-C8-C7	111.46(14)	C9-C18-C6	117.23(14)
C19-C9-C18	121.16(15)	C9-C19-C5	127.59(16)
C14-C10-C5	122.26(16)		

Table S5 Contacts (Å, °) in the asymmetric unit.

D-H···A	D-H	H···A	D···A	D-H···A
C10-H10··· C10-H10[a, i]	0.930(2)	2.877(2)	2.877(2)	117.8(1)
C7-H7···O3[ii]	0.930(2)	2.424(1)	3.262(2)	149.8(1)
C17-H17···S1[iii]	0.929(2)	2.949(1)	3.621(2)	130.3(1)
C15-H15B···Cl2[iv]	0.961(2)	2.787(1)	3.370(2)	119.8(1)