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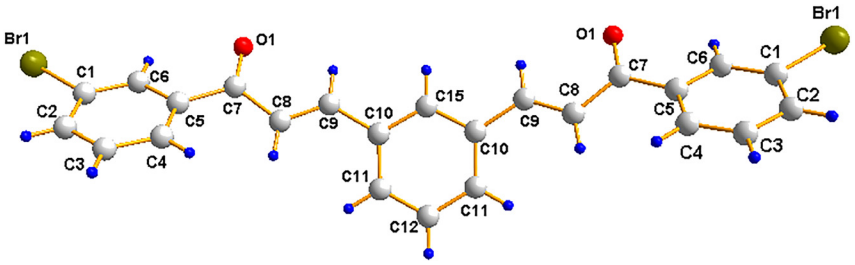
Synthesis and crystal structure of (2*E*,2′*E*)-3,3′-(1,3-phenylene)bis(1-(3-bromophenyl)prop-2-en-1-one), $C_{24}H_{16}Br_2O_2$



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Abstract

$C_{24}H_{16}Br_2O_2$, orthorhombic, *Pnma* (no. 62), a = 7.407(3) Å, b = 44.336(16) Å, c = 6.046(2) Å, V = 944.8(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0602, $wR_{ref}(F^2)$ = 0.1315, T = 293 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.20 × 0.14 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	4.10 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.0°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7399, 1779, 0.109
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1183
$N(param)_{refined}$:	130
Programs:	Bruker [1], SHELX [2], Diamond [3]

Source of material

The target compound (2*E*,2′*E*)-3,3′-(1,3-phenylene)bis(1-(3-bromophenyl)prop-2-en-1-one) (PBP) was synthesized according to the procedure reported in ref. [4]. A base catalyzed condensation of 3-bromoacetophenon (2 equivalents) and isophthalaldehyde (1 equivalent) in ethanol in presence of NaOH at room temperature resulted in the PBP in good yield (85%). Good quality colorless block crystals were obtained by slow evaporation of the ethyl acetate solution.

Experimental details

The hydrogen atoms bonded to the carbon atoms were placed in calculated positions and refined as riding mode, with C–H = 0.96 Å with U_{iso}(H) = 1.2 U_{eq}(C).

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*Y*	*z*	U_{iso}*/U_{eq}
Br1	0.33707 (10)	0.02317 (2)	0.33389 (13)	0.0622 (3)
O1	0.2911 (8)	0.14332 (10)	0.4304 (8)	0.0741 (17)
C1	0.3569 (8)	0.05838 (12)	0.1574 (11)	0.0453 (15)
C2	0.4218 (10)	0.05592 (15)	−0.0586 (12)	0.0562 (18)
H2	0.4492	0.0371	−0.1185	0.067*
C3	0.4440 (10)	0.08155 (16)	−0.1802 (12)	0.062 (2)
H3	0.4919	0.0804	−0.3221	0.074*
C4	0.3962 (10)	0.10920 (14)	−0.0943 (11)	0.0521 (18)
H4	0.4084	0.1264	−0.1809	0.063*
C5	0.3299 (9)	0.11171 (13)	0.1196 (11)	0.0474 (16)
C6	0.3108 (9)	0.08564 (12)	0.2468 (12)	0.0467 (16)
H6	0.2672	0.0868	0.3908	0.056*
C7	0.2874 (10)	0.14117 (13)	0.2288 (13)	0.0519 (18)
C8	0.2396 (10)	0.16735 (13)	0.0899 (12)	0.0548 (18)
H8	0.2185	0.1647	−0.0604	0.066*
C9	0.2267 (9)	0.19450 (12)	0.1772 (11)	0.0479 (16)
H9	0.2527	0.1960	0.3273	0.057*
C10	0.1760 (9)	0.22249 (12)	0.0655 (11)	0.0452 (15)
C11	0.0960 (9)	0.22306 (13)	−0.1432 (11)	0.0491 (16)
H11	0.0694	0.2050	−0.2140	0.059*
C12	0.0554 (13)	0.2500	−0.2467 (17)	0.054 (3)
H12	0.0010	0.2500	−0.3853	0.065*
C15	0.2110 (12)	0.2500	0.1673 (14)	0.041 (2)
H15	0.2598	0.2500	0.3090	0.050*

Comment

Chalcones are well known organic compounds and a major component of some natural products, which have attracted immense interest owing to their characteristic biological activities namely, anti-cancer [5], anti-microbial [6], anti-inflammatory [7], anti-protozoal [8], anti-oxidant [9] and anti-malarial [10] etc. The presence of the double bond believe to impart bioactive characteristic to the chalcone and removal of double bonds will make them biological inactive. Structural modification, biological active and facile preparation are some of the characteristics that differentiate chalcones from the plethora of other bioactive molecules. The crystals of the PBP were subjected to single crystal X-ray diffraction (SXRD) to determine the non-covalent forces and molecular stacking in the solid state. The crystal structure of the title compound is mainly established by the hydrogen bonds C4–H4···O1 (2.615 Å) between two neighboring molecules to form a sheet like structure along the *a* axis. Additionally, C12–H12···π interaction (2.740 Å) along *c* keeps the stack together. Thus, these two different interactions enhance each other, and in turn stabilize the overall crystal structure. All parameters are in expected ranges [11].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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