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The crystal structure of 2,6-di-*tert*-butyl-4-(phenyl(phenylsulfonyl)methyl)phenol, C₂₇H₃₂O₃S

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.35 × 0.3 × 0.28 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	1.37 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	67.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	42113, 8633, 0.035
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 7324
$N(\text{param})_{\text{refined}}$:	573
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

One of the two crystallographically molecules forming the asymmetric unit 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.

Source of material

To a stirring solution of 4-benzylidene-2,6-di-*tert*-butylcyclohexa-2,5-dienol (177 mg, 0.6 mmol) in anhydrous toluene (2 mL) were added sodium benzenesulfinate (82 mg, 0.5 mmol) and acetic acid (30 mg, 0.5 mmol). The mixture was stirred at 65 °C. After the completion of reaction, monitored by TLC, the mixture was washed by water, dried over by anhydrous magnesium sulfate and concentrated *in vacuo*. The residue was then purified by flash chromatography (petroleum ether/ethyl acetate 10:1) on silica gel to afford the title compound as white solid in yield 75%.

Experimental details

All hydrogen atoms were placed geometrically on calculated positions using a riding model with the help of the SHELX program [2].

Comment

The diarylmethyl sulfones as one of the most important sulfur-containing compounds are widely present in many biologically active natural products and pharmaceuticals [4–7]. For example, 2-(1-((4-chlorophenyl)sulfonyl)cyclohexyl)-1,4-difluorobenzene as a γ -secretase inhibitor show high potential in the treatment of Alzheimer's disease [4]. 4,4',4''-((Phenylsulfonyl)methanetriyl)tris(fluorobenzene) is useful

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Abstract

C₂₇H₃₂O₃S, triclinic, $P\bar{1}$, $a = 12.2441(2)$ Å, $b = 14.9350(2)$ Å, $c = 15.2081(3)$ Å, $\alpha = 73.6710(16)^\circ$, $\beta = 70.1267(17)^\circ$, $\gamma = 70.7828(15)^\circ$, $V = 2424.41(8)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0442$, $wR_{\text{ref}}(F^2) = 0.1319$, $T = 297.1(2)$ K.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
S1	0.44215(4)	0.98322(3)	0.19627(3)	0.04365(13)
S2	0.38627(3)	0.32632(3)	0.01628(3)	0.03848(12)
O1	0.42680(13)	1.03546(10)	0.10413(10)	0.0606(4)
O2	0.39315(13)	1.03550(10)	0.27304(11)	0.0608(4)
O3	0.59990(15)	0.63910(11)	0.51725(11)	0.0656(4)
H3	0.574275	0.662224	0.565578	0.098*
O4	0.39557(12)	0.42414(9)	−0.01926(9)	0.0513(3)
O5	0.44495(12)	0.25817(10)	−0.04659(9)	0.0512(3)
O6	0.08672(13)	0.46209(11)	0.41683(10)	0.0624(4)
H6A	0.096791	0.514086	0.415679	0.075*
C1	0.59806(16)	0.93277(13)	0.18464(13)	0.0435(4)
C2	0.6428(2)	0.92150(17)	0.25992(15)	0.0594(5)
H2	0.592218	0.941231	0.316229	0.071*
C3	0.7645(2)	0.8802(1)	0.25027(19)	0.0750(7)
H3A	0.796068	0.871613	0.300623	0.090*
C4	0.8382(2)	0.8522(2)	0.1672(2)	0.0803(8)
H4	0.919832	0.824349	0.161195	0.096*
C5	0.7925(2)	0.8649(2)	0.0927(2)	0.0832(8)
H5	0.843526	0.846151	0.036082	0.100*
C6	0.67104(18)	0.90549(17)	0.10060(16)	0.0621(6)
H6	0.639844	0.913970	0.050090	0.074*
C7	0.38258(15)	0.87788(12)	0.22931(12)	0.0404(4)
H7	0.421374	0.843552	0.175880	0.049*
C8	0.24962(16)	0.91356(13)	0.23391(13)	0.0445(4)
C9	0.2162(2)	0.9211(2)	0.15421(18)	0.0750(7)
H9	0.274338	0.901516	0.100299	0.090*
C10	0.0965(3)	0.9576(3)	0.1531(2)	0.0970(10)
H10	0.075705	0.963206	0.098009	0.116*
C11	0.0094(2)	0.98515(19)	0.2313(2)	0.0741(7)
H11	−0.070470	1.009889	0.230059	0.089*
C12	0.0411(2)	0.9760(2)	0.3109(2)	0.0820(8)
H12	−0.017871	0.993658	0.365205	0.098*
C13	0.1603(2)	0.9406(2)	0.31261(17)	0.0757(7)
H13	0.180137	0.935045	0.368114	0.091*
C14	0.42527(14)	0.81073(12)	0.31344(12)	0.0366(3)
C15	0.51366(14)	0.72653(12)	0.29622(12)	0.0373(4)
H15	0.534256	0.708979	0.237497	0.045*
C16	0.57255(14)	0.66747(12)	0.36373(12)	0.0387(4)
C17	0.53812(16)	0.69617(13)	0.45185(12)	0.0422(4)
C18	0.44690(15)	0.77936(13)	0.47342(12)	0.0412(4)
C19	0.39255(15)	0.83563(13)	0.40164(12)	0.0413(4)
H19	0.332374	0.891689	0.413507	0.050*
C20	0.67560(16)	0.57738(13)	0.33906(14)	0.0465(4)
C21	0.6930(2)	0.56318(18)	0.23892(17)	0.0732(7)
H21A	0.619538	0.556883	0.234599	0.110*
H21B	0.755886	0.505805	0.226319	0.110*
H21C	0.714498	0.617954	0.193001	0.110*
C22	0.6491(2)	0.48547(14)	0.40810(18)	0.0635(6)
H22A	0.640025	0.490752	0.471815	0.095*
H22B	0.714415	0.430763	0.391173	0.095*
H22C	0.576243	0.477263	0.404598	0.095*
C23	0.79472(18)	0.58929(17)	0.3414(2)	0.0703(6)
H23A	0.810676	0.647136	0.298168	0.106*
H23B	0.858966	0.534594	0.322870	0.106*
H23C	0.788803	0.593575	0.404796	0.106*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C24	0.41070(19)	0.81336(15)	0.56872(13)	0.0539(5)
C25	0.3702(4)	0.7370(2)	0.65414(17)	0.1053(11)
H25A	0.305630	0.719574	0.646479	0.158*
H25B	0.343231	0.762502	0.711412	0.158*
H25C	0.436444	0.680798	0.658175	0.158*
C26	0.5155(3)	0.8403(2)	0.5792(2)	0.0852(8)
H26A	0.583908	0.785273	0.576811	0.128*
H26B	0.492440	0.860367	0.639058	0.128*
H26C	0.535814	0.892225	0.528194	0.128*
C27	0.3066(3)	0.9051(2)	0.57383(19)	0.0898(9)
H27A	0.330508	0.956483	0.523762	0.135*
H27B	0.286128	0.923224	0.634360	0.135*
H27C	0.238105	0.893104	0.566580	0.135*
C28	0.23134(15)	0.32853(14)	0.06189(12)	0.0426(4)
C29	0.19861(18)	0.24253(16)	0.09473(15)	0.0535(5)
H29	0.256180	0.184187	0.087568	0.064*
C30	0.0787(2)	0.2444(2)	0.13855(17)	0.0671(6)
H30	0.055094	0.187017	0.161623	0.080*
C31	−0.00560(19)	0.3317(2)	0.14778(18)	0.0754(7)
H31	−0.086094	0.332757	0.176980	0.090*
C32	0.0275(2)	0.4165(2)	0.1147(2)	0.0781(7)
H32	−0.030488	0.474841	0.120771	0.094*
C33	0.14709(19)	0.41577(17)	0.07210(16)	0.0627(6)
H33	0.170420	0.473225	0.050652	0.075*
C34	0.43714(14)	0.27618(12)	0.12415(11)	0.0345(3)
H34	0.428427	0.209951	0.144327	0.041*
C35	0.57092(14)	0.26685(12)	0.09930(11)	0.0371(4)
C36	0.64811(17)	0.17622(16)	0.09203(17)	0.0604(6)
H36	0.616727	0.124492	0.100805	0.072*
C37	0.7710(2)	0.16083(19)	0.0720(2)	0.0765(7)
H37	0.821466	0.099134	0.068118	0.092*
C38	0.81849(18)	0.23681(19)	0.05778(17)	0.0677(6)
H38	0.901143	0.227219	0.043610	0.081*
C39	0.74286(19)	0.32671(18)	0.06469(17)	0.0620(5)
H39	0.774672	0.378211	0.055869	0.074*
C40	0.61994(17)	0.34248(15)	0.08457(14)	0.0512(5)
H40	0.570076	0.404415	0.088030	0.061*
C41	0.35119(13)	0.32898(12)	0.20331(11)	0.0351(3)
C42	0.33631(14)	0.42514(12)	0.20223(11)	0.0384(4)
H42	0.385528	0.459089	0.152745	0.046*
C43	0.24985(14)	0.47287(12)	0.27299(11)	0.0382(4)
C44	0.17607(14)	0.41899(13)	0.34580(11)	0.0400(4)
C45	0.18751(14)	0.32121(12)	0.34910(11)	0.0377(4)
C46	0.27686(14)	0.27869(12)	0.27659(11)	0.0354(3)
H46	0.287213	0.213982	0.277237	0.042*
C47	0.23521(16)	0.58057(13)	0.26831(12)	0.0434(4)
C48	0.3296(2)	0.62068(15)	0.18443(16)	0.0610(5)
H48A	0.408602	0.583763	0.189644	0.092*
H48B	0.319410	0.687000	0.185313	0.092*
H48C	0.320098	0.616414	0.125758	0.092*
C49	0.2521(2)	0.59557(17)	0.35844(15)	0.0650(6)
H49A	0.191002	0.575951	0.413094	0.097*
H49B	0.246084	0.662593	0.352738	0.097*
H49C	0.329901	0.557535	0.365707	0.097*
C50	0.1115(2)	0.64063(16)	0.25369(18)	0.0676(6)
H50A	0.106197	0.634488	0.194216	0.101*
H50B	0.101924	0.707259	0.252925	0.101*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H50C	0.049397	0.617587	0.304805	0.101*
C51	0.10364(16)	0.26347(14)	0.42672(12)	0.0450(4)
C52	0.1136(2)	0.25884(18)	0.52594(13)	0.0650(6)
H52A	0.195319	0.229128	0.528273	0.097*
H52B	0.062213	0.221457	0.573089	0.097*
H52C	0.089611	0.323047	0.538499	0.097*
C53	−0.02700(18)	0.30923(18)	0.42156(16)	0.0622(6)
H53A	−0.051803	0.374499	0.431456	0.093*
H53B	−0.078437	0.272679	0.469951	0.093*
H53C	−0.032263	0.309069	0.360050	0.093*
C54	0.1359(2)	0.15955(16)	0.41246(16)	0.0685(7)
H54A	0.129750	0.159960	0.351087	0.103*
H54B	0.081588	0.125779	0.461171	0.103*
H54C	0.216744	0.127670	0.416184	0.103*

as a potassium channel modulator [5]. 8-((Di(naphthalen-2-yl)methyl)sulfonyl)-4-methyl-1-(naphthalen-2-yl)-2,3,4,5-tetrahydro-1*H*-benzo[e][1,4]diazepine as an antidepressant drug has a wider therapeutic spectrum and can exert sufficient therapeutic effects in a short period [6]. 9-((4-Methoxyphenyl)sulfonyl)-9*H*-fluorene is a very selective and effective antimalarial agent, which shows pronounced activity against human skin cancer cells [7]. In addition, diarylmethylamines are also widely used as important synthetic intermediates in medicinal chemistry and materials science [8–10]. Our group has maintained a keen interest in the synthesis of the sulfones [11, 12] and diarylmethyl derivatives [13]. We first synthesized the 2,6-di-*tert*-butyl-4-(phenyl(phenylsulfonyl)methyl)phenol and obtained the crystal of it. Then we submitted the data to CCDC on 28th September, 2017. One month later, Zhu's group deposited another monoclinic crystal structure of the same compound with $P2_1/c$ space group with the Cambridge Crystallographic Data Center (CCDC no.: 1583037) [14]. There is only one molecule in the asymmetric unit of this monoclinic structure. Herein, we reported the crystal structure of the title compound. The geometry and labeling for the crystal structure of it is depicted in the figure. The title structure crystallizes in triclinic space group $P\bar{1}$. Thus, we obtained another modification of the title compound.

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