Crystal structure of bis{*tert*-butyl-[2-hydroxy-2-(3,5-dihydroxyphenyl)-ethyl]ammonium} sulfate, $C_{24}H_{40}N_2O_{10}S$

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Source of material: The compound (alternative name: *tert*butylsulfate) is commercially available.

$C_{24}H_{40}N_2O_{10}S$, triclinic, $P\bar{1}$ (No. 2), $a=9.970(7)$ Å, $b=11.204(4)$ Å, $c=13.397(6)$ Å, $\alpha=100.86(5)^\circ$, $\beta=104.40(6)^\circ$, $\gamma=101.54(4)^\circ$, $V=1374.8$ Å³, $Z=2$, $R(F)=0.073$, $R_w(F^2)=0.136$.

Table 1. Parameters used for the X-ray data collection

Crystal:	white, irregular prism, size 0.12 x 0.16 x 0.18 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ :	15.33 cm ⁻¹
Diffractometer:	STOE AED4
Scan mode:	$\omega/2\theta$
Temperature:	293 K
$2\theta_{max}$:	100°
$N(hkl)_{unique}$:	2794
Criterion for I_o :	$I_o > 3 \sigma(I_o)$
$N(param)_{refined}$:	125
Program:	SHELXS-86, SHELXTL, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
C(1)	2i	0.342(1)	0.4998(8)	0.7440(7)	0.044(6)
H(1)	2i	0.366(1)	0.5769(8)	0.7934(7)	0.053
C(2)	2i	0.252(1)	0.395(1)	0.7564(7)	0.046(6)
C(3)	2i	0.2168(9)	0.2800(9)	0.6827(9)	0.035(5)
H(3)	2i	0.157(1)	0.210(1)	0.691(1)	0.042
C(4)	2i	0.272(1)	0.2693(7)	0.5965(7)	0.011(4)
C(5)	2i	0.3615(9)	0.374(1)	0.5840(7)	0.030(5)
H(5)	2i	0.398(1)	0.367(1)	0.5264(8)	0.036
C(6)	2i	0.3969(9)	0.4891(8)	0.6578(9)	0.030(5)
C(7)	2i	0.225(2)	0.149(1)	0.515(1)	0.035(5)
H(7)	2i	0.278(2)	0.156(1)	0.463(1)	0.042
C(8)	2i	0.259(2)	0.042(1)	0.568(1)	0.022(5)
H(8A)	2i	0.362(2)	0.054(1)	0.592(1)	0.027
H(8B)	2i	0.223(2)	0.045(1)	0.629(1)	0.027
C(9)	2i	0.246(2)	-0.197(2)	0.520(1)	0.023(5)
C(10)	2i	0.153(2)	-0.312(2)	0.430(1)	0.058(7)
H(10A)	2i	0.168(2)	-0.301(2)	0.364(1)	0.088
H(10B)	2i	0.053(2)	-0.320(2)	0.425(1)	0.088
H(10C)	2i	0.178(2)	-0.386(2)	0.444(1)	0.088
C(11)	2i	0.398(2)	-0.179(1)	0.514(1)	0.042(6)
H(11A)	2i	0.399(2)	-0.175(1)	0.443(1)	0.063
H(11B)	2i	0.435(2)	-0.248(1)	0.531(1)	0.063
H(11C)	2i	0.458(2)	-0.102(1)	0.563(1)	0.063
C(12)	2i	0.230(2)	-0.204(1)	0.628(1)	0.037(5)
H(12A)	2i	0.130(2)	-0.216(1)	0.625(1)	0.056
H(12B)	2i	0.286(2)	-0.127(1)	0.679(1)	0.056
H(12C)	2i	0.262(2)	-0.274(1)	0.647(1)	0.056

Table 2. (Continued)

Atom	Site	x	y	z	U_{iso}
C(13)	2i	0.3901(9)	0.758(1)	0.1342(7)	0.033(5)
H(13)	2i	0.3290(9)	0.742(1)	0.1753(7)	0.039
C(14)	2i	0.403(1)	0.6594(7)	0.0599(8)	0.034(6)
C(15)	2i	0.494(1)	0.6833(8)	-0.0015(7)	0.033(5)
H(15)	2i	0.503(2)	0.617(1)	-0.0512(9)	0.040
C(16)	2i	0.5725(9)	0.806(1)	0.0115(7)	0.026(5)
C(17)	2i	0.560(1)	0.9041(7)	0.0858(8)	0.035(5)
H(17)	2i	0.612(1)	0.9859(8)	0.095(1)	0.042
C(18)	2i	0.468(1)	0.8802(9)	0.1472(7)	0.024(5)
C(19)	2i	0.666(2)	0.830(2)	-0.056(1)	0.041(6)
H(19)	2i	0.715(2)	0.920(2)	-0.034(1)	0.049
C(20)	2i	0.783(2)	0.754(2)	-0.044(1)	0.040(6)
H(20A)	2i	0.814(2)	0.750(2)	0.030(1)	0.048
H(20B)	2i	0.739(2)	0.669(2)	-0.087(1)	0.048
C(21)	2i	0.974(2)	0.720(2)	-0.140(2)	0.055(6)
C(22)	2i	0.878(2)	0.670(2)	-0.249(2)	0.089(8)
H(22A)	2i	0.789(2)	0.618(2)	-0.247(2)	0.134
H(22B)	2i	0.922(2)	0.621(2)	-0.291(2)	0.134
H(22C)	2i	0.859(2)	0.738(2)	-0.279(2)	0.134
C(23)	2i	0.996(2)	0.617(2)	-0.075(1)	0.063(6)
H(23A)	2i	1.061(2)	0.657(2)	-0.005(1)	0.094
H(23B)	2i	1.036(2)	0.557(2)	-0.111(1)	0.094
H(23C)	2i	0.906(2)	0.575(2)	-0.070(1)	0.094
C(24)	2i	1.118(2)	0.804(2)	-0.132(1)	0.073(7)
H(24A)	2i	1.175(2)	0.833(2)	-0.059(1)	0.109

Table 2. (Continued)

Atom	Site	x	y	z	U_{iso}
H(24B)	2i	1.104(2)	0.875(2)	-0.160(1)	0.109
H(24C)	2i	1.167(2)	0.757(2)	-0.172(1)	0.109
N(1)	2i	0.193(1)	-0.081(1)	0.4908(9)	0.036(4)
H(1A)	2i	0.208(1)	-0.075(1)	0.4283(9)	0.043
H(1B)	2i	0.098(1)	-0.099(1)	0.4804(9)	0.043
N(2)	2i	0.912(1)	0.807(1)	-0.075(1)	0.034(4)
H(2A)	2i	0.982(1)	0.849(1)	-0.014(1)	0.040
H(2B)	2i	0.890(1)	0.864(1)	-0.111(1)	0.040
O(1)	2i	0.080(1)	0.120(1)	0.4635(8)	0.045(4)
H(1A)	2i	0.056(1)	0.053(1)	0.4187(8)	0.068
O(2)	2i	0.197(1)	0.414(1)	0.8388(8)	0.054(4)
H(2)	2i	0.146(1)	0.348(1)	0.8395(8)	0.081
O(3)	2i	0.492(1)	0.591(1)	0.6477(9)	0.062(4)
H(3A)	2i	0.503(1)	0.652(1)	0.6961(9)	0.094
O(4)	2i	0.588(1)	0.7999(9)	-0.1639(9)	0.041(4)
H(4)	2i	0.644(1)	0.8148(9)	-0.1986(9)	0.062
O(5)	2i	0.320(1)	0.543(1)	0.0487(8)	0.056(4)
H(5A)	2i	0.334(1)	0.493(1)	0.0017(8)	0.084
O(6)	2i	0.456(1)	0.9798(9)	0.2208(8)	0.046(4)
H(6)	2i	0.400(1)	0.9531(9)	0.2515(8)	0.068
O(7)	2i	0.226(1)	-0.057(1)	0.2938(9)	0.046(4)
O(8)	2i	0.025(1)	-0.227(1)	0.1807(8)	0.043(4)
O(9)	2i	0.100(1)	-0.0425(9)	0.1238(8)	0.041(4)
O(10)	2i	0.001(1)	-0.028(1)	0.2729(9)	0.052(4)
S	2i	0.0859(6)	-0.0890(5)	0.2154(4)	0.044(2)

References

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