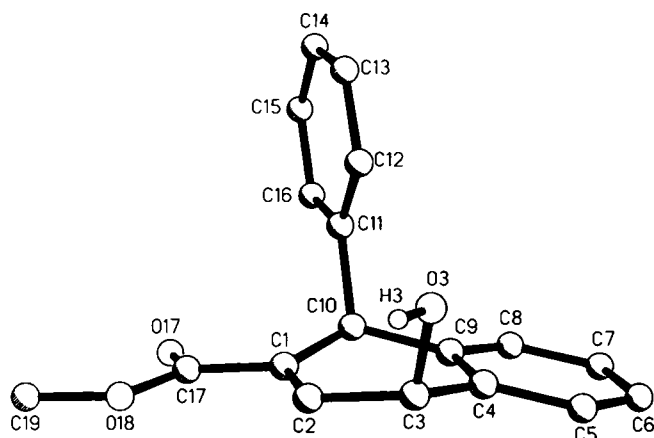


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Crystal:	colorless plate, size 0.45 x 0.65 x 0.2 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.90 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	3297
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	194
Program:	SHELXTL-plus

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2)	4e	0.5748(1)	0.3343(2)	0.0065(1)	0.08
H(3A)	4e	0.6084(2)	0.5896(2)	-0.0437(2)	0.08
H(3)	4e	0.715(2)	0.429(4)	-0.075(2)	0.11(1)
H(5)	4e	0.7055(2)	0.8532(3)	-0.0075(2)	0.08
H(6)	4e	0.7795(2)	1.0588(3)	0.1205(2)	0.08
H(7)	4e	0.8282(2)	1.0066(3)	0.3087(2)	0.08
H(8)	4e	0.8022(2)	0.7490(2)	0.3667(2)	0.08
H(10)	4e	0.7006(1)	0.4945(2)	0.3107(1)	0.08
H(12)	4e	0.8657(2)	0.3842(3)	0.1768(2)	0.08
H(13)	4e	1.0187(2)	0.2382(3)	0.2607(2)	0.08
H(14)	4e	1.0760(2)	0.1589(3)	0.4449(2)	0.08
H(15)	4e	0.9806(2)	0.2246(3)	0.5455(2)	0.08
H(16)	4e	0.8256(2)	0.3666(3)	0.4618(2)	0.08
H(19A)	4e	0.4728(2)	-0.0709(3)	0.0908(2)	0.08
H(19B)	4e	0.4702(2)	0.0237(3)	0.1920(2)	0.08
H(19C)	4e	0.5683(2)	-0.0734(3)	0.2035(2)	0.08

$\text{C}_{18}\text{H}_{16}\text{O}_3$, monoclinic, $P12_1/c1$ (No. 14), $a = 14.304(1) \text{ \AA}$, $b = 8.219(1) \text{ \AA}$, $c = 13.296(2) \text{ \AA}$, $\beta = 113.79(1)^\circ$, $V = 1430.3 \text{ \AA}^3$, $Z = 4$, $R(F) = 0.054$, $R_w(F) = 0.054$.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4e	0.6512(1)	0.3746(2)	0.1657(1)	0.0302(8)	0.0295(9)	0.0363(9)	0.0002(7)	0.0143(7)	0.0014(7)
C(2)	4e	0.6237(1)	0.4052(2)	0.0590(1)	0.038(1)	0.036(1)	0.034(1)	-0.0055(8)	0.0113(8)	-0.0033(8)
C(3)	4e	0.6652(2)	0.5448(2)	0.0173(2)	0.046(1)	0.038(1)	0.0309(9)	-0.0046(8)	0.0126(8)	0.0002(8)
O(3)	4e	0.7441(1)	0.4886(2)	-0.0150(1)	0.068(1)	0.055(1)	0.0456(8)	-0.0148(8)	0.0331(8)	-0.0161(8)
C(4)	4e	0.7110(1)	0.6758(2)	0.1026(2)	0.039(1)	0.0316(9)	0.0365(9)	-0.0001(8)	0.0161(8)	-0.0006(8)
C(5)	4e	0.7259(2)	0.8310(3)	0.0693(2)	0.053(1)	0.035(1)	0.046(1)	0.0018(9)	0.024(1)	0.0053(9)
C(6)	4e	0.7692(2)	0.9528(3)	0.1447(2)	0.061(1)	0.028(1)	0.067(1)	-0.0017(9)	0.035(1)	0.000(1)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(7)	4e	0.7980(2)	0.9219(3)	0.2557(2)	0.052(1)	0.035(1)	0.062(1)	-0.0078(9)	0.030(1)	-0.015(1)
C(8)	4e	0.7830(2)	0.7693(2)	0.2898(2)	0.043(1)	0.038(1)	0.040(1)	-0.0019(8)	0.0169(8)	-0.0081(9)
C(9)	4e	0.7404(1)	0.6436(2)	0.2142(1)	0.0330(9)	0.0285(9)	0.0362(9)	0.0008(7)	0.0147(8)	-0.0025(8)
C(10)	4e	0.7273(1)	0.4772(2)	0.2559(1)	0.0340(9)	0.0336(9)	0.0291(8)	-0.0002(7)	0.0129(7)	-0.0009(7)
C(11)	4e	0.8298(1)	0.3880(2)	0.3110(1)	0.0318(9)	0.032(1)	0.0335(9)	-0.0036(7)	0.0102(7)	-0.0015(7)
C(12)	4e	0.8882(2)	0.3507(3)	0.2521(2)	0.038(1)	0.046(1)	0.042(1)	0.0011(9)	0.0164(8)	0.0044(9)
C(13)	4e	0.9792(2)	0.2650(3)	0.3021(2)	0.039(1)	0.057(1)	0.064(1)	0.005(1)	0.024(1)	0.003(1)
C(14)	4e	1.0132(2)	0.2180(3)	0.4108(2)	0.036(1)	0.061(2)	0.060(1)	0.005(1)	0.007(1)	0.005(1)
C(15)	4e	0.9568(2)	0.2561(3)	0.4697(2)	0.052(1)	0.075(2)	0.038(1)	0.009(1)	0.004(1)	0.008(1)
C(16)	4e	0.8649(2)	0.3408(3)	0.4200(2)	0.045(1)	0.061(1)	0.034(1)	0.005(1)	0.0125(9)	0.000(1)
C(17)	4e	0.6092(1)	0.2330(2)	0.2042(2)	0.0295(9)	0.033(1)	0.041(1)	0.0033(7)	0.0135(8)	0.0037(8)
O(17)	4e	0.6241(1)	0.2106(2)	0.2994(1)	0.0553(9)	0.0460(8)	0.0430(8)	-0.0021(7)	0.0216(7)	0.0087(7)
O(18)	4e	0.5522(1)	0.1348(2)	0.1226(1)	0.0534(9)	0.0427(9)	0.0499(8)	-0.0180(7)	0.0169(7)	-0.0002(7)
C(19)	4e	0.5125(2)	-0.0085(3)	0.1549(2)	0.060(1)	0.046(1)	0.073(2)	-0.022(1)	0.021(1)	0.005(1)

References

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2. Sheldrick, G. M.: Program Package SHELXTL-plus. Release 4.1. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.