Table 1. Crystal data and structure refinement for C14 H12 O3.

Identification code	dyker19
Empirical formula	C14 H12 O3
Formula weight	228.24
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.592(4) A alpha = 90 deg. b = 6.912(6) A beta = 94.25(3) deg. c = 15.076(8) A gamma = 90 deg.
Volume	1100.6(11) A^3
Z, Calculated density	4, 1.377 Mg/m^3
Absorption coefficient	0.097 mm^-1
F(000)	480
Crystal size	0.49 x 0.37 x 0.35 mm
Theta range for data collection	3.52 to 25.25 deg.
Limiting indices	-12<=h<=12, -6<=k<=8, -18<=l<=18
Reflections collected / unique	8305 / 1991 [R(int) = 0.0435]
Completeness to theta = 25.25	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1991 / 0 / 154
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0412, wR2 = 0.1095
R indices (all data)	R1 = 0.0521, wR2 = 0.1172
Largest diff. peak and hole	0.234 and -0.192 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for C14 H12 O3.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(51)	5656(1)	4796(2)	4004(1)	33(1)
O(12)	4994(1)	8440(2)	2481(1)	23(1)
C(5)	5686(1)	6405(2)	3691(1)	21(1)
C(5A)	6858(1)	7613(2)	3748(1)	22(1)
C(6)	7987(2)	6894(3)	4162(1)	28(1)
C(7)	9071(2)	8022(3)	4199(1)	34(1)
C(8)	9028(2)	9844(3)	3835(1)	35(1)
C(9)	7907(2)	10582(3)	3426(1)	31(1)
C(9A)	6820(2)	9458(2)	3375(1)	24(1)
C(10)	5560(2)	10109(2)	2934(1)	25(1)
C(11)	4626(2)	10539(2)	3630(1)	24(1)
C(11A)	4036(1)	8926(2)	3800(1)	22(1)
C(1)	3050(1)	8426(2)	4417(1)	25(1)
O(2)	2099(1)	7217(2)	3976(1)	30(1)
C(3)	2646(2)	5514(2)	3641(1)	29(1)
C(4)	3484(2)	5954(2)	2883(1)	25(1)
C(4A)	4517(1)	7354(2)	3200(1)	20(1)

Table 3. Bond lengths [A] and angles [deg] for C14 H12 O3.

O(51)-C(5)	1.209(2)
O(12)-C(4A)	1.4398(19)
O(12)-C(10)	1.447(2)
C(5)-C(5A)	1.493(2)
C(5)-C(4A)	1.542(2)
C(5A)-C(9A)	1.393(2)
C(5A)-C(6)	1.398(2)
C(6)-C(7)	1.386(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.373(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.393(3)
C(8)-H(8)	0.9500
C(9)-C(9A)	1.387(2)
C(9)-H(9)	0.9500
C(9A)-C(10)	1.515(2)
C(10)-C(11)	1.524(2)
C(10)-H(10)	1.0000
C(11)-C(11A)	1.312(2)
C(11)-H(11)	0.9500
C(11A)-C(1)	1.490(2)
C(11A)-C(4A)	1.525(2)
C(1)-O(2)	1.4339(19)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
O(2)-C(3)	1.421(2)
C(3)-C(4)	1.529(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(4A)	1.512(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900

C(4A)-O(12)-C(10)	102.53(11)
O(51)-C(5)-C(5A)	122.49(14)
O(51)-C(5)-C(4A)	122.38(13)
C(5A)-C(5)-C(4A)	115.13(13)
C(9A)-C(5A)-C(6)	120.23(14)
C(9A)-C(5A)-C(5)	119.31(14)
C(6)-C(5A)-C(5)	120.46(15)
C(7)-C(6)-C(5A)	119.79(17)
C(7)-C(6)-H(6)	120.1
C(5A)-C(6)-H(6)	120.1
C(8)-C(7)-C(6)	119.81(16)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	120.95(15)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(9A)-C(9)-C(8)	119.78(17)
C(9A)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(9A)-C(5A)	119.43(16)
C(9)-C(9A)-C(10)	124.00(16)
C(5A)-C(9A)-C(10)	116.57(13)
O(12)-C(10)-C(9A)	106.90(13)
O(12)-C(10)-C(11)	102.31(12)

C(9A)-C(10)-C(11)	110.57(13)
O(12)-C(10)-H(10)	112.2
C(9A)-C(10)-H(10)	112.2
C(11)-C(10)-H(10)	112.2
C(11A)-C(11)-C(10)	108.10(14)
C(11A)-C(11)-H(11)	125.9
C(10)-C(11)-H(11)	125.9
C(11)-C(11A)-C(1)	133.18(15)
C(11)-C(11A)-C(4A)	107.78(14)
C(1)-C(11A)-C(4A)	119.04(14)
O(2)-C(1)-C(11A)	110.27(13)
O(2)-C(1)-H(1A)	109.6
C(11A)-C(1)-H(1A)	109.6
O(2)-C(1)-H(1B)	109.6
C(11A)-C(1)-H(1B)	109.6
H(1A)-C(1)-H(1B)	108.1
C(3)-O(2)-C(1)	110.92(12)
O(2)-C(3)-C(4)	112.06(13)
O(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3A)	109.2
O(2)-C(3)-H(3B)	109.2
C(4)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(4A)-C(4)-C(3)	109.73(13)
C(4A)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4A)	109.7
C(4A)-C(4)-H(4B)	109.7
C(3)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
O(12)-C(4A)-C(4)	112.46(12)
O(12)-C(4A)-C(11A)	103.06(13)
C(4)-C(4A)-C(11A)	112.22(13)
O(12)-C(4A)-C(5)	105.60(12)
C(4)-C(4A)-C(5)	114.61(13)
C(11A)-C(4A)-C(5)	108.05(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for C14 H12 O3.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(51)	28(1)	24(1)	46(1)	8(1)	-4(1)	1(1)
O(12)	24(1)	25(1)	21(1)	2(1)	1(1)	-3(1)
C(5)	20(1)	21(1)	21(1)	-3(1)	3(1)	2(1)
C(5A)	17(1)	29(1)	21(1)	-3(1)	4(1)	-1(1)
C(6)	19(1)	40(1)	25(1)	-4(1)	4(1)	4(1)
C(7)	16(1)	59(1)	27(1)	-8(1)	2(1)	0(1)
C(8)	24(1)	57(1)	26(1)	-11(1)	9(1)	-16(1)
C(9)	30(1)	38(1)	25(1)	-3(1)	9(1)	-12(1)
C(9A)	23(1)	30(1)	19(1)	-4(1)	6(1)	-4(1)
C(10)	28(1)	21(1)	25(1)	3(1)	0(1)	-6(1)
C(11)	26(1)	20(1)	27(1)	0(1)	-2(1)	3(1)
C(11A)	17(1)	23(1)	25(1)	0(1)	-5(1)	4(1)
C(1)	20(1)	28(1)	27(1)	-5(1)	1(1)	1(1)
O(2)	16(1)	36(1)	39(1)	-5(1)	3(1)	-2(1)
C(3)	23(1)	28(1)	35(1)	-5(1)	1(1)	-6(1)
C(4)	21(1)	26(1)	28(1)	-3(1)	-1(1)	-2(1)
C(4A)	17(1)	21(1)	21(1)	1(1)	1(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for C14 H12 O3.

	x	y	z	U(eq)
H(6)	8011	5636	4416	33
H(7)	9842	7536	4475	40
H(8)	9774	10612	3862	42
H(9)	7888	11851	3184	37
H(10)	5653	11224	2521	30
H(11)	4493	11762	3895	29
H(1A)	3447	7743	4943	30
H(1B)	2654	9626	4624	30
H(3A)	1962	4617	3424	34
H(3B)	3159	4861	4128	34
H(4A)	3866	4741	2678	30
H(4B)	2965	6523	2375	30