Supplementary material for:
(16 pages)

A Carbon Centered Radical Unreactive Towards Oxygen: Unusual Radical Stabilization by a Lactone Ring

J. C. Scaiano*1, Alan Martin1, Glenn P. A. Yap1 and K.U. Ingold2

1Department of Chemistry
University of Ottawa
10 Marie Curie
Ottawa, Ontario, K1N 6N5, Canada

2Steacie Institute for Molecular Sciences
National Research Council
Ottawa, Ontario, K1A 0R6, Canada

Table 1. Crystal data and structure refinement for ts003 (HP-136).

Identification code	ts003
Empirical formula	C24 H30 O2
Formula weight	350.48
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.791(3) A alpha = 90 deg. b = 10.797(2) A beta = 108.174(3) deg. c = 14.412(3) A gamma = 90 deg.
Volume	2038.9(6) A^3
Z, Calculated density	4, 1.142 Mg/m^3
Absorption coefficient	0.071 mm^-1
F(000)	760
Crystal size	0.3 x 0.3 x 0.2 mm
Theta range for data collection	2.40 to 22.49 deg.
Limiting indices	-14<=h<=14, 0<=k<=11, 0<=l<=15
Reflections collected / unique	15943 / 2654 [R(int) = 0.0802]
Completeness to theta = 22.49	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2654 / 0 / 264

Goodness-of-fit on F^2 1.040

Final R indices [I>2sigma(I)] R1 = 0.0492, wR2 = 0.1287

R indices (all data) R1 = 0.0647, wR2 = 0.1330

Extinction coefficient 0.020(3)

Largest diff. peak and hole 0.185 and -0.194 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ts003.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1377(1)	3831(2)	1147(1)	43(1)
C(2)	2012(2)	4504(2)	774(2)	47(1)
C(3)	2783(2)	5217(2)	1590(2)	38(1)
C(4)	2866(2)	5167(2)	3430(2)	37(1)
C(5)	2422(2)	4687(2)	4091(2)	37(1)
C(6)	1598(2)	3887(2)	3742(2)	39(1)
C(7)	1171(2)	3537(2)	2772(2)	35(1)
C(8)	1657(2)	4056(2)	2158(2)	34(1)
C(9)	2470(2)	4844(2)	2455(2)	34(1)
O(2A)	1933(2)	4458(2)	-73(1)	65(1)
C(5A)	2824(2)	5008(2)	5179(2)	49(1)
C(5B)	3679(7)	5956(6)	5397(4)	107(4)
C(5C)	3115(6)	3900(5)	5777(4)	67(2)
C(5D)	1922(6)	5659(7)	5467(4)	94(3)
C(5E)	2445(18)	4082(18)	5831(11)	94(6)
C(5F)	2599(14)	6221(12)	5371(9)	75(5)
C(5G)	4044(8)	4775(17)	5551(8)	81(6)
C(7A)	270(2)	2645(2)	2415(2)	47(1)
C(7B)	632(2)	1468(2)	2040(3)	79(1)
C(7C)	-584(2)	3234(3)	1581(2)	59(1)
C(7D)	-170(2)	2306(3)	3227(3)	78(1)
C(1')	3866(2)	4915(2)	1629(2)	36(1)
C(2')	4455(2)	5766(2)	1321(2)	37(1)
C(3')	5431(2)	5502(2)	1303(2)	37(1)

C(4')	5833(2)	4324(2)	1592(2)	37(1)
C(5')	5245(2)	3479(2)	1902(2)	40(1)
C(6')	4279(2)	3763(2)	1929(2)	39(1)
C(3'')	6037(2)	6467(2)	973(2)	52(1)
C(4'')	6882(2)	3980(3)	1582(2)	51(1)

Table 3. Bond lengths [A] and angles [deg] for ts003.

O(1)-C(2)	1.370(3)
O(1)-C(8)	1.406(3)
C(2)-O(2A)	1.192(3)
C(2)-C(3)	1.525(4)
C(3)-C(9)	1.495(3)
C(3)-C(1')	1.513(3)
C(4)-C(5)	1.384(3)
C(4)-C(9)	1.385(3)
C(5)-C(6)	1.391(3)
C(5)-C(5A)	1.530(3)
C(6)-C(7)	1.389(3)
C(7)-C(8)	1.384(3)
C(7)-C(7A)	1.528(3)
C(8)-C(9)	1.366(3)
C(5A)-C(5F)	1.394(12)
C(5A)-C(5C)	1.455(6)
C(5A)-C(5B)	1.519(6)
C(5A)-C(5E)	1.570(14)
C(5A)-C(5D)	1.592(6)
C(5A)-C(5G)	1.618(11)
C(7A)-C(7D)	1.521(4)
C(7A)-C(7B)	1.525(4)
C(7A)-C(7C)	1.534(4)
C(1')-C(6')	1.380(3)
C(1')-C(2')	1.388(3)
C(2')-C(3')	1.384(3)
C(3')-C(4')	1.398(3)
C(3')-C(3'')	1.501(3)
C(4')-C(5')	1.384(3)
C(4')-C(4'')	1.498(3)
C(5')-C(6')	1.379(3)
C(2)-O(1)-C(8)	108.25(19)
O(2A)-C(2)-O(1)	120.9(3)

O(2A)-C(2)-C(3)	129.1(3)
O(1)-C(2)-C(3)	110.0(2)
C(9)-C(3)-C(1')	116.7(2)
C(9)-C(3)-C(2)	101.2(2)
C(1')-C(3)-C(2)	111.23(19)
C(5)-C(4)-C(9)	119.0(2)
C(4)-C(5)-C(6)	118.1(2)
C(4)-C(5)-C(5A)	121.6(2)
C(6)-C(5)-C(5A)	120.4(2)
C(7)-C(6)-C(5)	125.1(2)
C(8)-C(7)-C(6)	113.3(2)
C(8)-C(7)-C(7A)	123.0(2)
C(6)-C(7)-C(7A)	123.7(2)
C(9)-C(8)-C(7)	124.4(2)
C(9)-C(8)-O(1)	111.4(2)
C(7)-C(8)-O(1)	124.2(2)
C(8)-C(9)-C(4)	120.0(2)
C(8)-C(9)-C(3)	109.2(2)
C(4)-C(9)-C(3)	130.8(2)
C(5F)-C(5A)-C(5C)	133.8(6)
C(5F)-C(5A)-C(5B)	62.1(7)
C(5C)-C(5A)-C(5B)	112.3(4)
C(5F)-C(5A)-C(5)	112.6(5)
C(5C)-C(5A)-C(5)	111.4(3)
C(5B)-C(5A)-C(5)	112.0(3)
C(5F)-C(5A)-C(5E)	110.1(10)
C(5C)-C(5A)-C(5E)	37.2(8)
C(5B)-C(5A)-C(5E)	133.5(7)
C(5)-C(5A)-C(5E)	112.8(6)
C(5F)-C(5A)-C(5D)	45.0(7)
C(5C)-C(5A)-C(5D)	107.6(3)
C(5B)-C(5A)-C(5D)	105.5(4)
C(5)-C(5A)-C(5D)	107.7(3)
C(5E)-C(5A)-C(5D)	72.0(9)
C(5F)-C(5A)-C(5G)	110.7(9)
C(5C)-C(5A)-C(5G)	67.0(6)
C(5B)-C(5A)-C(5G)	51.4(6)
C(5)-C(5A)-C(5G)	108.1(4)
C(5E)-C(5A)-C(5G)	102.0(9)
C(5D)-C(5A)-C(5G)	143.0(5)
C(7D)-C(7A)-C(7B)	108.9(3)
C(7D)-C(7A)-C(7)	111.7(2)
C(7B)-C(7A)-C(7)	108.9(2)
C(7D)-C(7A)-C(7C)	108.0(2)
C(7B)-C(7A)-C(7C)	108.9(2)

C(7)-C(7A)-C(7C)	110.3(2)
C(6')-C(1')-C(2')	118.1(2)
C(6')-C(1')-C(3)	120.8(2)
C(2')-C(1')-C(3)	121.0(2)
C(3')-C(2')-C(1')	122.6(2)
C(2')-C(3')-C(4')	118.6(2)
C(2')-C(3')-C(3'')	120.2(2)
C(4')-C(3')-C(3'')	121.2(2)
C(5')-C(4')-C(3')	118.6(2)
C(5')-C(4')-C(4'')	120.3(2)
C(3')-C(4')-C(4'')	121.1(2)
C(6')-C(5')-C(4')	122.1(2)
C(5')-C(6')-C(1')	120.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ts003.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

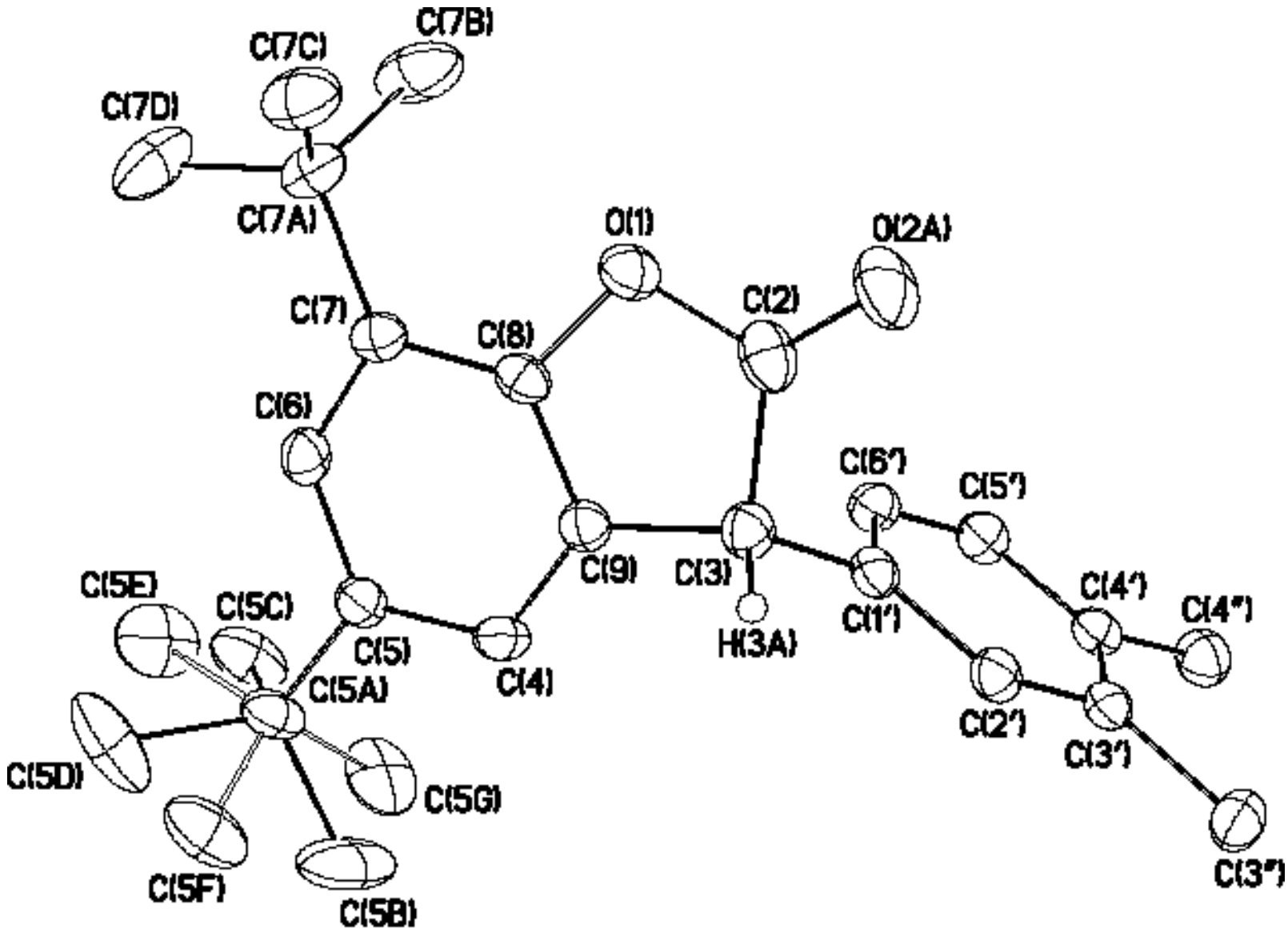
	U11	U22	U33	U23	U13	U12
O(1)	42(1)	50(1)	32(1)	-5(1)	6(1)	-2(1)
C(2)	47(2)	59(2)	35(2)	5(1)	13(1)	12(1)
C(3)	42(2)	37(1)	36(2)	2(1)	15(1)	1(1)
C(4)	42(1)	30(1)	37(2)	-4(1)	9(1)	-7(1)
C(5)	48(2)	32(1)	33(2)	-1(1)	15(1)	-2(1)
C(6)	47(2)	37(1)	39(2)	5(1)	21(1)	0(1)
C(7)	33(1)	29(1)	40(2)	0(1)	8(1)	1(1)
C(8)	35(1)	34(1)	28(2)	-3(1)	5(1)	4(1)
C(9)	39(1)	30(1)	35(2)	0(1)	14(1)	0(1)
O(2A)	61(1)	103(2)	30(1)	0(1)	11(1)	3(1)
C(5A)	76(2)	38(2)	31(2)	-4(1)	14(2)	-9(1)
C(5B)	178(8)	89(5)	41(3)	-19(3)	15(4)	-72(6)
C(5C)	103(5)	49(3)	39(3)	0(2)	8(3)	10(3)
C(5D)	156(7)	86(5)	46(3)	6(3)	43(4)	57(4)
C(5E)	155(18)	94(12)	35(7)	12(7)	32(11)	-33(13)

C(5F)	115(15)	63(9)	38(7)	-7(6)	13(8)	11(8)
C(5G)	60(8)	135(16)	32(7)	-18(7)	-11(5)	9(8)
C(7A)	35(2)	40(2)	61(2)	0(1)	10(1)	-6(1)
C(7B)	61(2)	37(2)	132(3)	-16(2)	20(2)	-7(1)
C(7C)	40(2)	57(2)	72(2)	-6(2)	4(2)	-3(1)
C(7D)	59(2)	84(2)	91(3)	18(2)	22(2)	-28(2)
C(1')	44(2)	38(1)	26(1)	-2(1)	13(1)	-3(1)
C(2')	50(2)	32(1)	32(2)	2(1)	17(1)	1(1)
C(3')	47(2)	37(1)	27(2)	-3(1)	12(1)	-7(1)
C(4')	43(2)	38(1)	28(1)	-5(1)	8(1)	-1(1)
C(5')	48(2)	35(1)	37(2)	2(1)	13(1)	3(1)
C(6')	50(2)	33(1)	35(2)	2(1)	14(1)	-6(1)
C(3'')	60(2)	45(2)	60(2)	2(1)	32(2)	-6(1)
C(4'')	48(2)	57(2)	50(2)	-5(1)	17(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ts003.

	x	y	z	U(eq)
H(3A)	2664	6117	1476	45
H(4A)	3428	5705	3640	45
H(6A)	1307	3557	4198	47
H(5BA)	4256	5611	5236	160
H(5BB)	3886	6169	6085	160
H(5BC)	3441	6694	5009	160
H(5CA)	3697	3515	5651	101
H(5CB)	2548	3324	5616	101
H(5CC)	3294	4124	6461	101
H(5DA)	1720	6411	5087	141
H(5DB)	2153	5862	6157	141
H(5DC)	1344	5100	5331	141
H(5EA)	1707	4126	5658	141
H(5EB)	2746	4302	6513	141
H(5EC)	2646	3246	5725	141
H(5FA)	1866	6345	5138	112
H(5FB)	2923	6792	5039	112
H(5FC)	2851	6372	6069	112
H(5GA)	4369	5326	5207	122

H(5GB)	4184	3922	5423	122
H(5GC)	4309	4936	6247	122
H(7BA)	65	895	1813	118
H(7BB)	1171	1087	2564	118
H(7BC)	890	1672	1505	118
H(7CA)	-1152	2661	1365	89
H(7CB)	-330	3421	1041	89
H(7CC)	-811	3992	1810	89
H(7DA)	-740	1744	2974	118
H(7DB)	-403	3051	3469	118
H(7DC)	352	1908	3755	118
H(2'A)	4180	6553	1116	45
H(5'A)	5512	2687	2100	48
H(6'A)	3902	3172	2151	47
H(3"A)	5638	7220	805	78
H(3"B)	6200	6166	406	78
H(3"C)	6662	6637	1496	78
H(4"A)	7028	3131	1803	77
H(4"B)	7379	4528	2015	77
H(4"C)	6919	4058	924	77


C(7B)
C(7C)
C(7D)
C(7A)
O(1)
O(2A)
C(7)
C(8)
C(2)
C(6)
C(6')
C(5')
C(9)
C(3)
C(4')
C(4'')
C(5E)
C(5C)
C(5)
C(1')
H(3A)
C(4)
C(5A)
C(2')
C(3')
C(5D)
C(5G)
C(5F)
C(5B)
C(3'')