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APPENDICES

APPENDICES A

Table A1 Crystallographic data and structure refinement for **D3**

Empirical formula	$C_{16}H_{14}O_4$
Formula weight	270.27
Temperature	293 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P2_1$
Unit cell dimensions	a = 6.6289(3) A alpha = 90 deg b = 8.7963(4) A beta = 99.4820(10) deg c = 11.3150(5) A gamma = 90 deg
Volume	650.76(5) $A^{\circ 3}$
Z, Calculated density	2,1.379 Mg/m^3
Absorption coefficient	0.099 mm^{-1}
F(000)	284
Theta range for data collection	1.82 to 30.41 deg
Limiting indices	-7<h<9, -12<k<12, -15<l<13
Reflections collected / unique	4783 / 3198 [R(int) = 0.0132]
Completeness to theta = 30.41	93.1%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3198/1/237
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0860
R indices (all data)	R1 = 0.0376, wR2 = 0.0885
Absolute structure parameter	1.9(8)
Largest diff. peak and hole	0.146 and -0.193 $e.A^{-3}$

Table A2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **D3**

	x	y	z	U (eq)
C(11b)	-1513(2)	6036(1)	3794(1)	35(1)
C(10a)	-453(2)	5697(2)	6632(1)	34(1)
C(6a)	-2800(2)	7369(2)	5516(1)	37(1)
C(6b)	-2448(2)	6233(2)	6527(1)	34(1)
C(4)	-3958(2)	4425(2)	2518(1)	40(1)
C(11a)	-958(2)	7039(2)	4876(1)	37(1)
C(7)	-3663(2)	5729(2)	7337(1)	40(1)
C(10)	419(2)	4712(2)	7533(1)	38(1)
C(1)	-56(2)	5610(2)	3090(1)	42(1)
C(4a)	-3482(2)	5431(2)	3473(1)	35(1)
C(8)	-2855(2)	4724(2)	8237(1)	43(1)
C(3)	-2454(2)	4001(2)	1866(1)	42(1)
C(2)	-495(2)	4609(2)	2149(1)	46(1)
C(9)	-829(2)	4247(2)	8342(1)	39(1)
C(6)	-4819(2)	7233(2)	4681(1)	43(1)
C(12)	1999(3)	2973(3)	9556(2)	58(1)
O(1)	-5041(1)	5787(1)	4083(1)	44(1)
O(2)	577(1)	6240(1)	5765(1)	40(1)
O(3)	-150(2)	3273(1)	9285(1)	52(1)
O(4)	-2994(2)	2988(2)	945(1)	55(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

Table A3 Bond distances of **D3**

	Distance (A°)		**Distance (A°)**
C(11b)-C(1)	1.4006(19)	C(11a)-O(2)	1.4851(16)
C(11b)-C(4a)	1.4007(16)	C(7)-C(8)	1.388(2)
C(11b)-C(11a)	1.5048(18)	C(10)-C(9)	1.3928(19)
C(10a)-O(2)	1.3701(15)	C(1)-C(2)	1.375(2)
C(10a)-C(10)	1.3894(19)	C(4a)-O(1)	1.3704(16)
C(10a)-C(6b)	1.3902(17)	C(8)-C(9)	1.393(2)
C(6a)-C(6b)	1.5076(19)	C(3)-O(4)	1.3730(18)
C(6a)-C(6)	1.511(2)	C(3)-C(2)	1.392(2)
C(6a)-C(11a)	1.5465(19)	C(9)-O(3)	1.3841(17)
C(6b)-C(7)	1.3885(19)	C(6)-O(1)	1.4369(19)
C(4)-C(3)	1.386(2)	C(12)-O(3)	1.431(2)
C(4)-C(4a)	1.392(2)		

Table A4 Bond angles of **D3**

	Angle (deg)		**Angle (deg)**
C(1)-C(11b)-C(4a)	116.81(12)	C(10a)-C(10)-C(9)	116.42(12)
C(1)-C(11b)-C(11a)	121.37(11)	C(2)-C(1)-C(11b)	122.28(13)
C(4a)-C(11b)-C(11a)	121.77(11)	O(1)-C(4a)-C(4)	116.25(11)
O(2)-C(10a)-C(10)	123.11(11)	O(1)-C(4a)-C(11b)	122.05(12)
O(2)-C(10a)-C(6b)	113.56(11)	C(4)-C(4a)-C(11b)	121.70(12)
C(10)-C(10a)-C(6b)	123.33(12)	C(7)-C(8)-C(9)	120.31(13)
C(6b)-C(6a)-C(6)	115.64(12)	O(4)-C(3)-C(4)	117.32(13)
C(6b)-C(6a)-C(11a)	101.28(10)	O(4)-C(3)-C(2)	122.70(14)
C(6)-C(6a)-C(11a)	112.26(12)	C(4)-C(3)-C(2)	119.98(13)
C(7)-C(6b)-C(10a)	118.81(12)	C(1)-C(2)-C(3)	119.62(14)
C(7)-C(6B)-C(6A)	132.69(12)	O(3)-C(9)-C(10)	122.36(13)
C(10a)-C(6b)-C(6a)	108.43(11)	O(3)-C(9)-C(8)	116.04(13)
C(3)-C(4)-C(4a)	119.57(12)	C(10)-C(9)-C(8)	121.60(13)
O(2)-C(11a)-C(11b)	108.77(11)	O(1)-C(6)-C(6a)	112.11(12)
O(2)-C(11a)-C(6a)	106.09(11)	C(4a)-O(1)-C(6)	114.32(11)
C(11b)-C(11a)-C(6a)	112.61(10)	C(10a)-O(2)-C(11a)	106.47(10)
C(8)-C(7)-C(6b)	119.49(12)	C(9)-O(3)-C(12)	117.71(13)

APPENDICES B

Table B1 Radical scavenging effect on DPPH radical

Sample	Concentration (mM)	% radical scavenging
D4	0.0625	9.93
	0.125	15.60
	0.25	28.98
	0.5	68.35
	1	51.09
D5	0.0625	9.19
	0.125	23.67
	0.25	48.80
	0.5	64.90
	1	73.72
D7	0.0625	-1.11
	0.125	7.73
	0.25	28.60
	0.5	54.02
	1	71.65
D8	0.0625	2.75
	0.125	15.65
	0.25	34.69
	0.5	55.95
	1	57.35
BHA	0.0625	25.51
	0.125	57.71
	0.25	73.69
	0.5	87.12
	1	90.59

VITA

Miss Sujittra Deesamer was born on January 3, 1976 in Angthong Province, Thailand. She received a Bachelor and Master Degree of Science in Chemistry from Chulalongkorn University in 1998 and 2001. Since then, she has been a graduate student studying Organic Chemistry as her major course at Chulalongkorn University. During her studies towards the Doctor Philosophy's Degree, she was awarded a teaching assistant scholarship by the Faculty of Science during 2001-2002 and was supported by the Thailand Research Fund for the 2002 Royal Golden Jubilee Ph.D.

Her present address is 66/4 Tesabal 7 Road, Amphur Maung, Angthong 14000, Tel. 06-9896689.