Table 1. Crystal data and structure refinement for dd39ys.

Identification code	dd39ys	
Empirical formula	C40 H28 Br2 O2	
Formula weight	700.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.54060(10) Å	α= 90°.
	b = 15.6871(3) Å	β= 95.8868(7)°.
	c = 14.5668(3) Å	γ = 90°.
Volume	1486.72(5) $Å^3$	
Z	2	
Density (calculated)	1.565 Mg/m^3	
Absorption coefficient	2.763 mm^{-1}	
F(000)	708	
Crystal size	0.105 x 0.067 x 0.044 mm^3	
Theta range for data collection	2.597 to 26.373°.	
Index ranges	-8<=h<=8, -19<=k<=19, -18<=l<=18	
Reflections collected	19489	
Independent reflections	3044 [R(int) = 0.0284]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	07454 and 0.6904	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3044 / 0 / 202	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0544	
R indices (all data)	R1 = 0.0240, wR2 = 0.0558	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.410 and -0.254 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for dd39ys. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	6472(1)	5740(1)	3083(1)	16(1)
O(1)	1010(2)	7376(1)	4873(1)	24(1)
C(1)	457(3)	6651(1)	5024(1)	14(1)
C(2)	1569(3)	5913(1)	4661(1)	12(1)
C(3)	3290(3)	6097(1)	4185(1)	13(1)
C(4)	4279(3)	5453(1)	3786(1)	12(1)
C(5)	3658(3)	4586(1)	3856(1)	12(1)
C(6)	4667(3)	3904(1)	3456(1)	16(1)
C(7)	4015(3)	3080(1)	3547(1)	18(1)
C(8)	2321(3)	2877(1)	4033(1)	14(1)
C(9)	1308(3)	3536(1)	4444(1)	13(1)
C(10)	1953(3)	4401(1)	4356(1)	11(1)
C(11)	896(2)	5084(1)	4756(1)	11(1)
C(12)	1685(3)	1957(1)	4004(1)	14(1)
C(13)	177(3)	1690(1)	3313(1)	16(1)
C(14)	-249(3)	823(1)	3219(1)	17(1)
C(15)	793(3)	216(1)	3782(1)	17(1)
C(16)	2240(3)	497(1)	4483(1)	18(1)
C(17)	2702(3)	1361(1)	4609(1)	16(1)
C(18)	-951(3)	2318(1)	2666(1)	22(1)
C(19)	427(3)	-723(1)	3612(2)	24(1)
C(20)	4239(3)	1649(1)	5396(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for dd39ys.

Br(1)-C(4)	1.8993(17)
O(1)-C(1)	1.219(2)
C(1)-C(9)#1	1.484(2)
C(1)-C(2)	1.493(2)
C(2)-C(11)	1.384(2)
C(2)-C(3)	1.411(2)
C(3)-C(4)	1.361(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.427(2)
C(5)-C(6)	1.413(2)
C(5)-C(10)	1.423(2)
C(6)-C(7)	1.372(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.411(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.395(2)
C(8)-C(12)	1.502(2)
C(9)-C(10)	1.431(2)
C(9)-C(1)#1	1.484(2)
C(10)-C(11)	1.431(2)
C(11)-C(11)#1	1.457(3)
C(12)-C(13)	1.399(3)
C(12)-C(17)	1.403(2)
C(13)-C(14)	1.393(2)
C(13)-C(18)	1.504(2)
C(14)-C(15)	1.388(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.391(3)
C(15)-C(19)	1.509(2)
C(16)-C(17)	1.398(2)
C(16)-H(16)	0.9500
C(17)-C(20)	1.514(3)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800

C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

O(1)-C(1)-C(9)#1	122.64(16)
O(1)-C(1)-C(2)	119.64(16)
C(9)#1-C(1)-C(2)	117.72(14)
C(11)-C(2)-C(3)	121.23(15)
C(11)-C(2)-C(1)	121.47(15)
C(3)-C(2)-C(1)	117.25(15)
C(4)-C(3)-C(2)	119.77(16)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	121.70(16)
C(3)-C(4)-Br(1)	118.20(13)
C(5)-C(4)-Br(1)	120.05(13)
C(6)-C(5)-C(10)	118.76(15)
C(6)-C(5)-C(4)	122.90(16)
C(10)-C(5)-C(4)	118.34(15)
C(7)-C(6)-C(5)	120.63(16)
C(7)-C(6)-H(6)	119.7
C(5)-C(6)-H(6)	119.7
C(6)-C(7)-C(8)	121.97(16)
C(6)-C(7)-H(7)	119.0
C(8)-C(7)-H(7)	119.0
C(9)-C(8)-C(7)	118.68(16)
C(9)-C(8)-C(12)	125.52(16)
C(7)-C(8)-C(12)	115.67(15)
C(8)-C(9)-C(10)	120.44(16)
C(8)-C(9)-C(1)#1	120.47(15)
C(10)-C(9)-C(1)#1	119.09(15)
C(5)-C(10)-C(9)	119.51(15)

C(5)-C(10)-C(11)	119.48(15)
C(9)-C(10)-C(11)	121.01(15)
C(2)-C(11)-C(10)	119.44(15)
C(2)-C(11)-C(11)#1	119.95(18)
C(10)-C(11)-C(11)#1	120.60(18)
C(13)-C(12)-C(17)	120.43(16)
C(13)-C(12)-C(8)	118.67(16)
C(17)-C(12)-C(8)	120.68(16)
C(14)-C(13)-C(12)	118.78(17)
C(14)-C(13)-C(18)	119.87(16)
C(12)-C(13)-C(18)	121.34(16)
C(15)-C(14)-C(13)	122.03(17)
C(15)-C(14)-H(14)	119.0
C(13)-C(14)-H(14)	119.0
C(14)-C(15)-C(16)	118.23(16)
C(14)-C(15)-C(19)	120.83(17)
C(16)-C(15)-C(19)	120.90(17)
C(15)-C(16)-C(17)	121.67(17)
C(15)-C(16)-H(16)	119.2
C(17)-C(16)-H(16)	119.2
C(16)-C(17)-C(12)	118.77(16)
C(16)-C(17)-C(20)	120.45(16)
C(12)-C(17)-C(20)	120.78(15)
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-H(19A)	109.5
C(15)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(15)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5

C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for dd39ys. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	14(1)	16(1)	18(1)	1(1)	7(1)	-2(1)
O(1)	29(1)	10(1)	38(1)	0(1)	20(1)	-2(1)
C(1)	16(1)	11(1)	15(1)	0(1)	3(1)	0(1)
C(2)	11(1)	12(1)	12(1)	0(1)	1(1)	0(1)
C(3)	13(1)	11(1)	14(1)	2(1)	1(1)	-2(1)
C(4)	10(1)	15(1)	12(1)	2(1)	3(1)	-2(1)
C(5)	12(1)	12(1)	12(1)	0(1)	1(1)	0(1)
C(6)	15(1)	17(1)	19(1)	-1(1)	8(1)	-1(1)
C(7)	19(1)	13(1)	23(1)	-4(1)	9(1)	2(1)
C(8)	15(1)	12(1)	16(1)	0(1)	2(1)	0(1)
C(9)	13(1)	12(1)	14(1)	0(1)	3(1)	0(1)
C(10)	11(1)	12(1)	12(1)	0(1)	2(1)	0(1)
C(11)	11(1)	11(1)	10(1)	1(1)	1(1)	1(1)
C(12)	15(1)	10(1)	19(1)	-3(1)	7(1)	1(1)
C(13)	17(1)	14(1)	18(1)	-2(1)	7(1)	2(1)
C(14)	17(1)	17(1)	18(1)	-4(1)	4(1)	-2(1)
C(15)	20(1)	12(1)	22(1)	-2(1)	10(1)	-2(1)
C(16)	18(1)	13(1)	22(1)	2(1)	5(1)	2(1)
C(17)	14(1)	14(1)	20(1)	-2(1)	4(1)	0(1)
C(18)	27(1)	16(1)	23(1)	-2(1)	-2(1)	4(1)
C(19)	30(1)	12(1)	29(1)	-5(1)	7(1)	-3(1)
C(20)	22(1)	16(1)	29(1)	0(1)	-2(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for dd39ys.

	x	y	z	U(eq)
H(3)	3757	6667	4143	15
H(6)	5809	4018	3121	20
H(7)	4724	2633	3274	21
H(14)	-1286	640	2756	21
H(16)	2932	90	4886	21
H(18A)	-1314	2821	3013	33
H(18B)	-2206	2053	2369	33
H(18C)	-69	2489	2193	33
H(19A)	1426	-941	3213	35
H(19B)	-968	-809	3312	35
H(19C)	584	-1028	4202	35
H(20A)	5455	1886	5147	34
H(20B)	4646	1161	5793	34
H(20C)	3612	2087	5757	34

Table 6. Torsion angles [°] for dd39ys.

O(1)-C(1)-C(2)-C(11)	-174.96(17)
C(9)#1-C(1)-C(2)-C(11)	4.7(2)
O(1)-C(1)-C(2)-C(3)	2.6(3)
C(9)#1-C(1)-C(2)-C(3)	-177.80(15)
C(11)-C(2)-C(3)-C(4)	1.9(3)
C(1)-C(2)-C(3)-C(4)	-175.59(16)
C(2)-C(3)-C(4)-C(5)	-1.8(3)
C(2)-C(3)-C(4)-Br(1)	175.90(12)
C(3)-C(4)-C(5)-C(6)	-179.40(17)
Br(1)-C(4)-C(5)-C(6)	3.0(2)
C(3)-C(4)-C(5)-C(10)	0.2(3)
Br(1)-C(4)-C(5)-C(10)	-177.40(12)
C(10)-C(5)-C(6)-C(7)	0.1(3)
C(4)-C(5)-C(6)-C(7)	179.72(17)
C(5)-C(6)-C(7)-C(8)	0.4(3)
C(6)-C(7)-C(8)-C(9)	-1.1(3)
C(6)-C(7)-C(8)-C(12)	175.07(17)
C(7)-C(8)-C(9)-C(10)	1.3(3)
C(12)-C(8)-C(9)-C(10)	-174.40(16)
C(7)-C(8)-C(9)-C(1)#1	-178.92(16)
C(12)-C(8)-C(9)-C(1)#1	5.4(3)
C(6)-C(5)-C(10)-C(9)	0.2(2)
C(4)-C(5)-C(10)-C(9)	-179.47(15)
C(6)-C(5)-C(10)-C(11)	-179.18(15)
C(4)-C(5)-C(10)-C(11)	1.2(2)
C(8)-C(9)-C(10)-C(5)	-0.9(2)
C(1)#1-C(9)-C(10)-C(5)	179.33(15)
C(8)-C(9)-C(10)-C(11)	178.45(16)
C(1)#1-C(9)-C(10)-C(11)	-1.3(2)
C(3)-C(2)-C(11)-C(10)	-0.5(2)
C(1)-C(2)-C(11)-C(10)	176.90(15)
C(3)-C(2)-C(11)-C(11)#1	-179.49(18)
C(1)-C(2)-C(11)-C(11)#1	-2.1(3)
C(5)-C(10)-C(11)-C(2)	-1.0(2)

C(9)-C(10)-C(11)-C(2)	179.63(15)
C(5)-C(10)-C(11)-C(11)#1	177.93(18)
C(9)-C(10)-C(11)-C(11)#1	-1.4(3)
C(9)-C(8)-C(12)-C(13)	83.6(2)
C(7)-C(8)-C(12)-C(13)	-92.2(2)
C(9)-C(8)-C(12)-C(17)	-101.7(2)
C(7)-C(8)-C(12)-C(17)	82.5(2)
C(17)-C(12)-C(13)-C(14)	-1.9(3)
C(8)-C(12)-C(13)-C(14)	172.78(16)
C(17)-C(12)-C(13)-C(18)	179.19(17)
C(8)-C(12)-C(13)-C(18)	-6.2(3)
C(12)-C(13)-C(14)-C(15)	-0.9(3)
C(18)-C(13)-C(14)-C(15)	178.05(17)
C(13)-C(14)-C(15)-C(16)	2.9(3)
C(13)-C(14)-C(15)-C(19)	-174.73(18)
C(14)-C(15)-C(16)-C(17)	-2.1(3)
C(19)-C(15)-C(16)-C(17)	175.47(18)
C(15)-C(16)-C(17)-C(12)	-0.5(3)
C(15)-C(16)-C(17)-C(20)	178.20(17)
C(13)-C(12)-C(17)-C(16)	2.6(3)
C(8)-C(12)-C(17)-C(16)	-171.98(16)
C(13)-C(12)-C(17)-C(20)	-176.16(17)
C(8)-C(12)-C(17)-C(20)	9.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1