

Table 1. Crystal data and structure refinement for lec02.

Identification code	lec02	
Empirical formula	C <sub>33</sub> H <sub>32</sub> O <sub>2</sub>	
Formula weight	460.59	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	
Unit cell dimensions	a = 7.4211(4) Å	α = 90°.
	b = 14.9140(9) Å	β = 90°.
	c = 22.0856(13) Å	γ = 90°.
Volume	2444.4(2) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.252 g/cm <sup>3</sup>	
Absorption coefficient	0.76 cm <sup>-1</sup>	
F(000)	984	
Crystal size	0.40 x 0.20 x 0.20 mm <sup>3</sup>	
Theta range for data collection	2.29 to 28.26°.	
Index ranges	-9 <= h <= 9, -11 <= k <= 17, -28 <= l <= 29	
Reflections collected	11334	
Independent reflections	5062 [R(int) = 0.0341]	
Completeness to theta = 28.26°	88.4 %	
Absorption correction	Empirical from SADABS	
Max. and min. transmission	0.9850 and 0.9702	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5062 / 0 / 320	
Goodness-of-fit on F <sup>2</sup>	1.163	
Final R indices [I > 2σ(I)]	R1 = 0.0512, wR2 = 0.1470	
R indices (all data)	R1 = 0.0602, wR2 = 0.1562	
Absolute structure parameter	-0.3(16)	
Largest diff. peak and hole	0.175 and -0.199 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for lec02.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^0$  tensor.

	x	y	z	$U(\text{eq})$
C(1)	12474(3)	5016(2)	995(1)	32(1)
C(2)	11427(3)	5799(2)	994(1)	29(1)
C(3)	11199(3)	6234(2)	427(1)	34(1)
C(4)	12313(3)	5996(2)	-46(1)	43(1)
C(5)	13314(3)	5214(2)	-29(1)	47(1)
C(6)	13225(3)	4644(2)	469(1)	41(1)
C(7)	13504(4)	3640(2)	391(2)	64(1)
C(8)	12013(4)	3172(2)	7(2)	54(1)
C(9)	10325(3)	3728(2)	-47(1)	41(1)
C(10)	9236(3)	3894(2)	462(1)	40(1)
C(11)	8203(3)	4659(2)	497(1)	36(1)
C(12)	8199(3)	5291(2)	30(1)	39(1)
C(13)	8964(3)	5026(2)	-520(1)	44(1)
C(14)	10004(3)	4258(2)	-559(1)	45(1)
C(15)	7808(3)	6254(2)	182(1)	48(1)
C(16)	9580(4)	6816(2)	275(1)	44(1)
C(17)	14323(4)	4277(2)	1744(1)	53(1)
C(18)	9349(3)	5679(2)	1934(1)	29(1)
C(19)	10437(2)	6181(2)	1530(1)	28(1)
C(20)	10574(3)	7115(2)	1645(1)	32(1)
C(21)	9299(3)	7525(2)	2011(1)	40(1)
C(22)	8179(3)	7019(2)	2378(1)	39(1)
C(23)	8341(3)	6096(2)	2393(1)	33(1)
C(24)	7799(3)	5584(2)	2961(1)	40(1)
C(25)	9424(3)	5392(2)	3395(1)	43(1)
C(26)	11014(3)	5991(2)	3265(1)	36(1)
C(27)	12381(3)	5692(2)	2884(1)	36(1)
C(28)	13395(3)	6303(2)	2547(1)	39(1)
C(29)	13062(3)	7214(2)	2588(1)	45(1)
C(30)	11975(4)	7509(2)	3066(1)	49(1)
C(31)	10971(3)	6897(2)	3397(1)	46(1)

Table 3. Bond lengths [Å] and angles [°] for lec02.

C(1)-C(2)	1.403(3)	C(27)-C(28)	1.396(3)
C(1)-C(6)	1.404(3)	C(28)-C(29)	1.383(4)
C(1)-O(1)	1.406(3)	C(29)-C(30)	1.401(4)
C(2)-C(3)	1.420(3)	C(29)-C(32)	1.513(4)
C(2)-C(19)	1.506(3)	C(30)-C(31)	1.387(4)
C(3)-C(4)	1.379(3)	C(32)-C(33)	1.586(4)
C(3)-C(16)	1.520(3)		
C(4)-C(5)	1.384(4)	C(2)-C(1)-C(6)	123.2(2)
C(5)-C(6)	1.390(4)	C(2)-C(1)-O(1)	117.44(18)
C(6)-C(7)	1.520(4)	C(6)-C(1)-O(1)	118.8(2)
C(7)-C(8)	1.559(4)	C(1)-C(2)-C(3)	116.67(19)
C(8)-C(9)	1.507(4)	C(1)-C(2)-C(19)	125.73(19)
C(9)-C(14)	1.400(4)	C(3)-C(2)-C(19)	117.48(19)
C(9)-C(10)	1.407(3)	C(4)-C(3)-C(2)	118.6(2)
C(10)-C(11)	1.377(4)	C(4)-C(3)-C(16)	116.9(2)
C(11)-C(12)	1.397(3)	C(2)-C(3)-C(16)	123.44(19)
C(12)-C(13)	1.396(3)	C(3)-C(4)-C(5)	121.2(2)
C(12)-C(15)	1.503(4)	C(4)-C(5)-C(6)	120.8(2)
C(13)-C(14)	1.385(4)	C(5)-C(6)-C(1)	115.5(2)
C(15)-C(16)	1.573(4)	C(5)-C(6)-C(7)	120.4(3)
C(17)-O(1)	1.432(3)	C(1)-C(6)-C(7)	122.4(3)
C(18)-O(2)	1.367(3)	C(6)-C(7)-C(8)	113.9(2)
C(18)-C(23)	1.406(3)	C(9)-C(8)-C(7)	112.7(2)
C(18)-C(19)	1.418(3)	C(14)-C(9)-C(10)	116.7(2)
C(19)-C(20)	1.419(3)	C(14)-C(9)-C(8)	121.0(2)
C(20)-C(21)	1.388(3)	C(10)-C(9)-C(8)	120.7(2)
C(20)-C(33)	1.520(3)	C(11)-C(10)-C(9)	120.7(2)
C(21)-C(22)	1.384(4)	C(10)-C(11)-C(12)	121.2(2)
C(22)-C(23)	1.381(4)	C(13)-C(12)-C(11)	116.8(2)
C(23)-C(24)	1.522(3)	C(13)-C(12)-C(15)	122.9(2)
C(24)-C(25)	1.567(3)	C(11)-C(12)-C(15)	118.6(2)
C(25)-C(26)	1.508(3)	C(14)-C(13)-C(12)	121.0(2)
C(26)-C(31)	1.383(4)	C(13)-C(14)-C(9)	120.7(2)
C(26)-C(27)	1.392(3)	C(12)-C(15)-C(16)	112.2(2)

C(3)-C(16)-C(15)	112.6(2)	C(23)-C(24)-C(25)	113.12(18)
O(2)-C(18)-C(23)	115.24(19)	C(26)-C(25)-C(24)	112.1(2)
O(2)-C(18)-C(19)	123.11(19)	C(31)-C(26)-C(27)	117.2(2)
C(23)-C(18)-C(19)	121.5(2)	C(31)-C(26)-C(25)	121.4(2)
C(18)-C(19)-C(20)	116.54(19)	C(27)-C(26)-C(25)	119.7(2)
C(18)-C(19)-C(2)	125.0(2)	C(26)-C(27)-C(28)	120.4(2)
C(20)-C(19)-C(2)	118.50(18)	C(29)-C(28)-C(27)	120.6(2)
C(21)-C(20)-C(19)	119.2(2)	C(28)-C(29)-C(30)	117.5(3)
C(21)-C(20)-C(33)	117.9(2)	C(28)-C(29)-C(32)	120.7(3)
C(19)-C(20)-C(33)	121.7(2)	C(30)-C(29)-C(32)	120.3(3)
C(22)-C(21)-C(20)	120.7(2)	C(31)-C(30)-C(29)	120.0(3)
C(23)-C(22)-C(21)	120.4(2)	C(26)-C(31)-C(30)	121.3(2)
C(22)-C(23)-C(18)	118.0(2)	C(29)-C(32)-C(33)	112.9(2)
C(22)-C(23)-C(24)	119.8(2)	C(20)-C(33)-C(32)	112.2(2)
C(18)-C(23)-C(24)	120.8(2)	C(1)-O(1)-C(17)	116.65(19)

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for lec02. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	24(1)	34(1)	38(1)	0(1)	-1(1)	-2(1)
C(2)	25(1)	30(1)	31(1)	-2(1)	0(1)	-4(1)
C(3)	38(1)	32(1)	31(1)	3(1)	-2(1)	-9(1)
C(4)	41(1)	54(2)	34(1)	2(1)	2(1)	-16(1)
C(5)	28(1)	73(2)	40(1)	-16(1)	5(1)	-7(1)
C(6)	25(1)	48(2)	50(1)	-15(1)	-3(1)	3(1)
C(7)	52(2)	56(2)	84(2)	-33(2)	-19(2)	23(1)
C(8)	53(2)	43(2)	65(2)	-12(1)	-1(1)	5(1)
C(9)	38(1)	37(2)	47(1)	-10(1)	-2(1)	-6(1)
C(10)	42(1)	37(2)	40(1)	1(1)	-4(1)	-13(1)
C(11)	27(1)	45(2)	35(1)	-1(1)	0(1)	-9(1)
C(12)	26(1)	53(2)	39(1)	0(1)	-8(1)	-2(1)
C(13)	39(1)	65(2)	29(1)	1(1)	-10(1)	-7(1)
C(14)	39(1)	64(2)	32(1)	-13(1)	0(1)	-11(1)
C(15)	38(1)	55(2)	50(1)	7(1)	-5(1)	6(1)
C(16)	57(1)	39(2)	35(1)	5(1)	-9(1)	2(1)
C(17)	46(1)	56(2)	57(2)	6(1)	-4(1)	24(1)
C(18)	24(1)	31(1)	30(1)	1(1)	-6(1)	-3(1)
C(19)	23(1)	34(1)	28(1)	1(1)	-4(1)	1(1)
C(20)	30(1)	31(1)	34(1)	2(1)	-3(1)	0(1)
C(21)	39(1)	36(1)	45(1)	-4(1)	-2(1)	9(1)
C(22)	26(1)	52(2)	38(1)	-9(1)	-1(1)	7(1)
C(23)	24(1)	46(2)	31(1)	-1(1)	-2(1)	-2(1)
C(24)	31(1)	58(2)	30(1)	-3(1)	2(1)	-6(1)
C(25)	39(1)	55(2)	34(1)	6(1)	-1(1)	-2(1)
C(26)	31(1)	48(2)	29(1)	-1(1)	-5(1)	0(1)
C(27)	29(1)	43(2)	35(1)	0(1)	-7(1)	0(1)
C(28)	25(1)	54(2)	38(1)	-2(1)	-4(1)	-4(1)
C(29)	37(1)	46(2)	51(1)	-1(1)	-12(1)	-12(1)
C(30)	44(1)	45(2)	59(2)	-14(1)	-11(1)	-3(1)
C(31)	41(1)	55(2)	41(1)	-16(1)	-8(1)	0(1)

C(32)	49(2)	51(2)	66(2)	7(1)	-12(1)	-24(1)
C(33)	44(1)	32(2)	47(1)	-2(1)	4(1)	-7(1)
O(1)	32(1)	41(1)	52(1)	11(1)	0(1)	8(1)
O(2)	37(1)	34(1)	37(1)	2(1)	3(1)	-5(1)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for lec02.

	x	y	z	U(eq)
H(4A)	12395	6376	-390	51
H(5A)	14071	5065	-361	57
H(7A)	13542	3357	796	77
H(7B)	14686	3538	195	77
H(8A)	12491	3051	-404	64
H(8B)	11709	2590	195	64
H(10A)	9214	3474	785	48
H(11A)	7478	4759	845	43
H(13A)	8768	5379	-872	53
H(14A)	10504	4087	-938	54
H(15A)	7078	6278	557	57
H(15B)	7090	6524	-149	57
H(16A)	9837	7158	-100	52
H(16B)	9387	7253	605	52
H(17A)	14219	3935	2122	80
H(17B)	15039	4818	1816	80
H(17C)	14915	3907	1436	80
H(21A)	9193	8160	2011	48
H(22A)	7294	7307	2620	46
H(24A)	7246	5007	2840	48
H(24B)	6877	5934	3182	48
H(25A)	9032	5483	3819	51
H(25B)	9796	4758	3351	51
H(27A)	12626	5068	2852	43
H(28A)	14322	6091	2287	47
H(30A)	11925	8129	3164	59
H(31A)	10239	7104	3721	55
H(32A)	14764	7758	1949	66
H(32B)	13303	8460	2193	66
H(33A)	11911	8220	1301	49

H(33B)	12973	7302	1185	49
H(2A)	10290(50)	4510(20)	1800(14)	62(10)

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C(32)	13482(4)	7831(2)	2063(1)	55(1)
C(33)	12263(3)	7642(2)	1487(1)	41(1)
O(1)	12562(2)	4525(1)	1538(1)	42(1)
O(2)	9283(2)	4762(1)	1932(1)	36(1)

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