

Table 1. Crystal data and structure refinement for *d,l*-**24**.

Identification code	xrl080	
Empirical formula	C <sub>48</sub> H <sub>52</sub> O <sub>12</sub>	
Formula weight	820.90	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7968(16) Å	α = 74.601(15)°.
	b = 10.6351(18) Å	β = 85.273(15)°.
	c = 11.831(2) Å	γ = 74.752(15)°.
Volume	1029.4(3) Å <sup>3</sup>	
Z	1	
Density (calculated)	1.324 Mg/m <sup>3</sup>	
Absorption coefficient	0.095 mm <sup>-1</sup>	
F(000)	436	
Crystal size	0.3 x 0.4 x 0.4 mm <sup>3</sup>	
Theta range for data collection	4.11 to 22.49°.	
Index ranges	-9 ≤ h ≤ 9, -11 ≤ k ≤ 7, -12 ≤ l ≤ 12	
Reflections collected	5012	
Independent reflections	2648 [R(int) = 0.0367]	
Completeness to theta = 22.49°	97.8 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2648 / 0 / 285	
Goodness-of-fit on F <sup>2</sup>	1.223	
Final R indices [I > 2σ(I)]	R1 = 0.0912, wR2 = 0.2429	
R indices (all data)	R1 = 0.0933, wR2 = 0.2452	
Largest diff. peak and hole	0.543 and -0.349 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for *d,l*-**24**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
O(3)	5068(3)	3455(3)	2049(2)	34(1)
O(2)	6066(3)	5461(3)	2449(2)	33(1)
O(6)	-1461(3)	5301(3)	-4000(3)	40(1)
C(004)	4735(4)	5756(4)	1782(3)	29(1)
O(1)	4451(3)	8034(3)	1669(2)	35(1)
O(5)	-3275(4)	7564(3)	-5117(3)	42(1)
C(007)	3904(5)	7078(4)	1341(3)	29(1)
O(4)	-3063(4)	9987(3)	-4798(3)	45(1)
C(009)	-110(4)	7618(4)	-2686(3)	28(1)
C(010)	4241(4)	4716(4)	1518(3)	29(1)
C(011)	-1253(5)	6417(4)	-3725(3)	32(1)
C(012)	-213(5)	6409(4)	-2895(4)	34(1)
C(013)	-2202(5)	7644(4)	-4368(3)	33(1)
C(014)	2637(4)	7373(4)	610(3)	30(1)
C(015)	3007(4)	5018(4)	746(4)	31(1)
C(016)	3623(5)	9407(4)	1208(4)	38(1)
C(017)	-1026(5)	8820(4)	-3338(4)	32(1)
C(018)	1053(5)	7607(4)	-1783(4)	33(1)
C(019)	-1869(5)	7389(4)	549(4)	34(1)
C(020)	2213(4)	6347(4)	279(3)	29(1)
C(021)	-2078(5)	8832(4)	-4158(4)	34(1)
C(022)	-490(6)	4025(4)	-3412(4)	44(1)
C(023)	963(5)	8969(4)	-1675(4)	32(1)
C(024)	4604(5)	2354(4)	1805(4)	37(1)
C(025)	-667(5)	7100(4)	22(3)	29(1)
C(026)	851(5)	6651(4)	-552(3)	31(1)
C(027)	-3301(6)	8399(5)	-6272(4)	45(1)
C(028)	5704(5)	5176(4)	3682(4)	37(1)
C(029)	840(5)	10082(4)	-1597(4)	40(1)
C(030)	-2790(6)	11245(4)	-4773(4)	47(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for *d,l*-24.

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O(3)-C(010)	1.356(5)
O(3)-C(024)	1.439(5)
O(2)-C(004)	1.386(5)
O(2)-C(028)	1.435(5)
O(6)-C(011)	1.370(5)
O(6)-C(022)	1.429(5)
C(004)-C(007)	1.384(6)
C(004)-C(010)	1.403(6)
O(1)-C(007)	1.383(5)
O(1)-C(016)	1.430(5)
O(5)-C(013)	1.380(5)
O(5)-C(027)	1.417(5)
C(007)-C(014)	1.386(6)
O(4)-C(021)	1.373(5)
O(4)-C(030)	1.429(5)
C(009)-C(017)	1.385(6)
C(009)-C(012)	1.399(6)
C(009)-C(018)	1.535(6)
C(010)-C(015)	1.393(6)
C(011)-C(012)	1.394(6)
C(011)-C(013)	1.408(6)
C(013)-C(021)	1.383(6)
C(014)-C(020)	1.396(6)
C(015)-C(020)	1.386(5)
C(017)-C(021)	1.390(6)
C(018)-C(023)	1.469(6)
C(018)-C(026)	1.566(6)
C(019)-C(025)	1.193(6)
C(020)-C(026)	1.526(6)
C(023)-C(029)	1.188(6)
C(025)-C(026)	1.469(6)
C(010)-O(3)-C(024)	116.9(3)
C(004)-O(2)-C(028)	111.9(3)

C(011)-O(6)-C(022)	117.0(3)
O(2)-C(004)-C(007)	120.6(3)
O(2)-C(004)-C(010)	120.2(3)
C(007)-C(004)-C(010)	119.2(4)
C(007)-O(1)-C(016)	116.1(3)
C(013)-O(5)-C(027)	116.3(3)
O(1)-C(007)-C(004)	115.3(3)
O(1)-C(007)-C(014)	124.4(3)
C(004)-C(007)-C(014)	120.3(3)
C(021)-O(4)-C(030)	117.6(3)
C(017)-C(009)-C(012)	118.9(4)
C(017)-C(009)-C(018)	120.8(3)
C(012)-C(009)-C(018)	120.2(3)
O(3)-C(010)-C(015)	124.9(3)
O(3)-C(010)-C(004)	114.8(3)
C(015)-C(010)-C(004)	120.2(3)
O(6)-C(011)-C(012)	125.5(4)
O(6)-C(011)-C(013)	114.2(4)
C(012)-C(011)-C(013)	120.3(4)
C(011)-C(012)-C(009)	120.3(4)
O(5)-C(013)-C(021)	124.4(4)
O(5)-C(013)-C(011)	116.7(3)
C(021)-C(013)-C(011)	118.7(4)
C(007)-C(014)-C(020)	120.5(4)
C(020)-C(015)-C(010)	120.0(3)
C(009)-C(017)-C(021)	120.9(4)
C(023)-C(018)-C(009)	111.9(3)
C(023)-C(018)-C(026)	110.5(3)
C(009)-C(018)-C(026)	112.7(3)
C(015)-C(020)-C(014)	119.4(3)
C(015)-C(020)-C(026)	119.0(3)
C(014)-C(020)-C(026)	121.5(3)
O(4)-C(021)-C(013)	115.5(4)
O(4)-C(021)-C(017)	123.7(4)
C(013)-C(021)-C(017)	120.8(4)
C(029)-C(023)-C(018)	177.9(4)

C(019)-C(025)-C(026)	175.6(4)
C(025)-C(026)-C(020)	110.9(3)
C(025)-C(026)-C(018)	113.2(3)
C(020)-C(026)-C(018)	114.2(3)

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for *d,l*-**24**. 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 <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(3)	32(2)	29(2)	45(2)	-14(1)	-7(1)	-6(1)
O(2)	27(2)	40(2)	34(2)	-10(1)	-7(1)	-8(1)
O(6)	44(2)	36(2)	45(2)	-16(1)	-10(1)	-8(1)
C(004)	24(2)	36(2)	28(2)	-11(2)	-1(2)	-9(2)
O(1)	34(2)	32(2)	41(2)	-11(1)	-8(1)	-9(1)
O(5)	45(2)	46(2)	40(2)	-12(1)	-14(1)	-12(1)
C(007)	28(2)	34(2)	29(2)	-15(2)	1(2)	-11(2)
O(4)	49(2)	36(2)	49(2)	-14(1)	-17(2)	0(1)
C(009)	22(2)	36(2)	27(2)	-9(2)	-1(2)	-7(2)
C(010)	25(2)	29(2)	31(2)	-8(2)	1(2)	-7(2)
C(011)	34(2)	33(2)	32(2)	-15(2)	3(2)	-10(2)
C(012)	31(2)	34(2)	35(2)	-10(2)	-6(2)	-1(2)
C(013)	35(2)	35(2)	30(2)	-11(2)	-5(2)	-3(2)
C(014)	24(2)	30(2)	34(2)	-8(2)	-4(2)	-6(2)
C(015)	27(2)	32(2)	38(2)	-15(2)	-6(2)	-6(2)
C(016)	36(2)	32(2)	52(3)	-19(2)	-6(2)	-7(2)
C(017)	28(2)	36(2)	35(2)	-18(2)	5(2)	-7(2)
C(018)	33(2)	31(2)	35(2)	-10(2)	0(2)	-7(2)
C(019)	36(3)	30(2)	40(2)	-13(2)	-3(2)	-11(2)
C(020)	24(2)	40(2)	26(2)	-14(2)	0(2)	-5(2)
C(021)	34(2)	34(2)	33(2)	-12(2)	-6(2)	0(2)
C(022)	47(3)	32(2)	52(3)	-13(2)	-7(2)	-5(2)
C(023)	26(2)	37(3)	35(2)	-10(2)	-5(2)	-8(2)
C(024)	36(2)	27(2)	47(3)	-11(2)	-1(2)	-7(2)
C(025)	29(2)	33(2)	30(2)	-13(2)	-4(2)	-10(2)
C(026)	32(2)	27(2)	37(2)	-15(2)	-1(2)	-7(2)
C(027)	53(3)	46(3)	35(2)	-6(2)	-10(2)	-13(2)
C(028)	36(2)	41(2)	35(2)	-10(2)	-3(2)	-10(2)
C(029)	44(3)	33(3)	45(3)	-7(2)	-10(2)	-14(2)
C(030)	53(3)	31(2)	51(3)	-12(2)	-6(2)	0(2)