Polycyclic Aromatic Compounds via Radical Cyclizations of Benzannulated Enyne–Allenenes
Derived from Ireland–Claisen Rearrangement

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All reactions were conducted in oven-dried (120 °C) glassware under a nitrogen atmosphere. Diethyl ether (Et₂O) and tetrahydrofuran (THF) were distilled from benzophenone ketyl prior to use. Methylene chloride was distilled from CaH₂ prior to use. *n*-Butyllithium (2.5 M) in hexanes, 9-fluorenone (**8**), acetic anhydride, diisopropylamine, *tert*-butyldimethylsilyl chloride (1.0 M) in THF, hexamethylphosphoramide (HMPA), thionyl chloride, anhydrous aluminum chloride, benzophenone (**20**), 2,2-dimethylpropiophenone (**31**), 1-indanone, 1-tetralone, iodomethane, Pd(PPh₃)₂Cl₂, copper(I) iodide, triethylamine, phenylacetylene, (trimethylsilyl)acetylene, 1-bromo-2-iodobenzene, and 4*H*-cyclopenta[*def*]phenanthrene¹⁰ were purchased from chemical suppliers and were used as received. 1-(2-Ethynylphenyl)-2-phenylethyne for **9** was prepared as described previously.⁶ 4*H*-Cyclopenta[*def*]phenanthren-4-one (**18**)⁹ and 8,9-dihydrocyclopenta[*def*]phenanthren-4-one (**19**)¹² were prepared from 4*H*-cyclopenta[*def*]phenanthrene as reported previously. 1-Oxo-2,2-dimethyl-1,2,3,4-tetrahydronaphthalene (**37**)¹⁶ and 2,2-dimethyl-1-indanone (**38**)¹⁷ were prepared from 1-tetralone and 1-indanone, respectively, according to the reported procedures. Melting points were uncorrected. ¹H (270 MHz) and ¹³C (67.9 MHz) NMR spectra were recorded in CDCl₃ using CHCl₃ (¹H δ 7.26) and CDCl₃ (¹³C δ 77.00) as internal standards.

Propargylic Acetate 21. The same procedure was repeated as described for **10** except that 0.08 g (0.39 mmol) of **18** was treated with **9**, prepared from 0.140 g (0.69 mmol) of 1-(2-ethynylphenyl)-2-phenylethyne and 0.25 mL of a 2.5 M solution of *n*-butyllithium (0.63 mmol) in hexanes at 0 °C, followed by 0.064 g (0.63 mmol) of acetic anhydride to afford 0.143 g of **21** (0.32 mmol, 81%) as a light brown solid; mp 143–145 °C; IR 2214, 1749, 1226, 756 cm⁻¹; ¹H δ 8.07–8.03 (2 H, m), 7.87–7.82 (4 H, m), 7.60–7.47 (4 H, m), 7.35–7.20 (7 H, m), 2.08 (3 H, s);

^{13}C δ 169.4, 143.2, 135.7, 132.5, 131.7, 131.6, 128.5, 128.4, 128.2, 128.1, 127.9, 127.8, 126.0, 125.8, 125.4, 124.7, 123.3, 123.0, 93.2, 89.1, 87.8, 84.7, 81.1, 21.6.

Carboxylic Acid 24. The same procedure was repeated as described for **16** except that 0.143 g (0.32 mmol) of **21** was treated with LDA, prepared from 0.26 mL of a 2.5 M solution of *n*-butyllithium (0.65 mmol) in hexanes and 0.09 mL (0.65 mmol) of diisopropylamine, followed by 0.34 mL of HMPA and 0.65 mL of a 1.0 M solution of TBDMSCl (0.65 mmol) in THF.

Hydrolysis with a mixture of 2.3 mL of acetic acid and 0.8 mL water provided 0.10 g of **24** (0.22 mmol, 70%) as yellow crystals: mp 228–231 °C; IR 3500–2600 (br), 1703, 827, 750, 704 cm^{-1} ;

^1H δ 8.25 (1 H, d, J = 6.9 Hz), 8.01 (1 H, d, J = 8.4 Hz), 7.97 (1 H, t, J = 8.2 Hz), 7.86 (1 H, d, J = 8.7 Hz), 7.80 (1 H, t, J = 7.5 Hz), 7.73 (1 H, d, J = 7.7 Hz), 7.67–7.52 (7 H, m), 7.30 (1 H, t, J = 7.9 Hz), 7.12 (1 H, t, J = 7.5 Hz), 6.77 (1 H, d, J = 7.9 Hz), 5.14 (1 H, dd, J = 10.9, 2.6 Hz), 3.94 (1 H, dd, J = 16.4, 2.6 Hz), 2.79 (1 H, dd, J = 16.4, 10.5 Hz); ^{13}C δ 177.3, 146.7, 144.6, 141.1, 138.9, 137.8, 135.9, 135.2, 133.9, 132.7, 132.5, 131.3, 130.0, 128.9, 128.8, 128.3, 128.1, 127.9, 127.5, 127.4, 126.8, 126.7, 126.6, 125.8, 125.3, 124.78, 124.74, 124.66, 123.7, 42.2, 38.7; MS m/z 448 (M^+), 402, 389; HRMS calcd for $\text{C}_{33}\text{H}_{20}\text{O}_2$ 448.1463, found 448.1451.

Recrystallization of **24** from CH_2Cl_2 /2-propanol produced a crystal suitable for X-ray structure analysis.

Propargylic Acetate 22. The same procedure was repeated as described for **10** except that 0.177 g (0.86 mmol) of **19** was treated with **9**, prepared from 0.19 g (0.94 mmol) of 1-(2-ethynylphenyl)-2-phenylethyne and 0.36 mL of a 2.5 M solution of *n*-butyllithium (0.90 mmol) in hexanes, followed by 0.10 g (0.98 mmol) of acetic anhydride. A small sample of **22** was isolated as a light brown solid for structural elucidation: mp 146–148 °C; IR 2226, 1749, 1226, 756 cm^{-1} ; ^1H δ 7.71 (2 H, t, J = 4.0 Hz), 7.55–7.50 (2 H, m), 7.41–7.23 (7 H, m), 7.17–7.12 (4 H,

m), 3.21–3.02 (4 H, m), 2.07 (3 H, s); ^{13}C δ 169.3, 141.8, 137.2, 132.5, 131.7, 130.5, 128.8, 128.24, 128.20, 128.1, 127.9, 127.7, 125.9, 124.8, 124.1, 123.1, 93.2, 89.4, 87.9, 84.0, 81.0, 25.6, 21.6. As in the case of **32**, the rest of the crude acetate **22** was used for the next step without further purification.

Carboxylic Acid 25. The same procedure was repeated as described for **16** except that 0.386 g (0.86 mmol) of the crude acetate **22** was treated with LDA, prepared from 0.69 mL of a 2.5 M solution of *n*-butyllithium (1.73 mmol) in hexanes and 0.24 mL (1.73 mmol) of diisopropylamine, followed by 1 mL of HMPA and 1.73 mL of a 1.0 M solution of TBDMSCl (1.73 mmol) in THF. Hydrolysis with a mixture of 5 mL of acetic acid and 3 mL of water provided 0.141 g of **25** (0.31 mmol, 37% from **19**) as a yellow solid: mp 230–233 °C; IR 3500–2600 (br), 1708, 756, 703 cm^{-1} ; ^1H δ 7.79 (1 H, d, J = 7.4 Hz), 7.69 (1 H, d, J = 7.4 Hz), 7.63–7.54 (4 H, m), 7.51–7.46 (1 H, m), 7.42–7.29 (4 H, m), 7.22 (1 H, d, J = 7.7 Hz), 7.10 (1 H, t, J = 7.7 Hz), 6.72 (1 H, d, J = 7.9 Hz), 5.06 (1 H, dd, J = 10.4, 1.5 Hz), 3.83 (1 H, dd, J = 16.6, 2.5 Hz), 3.44–3.26, (4 H, m), 2.68 (1 H, dd, J = 16.6, 10.6 Hz); ^{13}C δ 178.1, 146.8, 143.7, 140.8, 138.5, 138.1, 137.8, 134.6, 134.2, 133.0, 132.0, 131.1, 130.0, 129.9, 129.8, 128.9, 128.8, 128.7, 128.3, 127.9, 127.5, 126.9, 126.0, 125.8, 124.6, 123.7, 122.0, 42.0, 38.6, 26.5, 26.2; MS m/z 450 (M^+), 404, 391; HRMS calcd for $\text{C}_{33}\text{H}_{22}\text{O}_2$ 450.1620, found 450.1615.

Carboxylic Acid 26. The same procedure was repeated as described for **25** except that 0.259 g (1.42 mmol) of benzophenone (**20**) was treated with **9**, prepared from 0.316 g (1.56 mmol) of 1-(2-ethynylphenyl)-2-phenylethyne and 0.62 mL of a 2.5 M solution of *n*-butyllithium (1.55 mmol) in hexanes, followed by 0.158 g (1.55 mmol) of acetic anhydride to provide the crude acetate **23**. The crude acetate **23** (0.606 g, 1.42 mmol) was treated with LDA, prepared from 1.20 mL of a 2.5 M solution of *n*-butyllithium (3.0 mmol) in hexanes and 0.42 mL (3.0 mmol) of

diisopropylamine, followed by 0.8 mL of HMPA and 3.0 mL of a 1.0 M solution of TBDMSCl (3.0 mmol) in THF. Hydrolysis with a mixture of 10 mL of acetic acid and 3.3 mL of water followed by flash column chromatography (silica gel/25% acetone in hexanes) provided 0.323 g of **26** (0.76 mmol, 53% from **20**) as a light yellow solid: mp 252–255 °C; IR 3500–2600 (br), 1696, 767, 703 cm^{-1} ; ^1H δ 7.72–7.35 (15 H, m), 7.20 (1 H, t, $J = 7.4$ Hz), 7.04 (1 H, t, $J = 7.5$ Hz), 6.44 (1 H, d, $J = 7.7$ Hz), 4.69 (1 H, dd, $J = 8.9, 3.2$ Hz), 2.75 (1 H, dd, $J = 16.6, 3.5$ Hz), 2.17 (1 H, dd, $J = 16.6, 9.2$ Hz); ^{13}C δ 177.2, 147.4, 141.2, 140.4, 138.9, 138.0, 136.2, 135.4, 133.34, 133.31, 131.8, 130.9, 130.1, 129.7, 129.5, 129.2, 129.1, 128.4, 127.88, 127.85, 127.6, 127.3, 126.5, 125.8, 125.52, 125.48, 124.1, 123.8, 42.5, 37.0; MS m/z 426 (M^+), 367; HRMS calcd for $\text{C}_{31}\text{H}_{22}\text{O}_2$ 426.1620, found 426.1632.

Ketone 30. The same procedure was repeated as described for **17** except that 0.106 g (0.249 mmol) of **26** was treated with 3 mL of thionyl chloride and 0.100 g (0.749 mmol) of anhydrous aluminum chloride to afford 0.071 g of **30** (0.174 mmol, 70%) as yellow crystals: mp 239–241 °C; IR 1682, 765, 700 cm^{-1} ; ^1H δ 8.18 (1 H, dd, $J = 7.9, 1.5$ Hz), 7.88 (1 H, dd, $J = 7.7, 1.2$ Hz), 7.76 (1 H, dd, $J = 7.9, 1.0$ Hz), 7.70–7.38 (11 H, m), 7.27 (1 H, td, $J = 7.4, 1.0$ Hz), 7.08 (1 H, t, $J = 7.7$ Hz), 6.52 (1 H, d, $J = 7.9$ Hz), 4.44 (1 H, dd, $J = 13.4, 4.5$ Hz), 3.59 (1 H, dd, $J = 19.2, 4.5$ Hz), 2.69 (1 H, dd, $J = 19.2, 13.5$ Hz); ^{13}C δ 204.2, 146.2, 143.3, 140.4, 140.1, 138.5, 135.8, 134.6, 134.4, 134.3, 131.7, 130.9, 130.6, 130.1, 129.8, 129.5, 129.2, 128.0, 127.83, 127.77, 127.4, 127.1, 125.9, 125.6, 125.3, 124.0, 123.9, 52.7, 42.0; MS m/z 408 (M^+), 393, 378, 302; HRMS calcd for $\text{C}_{31}\text{H}_{20}\text{O}$ 408.1514, found 408.1527. Recrystallization of **30** from CH_2Cl_2 /hexanes produced a crystal suitable for X-ray structure analysis.

Carboxylic Acids 41 and 42. The same procedure was repeated as described for **35** and **36** except that 0.571 g (3.28 mmol) of the ketone **37** was treated with **9**, prepared from 0.800 g (3.96

mmol) of 1-(2-ethynylphenyl)-2-phenylethyne and 1.57 mL of a 2.5 M solution of *n*-butyllithium (3.93 mmol) in hexanes, followed by 0.405 g (3.96 mmol) of acetic anhydride to provide the crude acetate **39** as a light brown liquid. The crude acetate **39** was treated with LDA, prepared from 2.62 mL of a 2.5 M solution of *n*-butyllithium (6.55 mmol) in hexanes and 0.92 mL (6.55 mmol) of diisopropylamine, followed by 2.0 mL of HMPA and 6.60 mL of a 1.0 M solution of TBDMSCl (6.60 mmol) in THF. Hydrolysis with a mixture of 15 mL of acetic acid and 5 mL of water provided 0.326 g of **41** (0.78 mmol, 24% from **37**) as an orange solid and 0.326 g of **42** (0.78 mmol, 24% from **37**) as a yellow solid. **41**: mp 164–167 °C; IR 3500–2600 (br), 1702, 726 cm^{-1} ; ^1H δ 7.74 (1 H, d, $J = 7.4$ Hz), 7.43–7.08 (11 H, m), 6.98 (1 H, t, $J = 7.4$ Hz), 3.43 (2 H, s), 3.12–2.98 (2 H, m), 2.04–1.93 (1 H, m), 1.85–1.76 (1 H, m), 1.13 (3 H, s), 1.03 (3 H, s); ^{13}C δ 174.9, 153.0, 152.1, 148.1, 147.4, 138.4, 135.0, 134.8, 129.9, 129.4, 129.2, 128.7, 128.5, 128.4, 126.5, 126.2, 123.7, 123.6, 120.1, 113.1, 68.8, 35.3, 34.7, 31.8, 27.4, 26.2, 26.0. **42**: mp 225–228 °C; IR 3500–2600 (br), 1708, 732 cm^{-1} ; ^1H δ 7.61–7.51 (4 H, m), 7.46–7.28 (5 H, m), 7.18 (1 H, td, $J = 7.4, 0.7$ Hz), 6.98 (1 H, t, $J = 7.7$ Hz), 6.25 (1 H, d, $J = 7.7$ Hz), 5.21 (1 H, dd, $J = 10.6, 2.0$ Hz), 3.57 (1 H, dd, $J = 16.7, 2.4$ Hz), 3.46 (1 H, ddd, $J = 17.1, 11.9, 5.2$ Hz), 3.12 (1 H, dt, $J = 13.1, 4.0$ Hz), 2.43 (1 H, dd, $J = 16.6, 10.6$ Hz), 2.09 (1 H, td, $J = 12.5, 4.9$ Hz), 1.94 (1 H, dt, $J = 12.9, 4.5$ Hz), 1.84 (3 H, s), 1.59 (3 H, s); ^{13}C δ 177.0, 148.2, 139.8, 139.6, 139.2, 139.0, 136.6, 135.4, 134.1, 133.3, 130.2, 129.35, 129.30, 129.0, 127.7, 127.3, 127.2, 125.1, 124.9, 124.8, 124.0, 123.4, 44.2, 42.6, 40.8, 36.3, 30.7, 28.9, 27.7.

Carboxylic Acids 43 and 44. The same procedure was repeated as described for **35** and **36** except that 0.522 g (3.26 mmol) of the ketone **38** was treated with **9**, prepared from 0.806 g (3.99 mmol) of 1-(2-ethynylphenyl)-2-phenylethyne and 1.60 mL of a 2.5 M solution of *n*-butyllithium (4.00 mmol) in hexanes, followed by 0.413 g (4.00 mmol) of acetic anhydride to provide the

crude acetate **40** as a light brown liquid. The crude acetate **40** was treated with LDA, prepared from 2.60 mL of a 2.5 M solution of *n*-butyllithium (6.50 mmol) in hexanes and 0.91 mL (6.49 mmol) of diisopropylamine, followed by 1.2 mL of HMPA and 6.50 mL of a 1.0 M solution of TBDMSCl (6.50 mmol) in THF. Hydrolysis with a mixture of 7 mL of acetic acid and 3 mL of water provided 0.132 g of **43** (0.327 mmol, 10% from **38**) as an orange solid and 0.662 g of **44** (1.64 mmol, 50% from **38**) as a yellow solid. **43**: mp 55–57 °C; IR 3500–2600 (br), 1708, 689 cm^{-1} ; ^1H δ 7.77 (1 H, d, $J = 7.2$ Hz), 7.40–7.17 (10 H, m), 7.10–7.06 (2 H, m), 3.47 (2 H, s), 3.21 (1 H, d, $J = 16.1$ Hz), 2.99 (1 H, d, $J = 16.1$ Hz), 1.25 (3 H, s); 1.16 (3 H, s), ^{13}C δ 176.3, 152.8, 152.4, 147.6, 145.8, 145.3, 141.3, 134.4, 129.6, 129.3, 128.8, 128.7, 127.9, 127.8, 126.9, 125.6, 124.9, 123.8, 123.7, 120.2, 113.6, 75.7, 47.3, 45.4, 31.9, 28.6, 24.7; MS m/z 404 (M^+), 389, 359, 345, 329; HRMS calcd for $\text{C}_{29}\text{H}_{24}\text{O}_2$ 404.1776, found 404.1775. **44**: mp 143–146 °C; IR 3500–2600 (br), 1708, 779, 703 cm^{-1} ; ^1H δ 7.63–7.47 (5 H, m), 7.40–7.35 (2 H, m), 7.30–7.24 (2 H, m), 7.20 (1 H, td, $J = 7.4, 1.0$ Hz), 7.02 (1 H, td, $J = 7.5, 0.9$ Hz), 6.52 (1 H, d, $J = 7.9$ Hz), 4.83 (1 H, dd, $J = 10.3, 2.4$ Hz), 3.57 (1 H, dd, $J = 16.6, 2.5$ Hz), 3.41 (1 H, d, $J = 16.6$ Hz), 3.31 (1 H, d, $J = 16.6$ Hz), 2.59 (1 H, dd, $J = 16.6, 10.1$ Hz), 1.76 (3 H, s), 1.65 (3 H, s); ^{13}C δ 177.4, 148.1, 147.0, 142.6, 140.1, 138.64, 138.58, 137.2, 137.0, 131.5, 131.3, 130.3, 130.0, 129.1, 128.9, 127.7, 127.6, 127.29, 127.26, 124.0, 123.8, 121.6, 119.5, 49.3, 45.2, 41.4, 41.2, 30.7, 28.6; MS m/z 404(M^+), 389, 358, 345, 330, 315; HRMS calcd for $\text{C}_{29}\text{H}_{24}\text{O}_2$ 404.1776, found 404.1769.

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Figure S1. ORTEP Drawing of the Crystal Structure of the Ketone 17.

Table 1. Crystal data and structure refinement for $C_{31}H_{18}O$.

Identification code	yyang3	<p>17</p>
Empirical formula	$C_{31}H_{18}O$	
Formula weight	406.45	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 8.409(1) \text{ Å}$ $\alpha = 76.20(1)^\circ$ $b = 9.978(2) \text{ Å}$ $\beta = 73.36(1)^\circ$ $c = 12.764(1) \text{ Å}$ $\gamma = 85.56(1)^\circ$	
Volume	$996.4(3) \text{ Å}^3$	
Z	2	
Density (calculated)	1.355 g/cm^3	
Absorption coefficient	0.80 cm^{-1}	
F(000)	424	
Crystal size	$0.16 \times 0.30 \times 0.32 \text{ mm}$	
θ range for data collection	2.10 to 24.00°	
Index ranges	$0 \leq h \leq 9, -11 \leq k \leq 11, -13 \leq l \leq 14$	
Reflections collected	3243	
Independent reflections	3014 ($R_{\text{int}} = 0.0615$)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3013 / 0 / 308	
Goodness-of-fit on F^2	1.027	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0610, wR_2 = 0.0996$	
R indices (all data)	$R_1 = 0.1686, wR_2 = 0.1367$	
Largest diff. peak and hole	0.150 and -0.147 eÅ^{-3}	

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{31}\text{H}_{18}\text{O}$.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
O	3263(5)	8925(3)	3157(3)	88(1)
C(1)	3937(20)	7667(9)	4778(6)	58(3)
C(2)	2863(18)	7075(9)	5932(7)	44(2)
C(1')	2795(53)	7896(21)	5014(23)	51(8)
C(2')	3785(45)	6808(22)	5745(20)	34(6)
C(3)	3557(6)	7088(4)	6926(3)	52(1)
C(4)	4230(6)	8180(4)	7132(4)	60(1)
C(5)	4565(6)	8023(5)	8152(4)	64(1)
C(6)	4266(6)	6799(5)	8939(4)	62(1)
C(7)	3592(5)	5686(4)	8740(3)	52(1)
C(8)	3235(5)	5826(4)	7730(3)	47(1)
C(9)	2624(5)	4828(4)	7246(3)	48(1)
C(10)	2182(5)	3439(4)	7645(3)	43(1)
C(11)	1829(5)	2723(4)	6880(3)	44(1)
C(12)	1404(5)	1309(4)	7085(4)	57(1)
C(13)	1178(6)	786(5)	6233(4)	64(1)
C(14)	1330(6)	1573(5)	5139(4)	61(1)
C(15)	1685(5)	2949(4)	4912(4)	47(1)
C(16)	1947(5)	4121(4)	3924(3)	50(1)
C(17)	1886(6)	4246(5)	2827(4)	65(1)
C(18)	2203(6)	5533(5)	2083(4)	71(2)
C(19)	2592(6)	6669(5)	2398(4)	66(1)
C(20)	2696(5)	6567(4)	3494(3)	51(1)
C(21)	3171(5)	7809(5)	3795(4)	55(1)
C(22)	2630(6)	5532(4)	6130(4)	56(1)
C(23)	1917(5)	3476(4)	5795(3)	44(1)
C(24)	2348(5)	5293(4)	4237(3)	44(1)
C(25)	2313(5)	4880(4)	5411(3)	44(1)
C(26)	2041(5)	2672(4)	8826(3)	46(1)
C(27)	843(6)	3057(4)	9702(4)	61(1)
C(28)	643(6)	2336(5)	10803(4)	68(1)
C(29)	1652(6)	1227(5)	11031(4)	69(2)
C(30)	2838(6)	830(5)	10179(4)	70(2)
C(31)	3052(6)	1556(4)	9072(4)	61(1)

Table 3. Interatomic distances [$\text{\AA}$] and bond angles [$^\circ$] for

O-C(21)	1.206(4)	C(1)-C(2)	1.50(2)
C(1)-C(21)	1.541(10)	C(2)-C(22)	1.519(9)
C(2)-C(3)	1.544(9)	C(1')-C(21)	1.52(3)
C(1')-C(2')	1.60(4)	C(2')-C(3)	1.55(2)
C(2')-C(22)	1.56(2)	C(3)-C(4)	1.375(5)
C(3)-C(8)	1.410(5)	C(4)-C(5)	1.381(5)
C(5)-C(6)	1.371(5)	C(6)-C(7)	1.390(5)
C(7)-C(8)	1.379(5)	C(8)-C(9)	1.480(5)
C(9)-C(10)	1.398(5)	C(9)-C(22)	1.428(5)
C(10)-C(11)	1.443(5)	C(10)-C(26)	1.495(5)
C(11)-C(23)	1.394(5)	C(11)-C(12)	1.426(5)
C(12)-C(13)	1.378(5)	C(13)-C(14)	1.404(5)
C(14)-C(15)	1.372(5)	C(15)-C(23)	1.417(5)
C(15)-C(16)	1.478(5)	C(16)-C(17)	1.390(5)
C(16)-C(24)	1.415(5)	C(17)-C(18)	1.396(6)
C(18)-C(19)	1.380(6)	C(19)-C(20)	1.406(5)
C(20)-C(24)	1.388(5)	C(20)-C(21)	1.494(6)
C(22)-C(25)	1.337(5)	C(23)-C(25)	1.402(5)
C(24)-C(25)	1.450(5)	C(26)-C(31)	1.378(5)
C(26)-C(27)	1.383(6)	C(27)-C(28)	1.386(5)
C(28)-C(29)	1.369(6)	C(29)-C(30)	1.362(6)
C(30)-C(31)	1.393(5)		
C(2)-C(1)-C(21)	117.1(12)	C(2')-C(1')-C(21)	115(3)
C(1)-C(2)-C(3)	117.0(11)	C(1)-C(2)-C(22)	112.0(9)
C(3)-C(2)-C(22)	99.3(6)	C(1')-C(2')-C(3)	113(3)
C(1')-C(2')-C(22)	101(3)	C(3)-C(2')-C(22)	97(2)
C(4)-C(3)-C(8)	121.0(4)	C(4)-C(3)-C(2)	128.0(5)
C(8)-C(3)-C(2)	110.6(4)	C(4)-C(3)-C(2')	125.0(10)
C(8)-C(3)-C(2')	108.6(8)	C(3)-C(4)-C(5)	118.6(4)
C(6)-C(5)-C(4)	120.9(4)	C(5)-C(6)-C(7)	121.0(4)
C(8)-C(7)-C(6)	118.9(4)	C(7)-C(8)-C(3)	119.5(4)
C(7)-C(8)-C(9)	131.7(4)	C(3)-C(8)-C(9)	108.7(3)

C(10)-C(9)-C(22)	120.5(4)	C(10)-C(9)-C(8)	133.1(4)
C(22)-C(9)-C(8)	106.3(4)	C(9)-C(10)-C(11)	118.2(4)
C(9)-C(10)-C(26)	123.0(4)	C(11)-C(10)-C(26)	118.8(4)
C(23)-C(11)-C(12)	114.3(4)	C(23)-C(11)-C(10)	117.5(4)
C(12)-C(11)-C(10)	128.2(4)	C(13)-C(12)-C(11)	120.1(4)
C(12)-C(13)-C(14)	123.7(4)	C(15)-C(14)-C(13)	118.2(4)
C(14)-C(15)-C(23)	117.6(4)	C(14)-C(15)-C(16)	136.3(4)
C(23)-C(15)-C(16)	106.1(3)	C(17)-C(16)-C(24)	118.9(4)
C(17)-C(16)-C(15)	132.9(4)	C(24)-C(16)-C(15)	108.1(3)
C(16)-C(17)-C(18)	118.4(4)	C(19)-C(18)-C(17)	122.1(4)
C(18)-C(19)-C(20)	120.7(4)	C(24)-C(20)-C(19)	116.9(4)
C(24)-C(20)-C(21)	123.8(4)	C(19)-C(20)-C(21)	119.2(4)
O-C(21)-C(20)	120.6(4)	O-C(21)-C(1)	116.7(5)
O-C(21)-C(1')	113.0(8)	C(20)-C(21)-C(1)	121.2(4)
C(20)-C(21)-C(1')	120.8(9)	C(9)-C(22)-C(25)	121.9(4)
C(9)-C(22)-C(2)	111.9(4)	C(9)-C(22)-C(2')	109.4(9)
C(25)-C(22)-C(2)	126.0(5)	C(25)-C(22)-C(2')	122.9(9)
C(11)-C(23)-C(25)	123.9(4)	C(11)-C(23)-C(15)	126.0(4)
C(25)-C(23)-C(15)	110.0(4)	C(20)-C(24)-C(16)	122.8(4)
C(20)-C(24)-C(25)	129.7(4)	C(16)-C(24)-C(25)	107.5(3)
C(22)-C(25)-C(23)	117.9(4)	C(22)-C(25)-C(24)	133.7(4)
C(23)-C(25)-C(24)	108.3(4)	C(31)-C(26)-C(27)	118.4(4)
C(31)-C(26)-C(10)	121.7(4)	C(27)-C(26)-C(10)	119.8(4)
C(26)-C(27)-C(28)	121.2(4)	C(29)-C(28)-C(27)	119.6(5)
C(30)-C(29)-C(28)	120.1(4)	C(29)-C(30)-C(31)	120.5(5)
C(26)-C(31)-C(30)	120.2(4)		

The primed (') atoms correspond to the minor site of a two site disorder.

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for

$\text{C}_{31}\text{H}_{18}\text{O}$. The anisotropic displacement

factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}].$$

	U11	U22	U33	U23	U13	U12
O	123(3)	64(2)	67(2)	19(2)	-34(2)	-17(2)
C(1)	60(8)	48(5)	63(5)	5(4)	-22(5)	-13(5)
C(2)	46(6)	36(5)	48(5)	-4(3)	-16(5)	7(4)
C(1')	51(20)	33(10)	82(18)	-4(11)	-45(16)	8(13)
C(2')	28(15)	21(10)	50(14)	-2(9)	-17(12)	15(10)
C(3)	72(4)	39(3)	53(3)	-9(2)	-27(3)	-6(2)
C(4)	73(4)	45(3)	65(3)	-9(2)	-25(3)	-2(3)
C(5)	74(4)	56(3)	71(3)	-24(3)	-25(3)	-5(3)
C(6)	74(4)	62(3)	58(3)	-14(3)	-28(3)	-5(3)
C(7)	56(3)	52(3)	48(3)	-9(2)	-17(2)	1(2)
C(8)	51(3)	44(3)	44(3)	-9(2)	-13(2)	-5(2)
C(9)	57(3)	40(3)	44(3)	-7(2)	-13(2)	-5(2)
C(10)	43(3)	45(3)	37(3)	-9(2)	-8(2)	2(2)
C(11)	44(3)	39(3)	45(3)	-7(2)	-8(2)	-3(2)
C(12)	58(3)	44(3)	64(3)	-8(2)	-15(3)	-1(2)
C(13)	67(4)	47(3)	81(4)	-17(3)	-23(3)	-8(3)
C(14)	59(3)	63(3)	71(4)	-33(3)	-22(3)	4(3)
C(15)	41(3)	42(3)	58(3)	-17(2)	-12(2)	2(2)
C(16)	44(3)	64(3)	46(3)	-20(2)	-10(2)	3(2)
C(17)	58(4)	88(4)	58(3)	-25(3)	-24(3)	5(3)
C(18)	66(4)	104(5)	45(3)	-12(3)	-22(3)	4(3)
C(19)	62(4)	79(4)	50(3)	-3(3)	-14(3)	-1(3)
C(20)	43(3)	67(3)	41(3)	-10(2)	-14(2)	3(3)
C(21)	52(3)	59(3)	44(3)	5(3)	-9(2)	1(3)
C(22)	76(4)	43(3)	49(3)	0(2)	-22(3)	-8(3)
C(23)	42(3)	43(3)	50(3)	-18(2)	-13(2)	2(2)
C(24)	37(3)	53(3)	38(3)	-8(2)	-7(2)	5(2)
C(25)	52(3)	41(3)	39(3)	-6(2)	-14(2)	-3(2)
C(26)	47(3)	42(3)	46(3)	-1(2)	-11(2)	-7(2)
C(27)	63(4)	66(3)	49(3)	-6(3)	-16(3)	9(3)
C(28)	63(4)	84(4)	46(3)	-8(3)	-7(3)	5(3)
C(29)	66(4)	80(4)	49(3)	9(3)	-14(3)	-16(3)
C(30)	69(4)	61(3)	66(4)	13(3)	-17(3)	2(3)
C(31)	57(3)	59(3)	53(3)	1(2)	-5(3)	8(3)

Table 5. Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{31}\text{H}_{18}\text{O}$.

	x	y	z	U(eq)
H(1A)	4927(20)	7094(9)	4641(6)	70
H(1B)	4287(20)	8575(9)	4767(6)	70
H(2A)	1776(18)	7539(9)	6039(7)	53
H(1C)	1615(53)	7760(21)	5363(23)	62
H(1D)	3051(53)	8819(21)	5034(23)	62
H(2B)	4934(45)	6633(22)	5344(20)	41
H(4A)	4454(6)	9006(4)	6595(4)	72
H(5A)	5001(6)	8758(5)	8309(4)	77
H(6A)	4517(6)	6712(5)	9616(4)	75
H(7A)	3386(5)	4861(4)	9279(3)	62
H(12A)	1280(5)	740(4)	7796(4)	68
H(13A)	909(6)	-141(5)	6391(4)	77
H(14A)	1194(6)	1172(5)	4584(4)	73
H(17A)	1640(6)	3490(5)	2596(4)	78
H(18A)	2151(6)	5627(5)	1351(4)	86
H(19A)	2787(6)	7512(5)	1879(4)	79
H(27A)	159(6)	3814(4)	9549(4)	73
H(28A)	-173(6)	2604(5)	11383(4)	81
H(29A)	1528(6)	743(5)	11768(4)	83
H(30A)	3511(6)	68(5)	10339(4)	84
H(31A)	3878(6)	1288(4)	8498(4)	74

Figure S2. ORTEP Drawing of the Crystal Structure of the Carboxylic Acid 24.

Table 1. Crystal data and structure refinement for $C_{33}H_{20}O_2$.

Identification code	yang6ccd	
Empirical formula	$C_{33}H_{20}O_2$	
Formula weight	448.49	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	$a = 21.478(2)$ Å	$\alpha = 90^\circ$
	$b = 6.8291(7)$ Å	$\beta = 104.651(2)^\circ$
	$c = 15.8755(15)$ Å	$\gamma = 90^\circ$
Volume, Z	$2252.8(4)$ Å ³ , 4	
Density (calculated)	1.322 g/cm ³	
Absorption coefficient	0.81 cm ⁻¹	
F(000)	936	
Crystal size	$0.12 \times 0.20 \times 0.30$ mm	
θ range for data collection	1.96 to 27.53°	
Limiting indices	$-27 \leq h \leq 26$, $-8 \leq k \leq 8$, $-20 \leq l \leq 20$	
Reflections collected	15510	
Independent reflections	5125 ($R_{int} = 0.0525$)	
Completeness to $\theta = 27.53^\circ$	98.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5125 / 0 / 317	
Goodness-of-fit on F^2	0.931	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0537$, $wR2 = 0.1227$	
R indices (all data)	$R1 = 0.1554$, $wR2 = 0.1574$	
Largest diff. peak and hole	0.144 and -0.149 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{33}\text{H}_{20}\text{O}_2$.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	338(1)	12979(4)	10670(1)	126(1)
O(2)	446(1)	14028(4)	9407(1)	122(1)
C(1)	1707(1)	12352(3)	9834(1)	69(1)
C(2)	2090(1)	13765(3)	10499(1)	64(1)
C(3)	1890(1)	15512(4)	10795(2)	79(1)
C(4)	2317(2)	16585(4)	11429(2)	83(1)
C(5)	2934(2)	15939(3)	11743(2)	79(1)
C(6)	3151(1)	14229(3)	11443(2)	69(1)
C(7)	2723(1)	13110(3)	10824(1)	60(1)
C(8)	2811(1)	11246(3)	10387(1)	61(1)
C(9)	3356(1)	10055(3)	10486(2)	68(1)
C(10)	3297(1)	8351(3)	9937(2)	74(1)
C(11)	3757(2)	6815(4)	9927(2)	91(1)
C(12)	3609(2)	5195(4)	9391(2)	107(1)
C(13)	2988(2)	4915(4)	8803(2)	103(1)
C(14)	2707(3)	3349(5)	8216(2)	127(2)
C(15)	2083(3)	3389(6)	7741(3)	138(2)
C(16)	1651(3)	4995(6)	7790(2)	114(1)
C(17)	990(3)	5322(7)	7369(2)	137(2)
C(18)	687(2)	6985(7)	7535(2)	134(1)
C(19)	992(2)	8454(5)	8125(2)	108(1)
C(20)	1627(2)	8196(4)	8566(2)	88(1)
C(21)	1923(2)	6483(4)	8356(2)	95(1)
C(22)	2565(2)	6415(4)	8822(2)	91(1)
C(23)	2705(2)	8068(3)	9363(2)	76(1)
C(24)	2138(1)	9223(4)	9244(2)	76(1)
C(25)	2202(1)	10832(3)	9776(1)	67(1)
C(26)	1129(1)	11466(4)	10095(2)	78(1)
C(27)	602(1)	12915(4)	10046(2)	84(1)
C(28)	3971(1)	10425(3)	11144(2)	71(1)
C(29)	3998(1)	10410(3)	12030(2)	75(1)
C(30)	4569(2)	10696(4)	12643(2)	88(1)
C(31)	5132(2)	10987(4)	12395(2)	98(1)
C(32)	5117(2)	10994(4)	11524(3)	99(1)
C(33)	4542(1)	10727(4)	10900(2)	86(1)

Table 3. Interatomic distances [Å] and bond angles [°] for C₃₃H₂₀O₂.

O(1)-C(27)	1.261(3)	O(2)-C(27)	1.244(3)
C(1)-C(25)	1.505(3)	C(1)-C(2)	1.510(3)
C(1)-C(26)	1.531(3)	C(2)-C(3)	1.390(3)
C(2)-C(7)	1.401(3)	C(3)-C(4)	1.388(3)
C(4)-C(5)	1.366(3)	C(5)-C(6)	1.385(3)
C(6)-C(7)	1.392(3)	C(7)-C(8)	1.484(3)
C(8)-C(9)	1.403(3)	C(8)-C(25)	1.444(3)
C(9)-C(10)	1.439(3)	C(9)-C(28)	1.483(3)
C(10)-C(23)	1.379(3)	C(10)-C(11)	1.445(3)
C(11)-C(12)	1.383(4)	C(12)-C(13)	1.434(4)
C(13)-C(22)	1.376(4)	C(13)-C(14)	1.446(5)
C(14)-C(15)	1.363(5)	C(15)-C(16)	1.451(6)
C(16)-C(21)	1.385(4)	C(16)-C(17)	1.425(5)
C(17)-C(18)	1.368(5)	C(18)-C(19)	1.415(5)
C(19)-C(20)	1.378(4)	C(20)-C(21)	1.410(4)
C(20)-C(24)	1.502(4)	C(21)-C(22)	1.391(4)
C(22)-C(23)	1.404(4)	C(23)-C(24)	1.422(3)
C(24)-C(25)	1.372(3)	C(26)-C(27)	1.490(3)
C(28)-C(33)	1.392(3)	C(28)-C(29)	1.393(3)
C(29)-C(30)	1.372(3)	C(30)-C(31)	1.377(4)
C(31)-C(32)	1.375(4)	C(32)-C(33)	1.386(4)
C(25)-C(1)-C(2)	102.46(19)	C(25)-C(1)-C(26)	112.2(2)
C(2)-C(1)-C(26)	113.46(18)	C(3)-C(2)-C(7)	120.3(2)
C(3)-C(2)-C(1)	128.7(2)	C(7)-C(2)-C(1)	111.06(19)
C(4)-C(3)-C(2)	119.6(2)	C(5)-C(4)-C(3)	119.8(2)
C(4)-C(5)-C(6)	121.7(3)	C(5)-C(6)-C(7)	119.2(2)
C(6)-C(7)-C(2)	119.4(2)	C(6)-C(7)-C(8)	131.5(2)
C(2)-C(7)-C(8)	109.1(2)	C(9)-C(8)-C(25)	123.4(2)
C(9)-C(8)-C(7)	130.2(2)	C(25)-C(8)-C(7)	106.4(2)
C(8)-C(9)-C(10)	117.2(2)	C(8)-C(9)-C(28)	123.3(2)
C(10)-C(9)-C(28)	119.4(2)	C(23)-C(10)-C(9)	116.0(2)
C(23)-C(10)-C(11)	114.2(3)	C(9)-C(10)-C(11)	129.7(3)
C(12)-C(11)-C(10)	122.5(3)	C(11)-C(12)-C(13)	122.6(3)
C(22)-C(13)-C(12)	113.4(3)	C(22)-C(13)-C(14)	113.2(4)
C(12)-C(13)-C(14)	133.3(4)	C(15)-C(14)-C(13)	122.3(4)
C(14)-C(15)-C(16)	122.6(4)	C(21)-C(16)-C(17)	113.3(4)
C(21)-C(16)-C(15)	114.8(4)	C(17)-C(16)-C(15)	131.9(4)
C(18)-C(17)-C(16)	120.4(4)	C(17)-C(18)-C(19)	123.6(4)
C(20)-C(19)-C(18)	118.6(4)	C(19)-C(20)-C(21)	115.7(3)
C(19)-C(20)-C(24)	138.9(3)	C(21)-C(20)-C(24)	105.4(3)
C(16)-C(21)-C(22)	121.3(4)	C(16)-C(21)-C(20)	128.4(4)
C(22)-C(21)-C(20)	110.3(3)	C(13)-C(22)-C(21)	125.8(3)
C(13)-C(22)-C(23)	124.9(4)	C(21)-C(22)-C(23)	109.2(3)
C(10)-C(23)-C(22)	122.4(3)	C(10)-C(23)-C(24)	128.7(2)
C(22)-C(23)-C(24)	108.7(3)	C(25)-C(24)-C(23)	114.4(2)
C(25)-C(24)-C(20)	139.2(3)	C(23)-C(24)-C(20)	106.3(2)
C(24)-C(25)-C(8)	120.2(2)	C(24)-C(25)-C(1)	128.9(2)
C(8)-C(25)-C(1)	110.9(2)	C(27)-C(26)-C(1)	112.4(2)
O(2)-C(27)-O(1)	122.6(3)	O(2)-C(27)-C(26)	119.5(2)
O(1)-C(27)-C(26)	118.0(2)	C(33)-C(28)-C(29)	117.8(3)
C(33)-C(28)-C(9)	121.3(2)	C(29)-C(28)-C(9)	120.9(2)
C(30)-C(29)-C(28)	121.1(2)	C(29)-C(30)-C(31)	120.6(3)

C(32)-C(31)-C(30)

119.3 (3)

C(31)-C(32)-C(33)

120.5 (3)

C(32)-C(33)-C(28)

120.7 (3)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for

$\text{C}_{33}\text{H}_{20}\text{O}_2$. The anisotropic displacement

factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}].$$

	U11	U22	U33	U23	U13	U12
O(1)	123(2)	167(2)	106(2)	55(1)	64(1)	62(2)
O(2)	120(2)	168(2)	87(1)	50(1)	40(1)	60(2)
C(1)	79(2)	72(2)	62(1)	8(1)	27(1)	8(1)
C(2)	82(2)	59(2)	60(1)	4(1)	33(1)	5(1)
C(3)	92(2)	69(2)	85(2)	11(2)	41(2)	22(2)
C(4)	116(2)	57(2)	90(2)	-3(2)	51(2)	10(2)
C(5)	103(2)	58(2)	85(2)	-5(1)	41(2)	-5(2)
C(6)	80(2)	53(1)	84(2)	0(1)	37(1)	-3(1)
C(7)	72(2)	52(1)	63(1)	3(1)	31(1)	1(1)
C(8)	75(2)	55(1)	63(1)	3(1)	35(1)	1(1)
C(9)	82(2)	56(1)	79(2)	5(1)	45(1)	3(1)
C(10)	99(2)	58(2)	79(2)	0(1)	50(2)	6(2)
C(11)	125(2)	65(2)	110(2)	6(2)	79(2)	15(2)
C(12)	173(3)	63(2)	120(3)	6(2)	106(3)	18(2)
C(13)	189(4)	61(2)	90(2)	-7(2)	89(2)	-9(2)
C(14)	250(5)	66(2)	102(3)	-16(2)	116(3)	-25(3)
C(15)	270(6)	85(3)	91(3)	-23(2)	106(3)	-55(4)
C(16)	201(4)	95(3)	63(2)	-15(2)	64(2)	-50(3)
C(17)	210(5)	143(4)	72(2)	-34(2)	61(3)	-82(4)
C(18)	165(4)	159(4)	77(2)	-31(2)	31(2)	-56(3)
C(19)	133(3)	120(3)	68(2)	-10(2)	21(2)	-28(2)
C(20)	124(3)	84(2)	60(2)	-6(2)	33(2)	-19(2)
C(21)	159(3)	77(2)	60(2)	-10(2)	48(2)	-25(2)
C(22)	158(3)	60(2)	73(2)	-5(2)	65(2)	-7(2)
C(23)	115(2)	57(2)	70(2)	-2(1)	49(2)	0(2)
C(24)	103(2)	65(2)	65(2)	-2(1)	33(1)	-5(2)
C(25)	87(2)	64(2)	59(1)	1(1)	34(1)	1(1)
C(26)	78(2)	88(2)	72(2)	10(1)	25(1)	7(2)
C(27)	75(2)	111(2)	67(2)	17(2)	21(1)	12(2)
C(28)	71(2)	56(2)	94(2)	3(1)	40(2)	7(1)
C(29)	79(2)	63(2)	91(2)	-1(1)	33(2)	-2(1)
C(30)	96(2)	67(2)	106(2)	5(2)	32(2)	1(2)
C(31)	88(2)	67(2)	138(3)	6(2)	25(2)	3(2)
C(32)	77(2)	79(2)	156(3)	5(2)	54(2)	4(2)
C(33)	82(2)	75(2)	115(2)	7(2)	51(2)	11(2)

Table 5. Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{33}\text{H}_{20}\text{O}_2$.

	x	y	z	U(eq)
H(1A)	84	13899	10599	189
H(1B)	1560	13017	9271	83
H(3)	1472	15960	10570	94
H(4)	2184	17742	11639	100
H(5)	3216	16665	12171	95
H(6)	3576	13834	11652	83
H(11)	4169	6918	10294	109
H(12)	3925	4250	9412	128
H(14)	2962	2278	8161	152
H(15)	1927	2346	7371	165
H(17)	764	4399	6979	165
H(18)	257	7160	7245	160
H(19)	769	9571	8213	129
H(26A)	964	10372	9714	94
H(26B)	1268	10969	10685	94
H(29)	3623	10203	12209	90
H(30)	4575	10693	13231	106
H(31)	5517	11177	12812	118
H(32)	5496	11180	11353	119
H(33)	4538	10748	10313	103

Figure S3. ORTEP Drawing of the Crystal Structure of the Ketone 30.

Table 1. Crystal data and structure refinement for $C_{31}H_{20}O$.

Identification code	yang9ccd	<p>30</p>
Empirical formula	$C_{31}H_{20}O$	
Formula weight	408.47	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	$a = 10.2468(9) \text{ Å}$ $\alpha = 90^\circ$ $b = 8.8322(8) \text{ Å}$ $\beta = 90.122(2)^\circ$ $c = 22.707(2) \text{ Å}$ $\gamma = 90^\circ$	
Volume, Z	$2055.0(3) \text{ Å}^3, 4$	
Density (calculated)	1.320 g/cm^3	
Absorption coefficient	0.78 cm^{-1}	
$F(000)$	856	
Crystal size	$0.20 \times 0.34 \times 0.40 \text{ mm}$	
θ range for data collection	1.79 to 27.52°	
Limiting indices	$-13 \leq h \leq 12, -11 \leq k \leq 11, -29 \leq l \leq 26$	
Reflections collected	14221	
Independent reflections	4708 ($R_{\text{int}} = 0.0318$)	
Completeness to $\theta = 27.52^\circ$	99.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4708 / 0 / 289	
Goodness-of-fit on F^2	1.050	
Final R indices $[I > 2\sigma(I)]$	$R1 = 0.0429, wR2 = 0.1094$	
R indices (all data)	$R1 = 0.0561, wR2 = 0.1174$	
Largest diff. peak and hole	0.241 and -0.165 eÅ^{-3}	

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{31}\text{H}_{20}\text{O}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	1586(1)	4184(1)	711(1)	66(1)
C(1)	2316(1)	4792(2)	1061(1)	43(1)
C(2)	3450(1)	5690(2)	836(1)	41(1)
C(3)	3286(2)	6265(2)	266(1)	53(1)
C(4)	4223(2)	7131(2)	-2(1)	60(1)
C(5)	5356(2)	7470(2)	301(1)	56(1)
C(6)	5545(1)	6912(2)	862(1)	46(1)
C(7)	4629(1)	5988(1)	1141(1)	39(1)
C(8)	4937(1)	5392(1)	1739(1)	36(1)
C(9)	6196(1)	4765(1)	1886(1)	37(1)
C(10)	7175(1)	4486(2)	1461(1)	42(1)
C(11)	8360(1)	3894(2)	1613(1)	45(1)
C(12)	8633(1)	3524(2)	2199(1)	48(1)
C(13)	7713(1)	3740(2)	2619(1)	45(1)
C(14)	6465(1)	4354(1)	2485(1)	37(1)
C(15)	5502(1)	4517(1)	2932(1)	37(1)
C(16)	4288(1)	5051(1)	2772(1)	36(1)
C(17)	3082(1)	5287(1)	3111(1)	37(1)
C(18)	2783(1)	5082(2)	3705(1)	46(1)
C(19)	1533(2)	5373(2)	3896(1)	55(1)
C(20)	575(2)	5880(2)	3512(1)	55(1)
C(21)	861(1)	6095(2)	2922(1)	47(1)
C(22)	2107(1)	5795(1)	2724(1)	38(1)
C(23)	2620(1)	5891(1)	2103(1)	36(1)
C(24)	1977(1)	4712(2)	1703(1)	40(1)
C(25)	4032(1)	5474(1)	2178(1)	35(1)
C(26)	5795(1)	4101(1)	3555(1)	38(1)
C(27)	6345(2)	5134(2)	3939(1)	56(1)
C(28)	6527(2)	4779(2)	4526(1)	63(1)
C(29)	6190(2)	3379(2)	4738(1)	54(1)
C(30)	5687(2)	2324(2)	4359(1)	53(1)
C(31)	5493(1)	2680(2)	3772(1)	48(1)

Table 3. Interatomic distances [Å] and bond angles [°] for C₃₁H₂₀O.

O(1)-C(1)	1.2143 (15)	C(1)-C(2)	1.498 (2)
C(1)-C(24)	1.5018 (19)	C(2)-C(3)	1.3995 (18)
C(2)-C(7)	1.4157 (17)	C(3)-C(4)	1.370 (2)
C(4)-C(5)	1.381 (2)	C(5)-C(6)	1.3801 (19)
C(6)-C(7)	1.3966 (19)	C(7)-C(8)	1.4914 (16)
C(8)-C(25)	1.3645 (18)	C(8)-C(9)	1.4420 (17)
C(9)-C(10)	1.4144 (19)	C(9)-C(14)	1.4337 (17)
C(10)-C(11)	1.3654 (18)	C(11)-C(12)	1.400 (2)
C(12)-C(13)	1.356 (2)	C(13)-C(14)	1.4217 (17)
C(14)-C(15)	1.4243 (19)	C(15)-C(16)	1.3781 (17)
C(15)-C(26)	1.4935 (16)	C(16)-C(25)	1.4227 (16)
C(16)-C(17)	1.4728 (18)	C(17)-C(18)	1.3953 (18)
C(17)-C(22)	1.4025 (17)	C(18)-C(19)	1.378 (2)
C(19)-C(20)	1.386 (2)	C(20)-C(21)	1.385 (2)
C(21)-C(22)	1.3807 (19)	C(22)-C(23)	1.5085 (18)
C(23)-C(25)	1.5025 (16)	C(23)-C(24)	1.5295 (16)
C(26)-C(27)	1.3809 (19)	C(26)-C(31)	1.3829 (19)
C(27)-C(28)	1.382 (2)	C(28)-C(29)	1.371 (2)
C(29)-C(30)	1.367 (2)	C(30)-C(31)	1.3849 (19)
O(1)-C(1)-C(2)	119.20 (13)	O(1)-C(1)-C(24)	118.10 (13)
C(2)-C(1)-C(24)	122.51 (11)	C(3)-C(2)-C(7)	119.01 (13)
C(3)-C(2)-C(1)	114.61 (11)	C(7)-C(2)-C(1)	126.37 (11)
C(4)-C(3)-C(2)	121.99 (13)	C(3)-C(4)-C(5)	119.30 (13)
C(6)-C(5)-C(4)	119.93 (14)	C(5)-C(6)-C(7)	122.21 (13)
C(6)-C(7)-C(2)	117.48 (11)	C(6)-C(7)-C(8)	118.51 (11)
C(2)-C(7)-C(8)	124.00 (12)	C(25)-C(8)-C(9)	117.45 (11)
C(25)-C(8)-C(7)	120.31 (11)	C(9)-C(8)-C(7)	122.21 (11)
C(10)-C(9)-C(14)	117.84 (11)	C(10)-C(9)-C(8)	123.06 (11)
C(14)-C(9)-C(8)	119.07 (12)	C(11)-C(10)-C(9)	121.79 (13)
C(10)-C(11)-C(12)	120.32 (13)	C(13)-C(12)-C(11)	119.95 (12)
C(12)-C(13)-C(14)	121.89 (13)	C(13)-C(14)-C(15)	120.60 (11)
C(13)-C(14)-C(9)	118.17 (12)	C(15)-C(14)-C(9)	121.21 (11)
C(16)-C(15)-C(14)	118.27 (11)	C(16)-C(15)-C(26)	120.86 (12)
C(14)-C(15)-C(26)	120.86 (11)	C(15)-C(16)-C(25)	120.21 (12)
C(15)-C(16)-C(17)	132.03 (11)	C(25)-C(16)-C(17)	107.75 (10)
C(18)-C(17)-C(22)	119.37 (12)	C(18)-C(17)-C(16)	132.27 (12)
C(22)-C(17)-C(16)	108.36 (11)	C(19)-C(18)-C(17)	119.08 (13)
C(18)-C(19)-C(20)	121.27 (14)	C(21)-C(20)-C(19)	120.17 (14)
C(22)-C(21)-C(20)	119.11 (13)	C(21)-C(22)-C(17)	120.99 (12)
C(21)-C(22)-C(23)	128.19 (12)	C(17)-C(22)-C(23)	110.78 (11)
C(25)-C(23)-C(22)	102.54 (9)	C(25)-C(23)-C(24)	108.34 (10)
C(22)-C(23)-C(24)	111.44 (10)	C(1)-C(24)-C(23)	116.38 (11)
C(8)-C(25)-C(16)	123.66 (11)	C(8)-C(25)-C(23)	125.81 (10)
C(16)-C(25)-C(23)	110.36 (11)	C(27)-C(26)-C(31)	117.87 (12)
C(27)-C(26)-C(15)	121.11 (12)	C(31)-C(26)-C(15)	121.00 (11)
C(26)-C(27)-C(28)	120.83 (14)	C(29)-C(28)-C(27)	120.60 (14)
C(30)-C(29)-C(28)	119.28 (13)	C(29)-C(30)-C(31)	120.29 (14)
C(26)-C(31)-C(30)	121.06 (13)		

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{31}\text{H}_{20}\text{O}$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}].$$

	U11	U22	U33	U23	U13	U12
O(1)	66(1)	81(1)	49(1)	-18(1)	-12(1)	-19(1)
C(1)	46(1)	43(1)	39(1)	-8(1)	-10(1)	3(1)
C(2)	45(1)	45(1)	32(1)	-4(1)	-6(1)	3(1)
C(3)	56(1)	67(1)	34(1)	1(1)	-11(1)	5(1)
C(4)	70(1)	76(1)	34(1)	13(1)	-6(1)	1(1)
C(5)	63(1)	64(1)	42(1)	12(1)	1(1)	-6(1)
C(6)	49(1)	52(1)	37(1)	3(1)	-4(1)	-3(1)
C(7)	44(1)	41(1)	31(1)	-2(1)	-4(1)	2(1)
C(8)	38(1)	36(1)	32(1)	0(1)	-7(1)	-3(1)
C(9)	38(1)	35(1)	37(1)	-1(1)	-5(1)	-4(1)
C(10)	42(1)	43(1)	40(1)	-1(1)	-3(1)	-3(1)
C(11)	41(1)	43(1)	53(1)	-4(1)	3(1)	-1(1)
C(12)	38(1)	45(1)	61(1)	6(1)	-5(1)	4(1)
C(13)	44(1)	44(1)	48(1)	7(1)	-10(1)	0(1)
C(14)	38(1)	35(1)	39(1)	1(1)	-8(1)	-2(1)
C(15)	42(1)	34(1)	35(1)	2(1)	-8(1)	-3(1)
C(16)	42(1)	34(1)	31(1)	0(1)	-6(1)	-3(1)
C(17)	44(1)	34(1)	33(1)	-3(1)	-4(1)	-1(1)
C(18)	55(1)	51(1)	33(1)	-3(1)	-4(1)	2(1)
C(19)	63(1)	66(1)	36(1)	-5(1)	7(1)	0(1)
C(20)	51(1)	68(1)	47(1)	-9(1)	7(1)	5(1)
C(21)	45(1)	51(1)	44(1)	-5(1)	-3(1)	6(1)
C(22)	44(1)	34(1)	36(1)	-3(1)	-3(1)	0(1)
C(23)	38(1)	36(1)	33(1)	1(1)	-5(1)	2(1)
C(24)	38(1)	41(1)	41(1)	-1(1)	-7(1)	-1(1)
C(25)	38(1)	34(1)	32(1)	0(1)	-6(1)	-1(1)
C(26)	39(1)	41(1)	34(1)	3(1)	-8(1)	2(1)
C(27)	78(1)	43(1)	46(1)	7(1)	-21(1)	-10(1)
C(28)	91(1)	53(1)	44(1)	-1(1)	-25(1)	-6(1)
C(29)	66(1)	60(1)	34(1)	7(1)	-8(1)	8(1)
C(30)	63(1)	49(1)	48(1)	14(1)	-6(1)	-3(1)
C(31)	59(1)	42(1)	43(1)	3(1)	-12(1)	-7(1)

Table 5. Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{31}\text{H}_{20}\text{O}$.

	x	y	z	U(eq)
H(3)	2510	6051	61	63
H(4)	4095	7491	-387	72
H(5)	5998	8079	125	67
H(6)	6317	7163	1064	55
H(10)	7005	4714	1064	50
H(11)	8996	3734	1321	55
H(12)	9453	3126	2302	58
H(13)	7906	3476	3011	54
H(18)	3427	4749	3971	56
H(19)	1325	5225	4295	66
H(20)	-271	6078	3652	66
H(21)	215	6440	2660	56
H(23)	2523	6925	1941	43
H(24A)	2214	3704	1849	48
H(24B)	1028	4813	1741	48
H(27)	6599	6091	3799	67
H(28)	6884	5504	4783	75
H(29)	6304	3146	5138	64
H(30)	5472	1354	4499	63
H(31)	5150	1944	3515	58