

Advanced
**Synthesis &
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Supporting Information

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Supporting Information for
Double Carbonylation Reactions of Enynols and Thiols to
form Thioester Substituted 6-Membered Ring Lactones

Hong Cao^{a,b}, Wen-Jing Xiao^{*,a} and Howard Alper^{*,b}

^a Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, 152 Luoyu Road, Wuhan, Hubei 430079, China; ^bCenter for Catalysis Research and Innovation, Department of Chemistry, University of Ottawa, 10 Marie Curie, Ottawa, Ontario K1N 6N5, Canada

howard.alper@uottawa.ca and wxiao@mail.ccnu.edu.cn

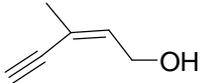
I, General .

Proton and carbon magnetic resonance spectra were recorded on a Bruker 300 MHz spectrometer. Chemical shifts are reported in ppm relative to tetramethylsilane as the internal standard. Mass spectra were obtained on a VG 7070E mass spectrometer. THF, toluene, and CH₂Cl₂ were distilled prior to use. All of the thiols employed in the reactions were purchased from Aldrich Chemical Co. and were used as received. 3-methyl-2-penten-4yn-1-ol, 3-ethyl-2-penten-4yn-1-ol, and 3-phenyl-2-penten-4yn-1-ol were prepared according to the literature.¹

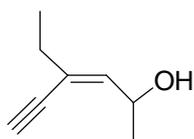
II, General Procedure for the Thiocarbonylation Reactions:

A mixture of **1** (3.0 mmol), thiol (1.0 mmol), Pd(OAc)₂ (0.05 mmol), PPh₃ (0.2 mmol) and THF (15 mL) was reacted in an autoclave at 500 psi of carbon monoxide for 36 h at 110 °C. The reaction mixture was cooled to room temperature and the excess CO was released. The mixture was filtered through Celite or silica gel, and concentrated by rotary evaporation. The separation and the purification of products were achieved by preparative TLC on silica gel using n-hexane-ethyl acetate (1:1) as the eluant .

III, Spectral data

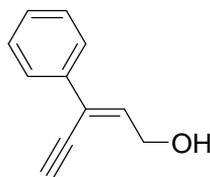
 ¹H NMR (300 MHz, CDCl₃) δ 1.81 (s, 1H), 1.87 (s, 3H), 3.14 (s, 1H), 4.30 (t, *J* = 6.0 Hz, 2H), 5.89-5.94 (t, *J* = 7.5 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 23.32, 35.01, 61.56, 82.13, 82.56, 120.17, 137.74; Spectral data are consistent with

literature.²



IR: ? 3296 cm^{-1} , 2966 cm^{-1} , 1251 cm^{-1} , 1081 cm^{-1} , 1000 cm^{-1} ; 962 cm^{-1} ;

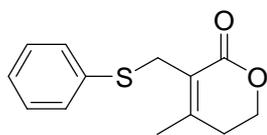
^1H NMR (300 MHz, CDCl_3) d 1.09 (t, $J = 7.5$ Hz, 3H), 1.27 (d, $J = 6.0$ Hz, 3H), 2.11-2.27 (m, 3H), 3.17 (s, 1H), 4.75-4.84 (m, 1H), 5.77 (d, $J = 7.5$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) d 13.12, 22.99, 30.29, 66.98, 81.54, 82.97, 124.69, 141.58; MS: m/e 124 (17, M^+), 109 (46), 95 (100);



^1H NMR (300 MHz, CDCl_3) d 2.89 (s, 1H), 4.62 (d, $J = 6.0$ Hz, 2H),

6.66 (t, $J = 6.0$ Hz, 1H), 7.35-7.67 (m, 5H); ^{13}C NMR (75 MHz, CDCl_3) d 61.09, 79.15, 84.25, 123.00, 125.49, 127.69, 136.03, 136.78; Spectral data are consistent with

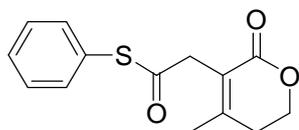
literature.³



IR: ? 1701 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 1.80 (s, 3H),

2.38-2.42 (t, $J = 6$ Hz, 2H), 3.90 (s, 2H), 4.26-4.30 (t, $J = 6$ Hz, 2H), 7.26-7.46 (m, 5H);

^{13}C NMR (75 MHz, CDCl_3) d 20.62, 31.11, 65.40, 110.66, 123.81, 129.23, 132.41, 135.90, 147.43, 153.56, 164.92;

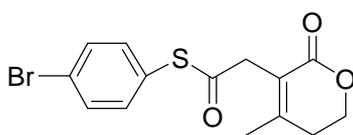


IR: ? 1701 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.03 (s, 3H),

2.50 (t, $J = 6.0$ Hz, 2H), 3.78 (s, 2H), 4.37 (t, $J = 6.0$ Hz, 2H), 7.41 (s, 5H); ^{13}C NMR

(75 MHz, CDCl_3) d 21.28, 31.13, 41.38, 65.51, 120.71, 127.89, 129.59, 129.86, 134.98, 155.34, 165.21, 195.03; Elemental analysis: calculate C 64.10, H 5.38; found C 64.21,

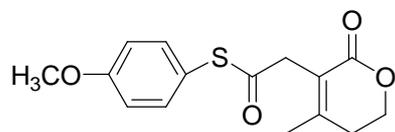
H 5.23;



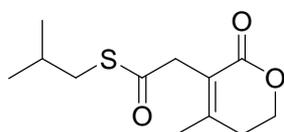
IR: ? 1701 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.02 (s,

3H), 2.55 (t, $J = 6.0$ Hz, 2H), 3.75 (s, 2H), 4.37 (t, $J = 6.0$ Hz, 2H), 7.24-7.53 (m, 4H);

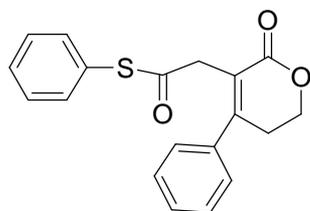
^{13}C NMR (75 MHz, CDCl_3) d 21.27, 31.12, 41.45, 65.53, 120.53, 124.50, 127.03, 132.76, 136.42, 155.60, 165.15, 194.35; Elemental analysis: calculate C 49.28, H 3.84; found C 49.51, H 3.84;



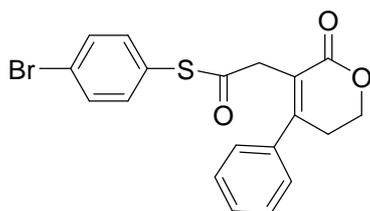
IR: ? 1701 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.04 (s, 3H), 2.51 (t, $J = 6.0$ Hz, 2H), 3.77 (s, 2H), 3.83 (s, 3H), 4.39 (t, $J = 6.0$ Hz, 2H); 6.93-7.35 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) d 21.26, 30.11, 31.16, 41.13, 55.75, 65.48, 115.26, 118.56, 120.87, 136.59, 155.04, 161.09, 196.05; Elemental analysis: calculated C 61.62, H 5.52; found C 61.31, H 5.51;



IR: ? 1737 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 0.96 (d, $J = 6.6$ Hz, 6H), 1.76-1.85 (m, 1H), 2.01 (s, 3H), 2.51 (t, $J = 6.0$ Hz, 2H), 2.80 (d, $J = 6.6$ Hz, 2H), 3.69 (s, 2H), 4.37-4.41 (t, $J = 6.0$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) d 21.17, 22.15, 29.07, 31.73, 37.75, 41.74, 65.72, 121.08, 154.71, 165.21, 196.85; Elemental analysis: calculate C 59.47, H 7.49; found C 59.73, H 7.55;

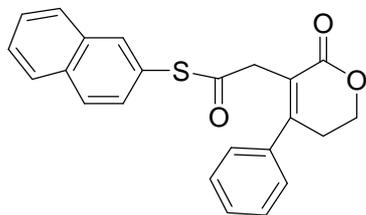


IR: ? 1709 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.82 (t, $J = 6.0$ Hz, 2H), 3.73 (s, 2H), 4.53 (t, $J = 6.0$ Hz, 2H), 7.30-7.44 (m, 10H); ^{13}C NMR (75 MHz, CDCl_3) d 31.35, 42.82, 65.97, 122.12, 127.34, 127.95, 129.34, 129.89, 135.03, 138.21, 155.97, 165.47, 195.66; Elemental analysis: calculate C 70.35, H 4.97; found C 70.13, H 4.89;

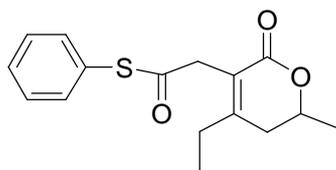


IR: ? 1709 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.82 (t, $J = 6.0$ Hz, 2H), 3.68 (s, 2H), 4.51 (t, $J = 6.0$ Hz, 2H), 7.23-7.52 (m, 9H); ^{13}C NMR (75

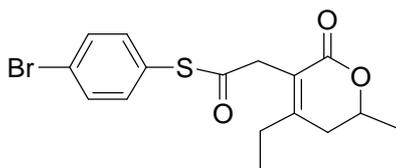
MHz, CDCl₃) d 31.34, 42.78, 65.90, 122.01, 124.53, 127.24, 129.32, 129.70, 132.74, 136.41, 138.09, 156.03, 165.32, 194.95; Elemental analysis: calculate C 56.59, H 3.75; found C 56.75, H 3.62;



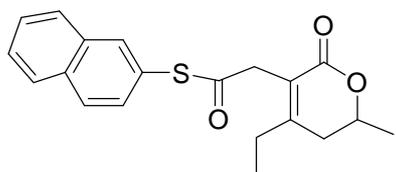
IR: ? 1704 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) d 2.84 (t, *J* = 6.0 Hz, 2H), 3.76 (s, 2H), 4.55 (t, *J* = 6.0 Hz, 2H), 7.28-7.97 (m, 12H); ¹³C NMR (75 MHz, CDCl₃) d 31.38, 42.84, 65.93, 122.23, 125.26, 126.94, 127.33, 127.57, 128.18, 128.42, 129.34, 129.69, 131.41, 133.77, 133.92, 134.92, 138.21, 153.88, 165.44, 195.88; Elemental analysis: calculated C 73.77, H 4.85; found C 73.91, H 4.88;



IR: ? 1701 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) d 1.12 (t, *J* = 7.5 Hz, 3H), 1.46 (d, *J* = 6.0 Hz, 3H), 2.28-2.41 (m, 4H), 3.77 (q, *J* = 7.5 Hz, 2H), 4.51-4.58 (m, 1H), 7.40 (s, 5H); ¹³C NMR (75 MHz, CDCl₃) d 11.88, 21.80, 27.79, 35.42, 41.11, 73.36, 119.52, 127.96, 129.59, 129.84, 134.99, 159.19, 166.11, 195.18 ;Elemental analysis: calculate C 66.18, H 6.25; found C 66.12, H 6.38;

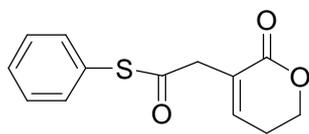


IR: ? 1701 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) d 1.13 (t, *J* = 7.5 Hz, 3H), 1.46 (d, *J* = 6.0 Hz, 3H), 2.32-2.45 (m, 4H), 3.83 (q, *J* = 7.5 Hz, 2H), 4.54-4.62 (m, 1H), 7.45-7.96 (m, 4H); ¹³C NMR (75 MHz, CDCl₃) d 11.89, 21.01, 27.80, 35.46, 41.15, 73.38, 119.44, 124.52, 127.04, 132.78, 136.43, 159.28, 194.58; Elemental analysis: calculate C 52.04, H 4.64; found C 52.20, H 4.68;

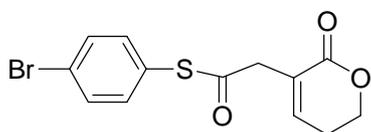


IR: ? 1701 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) d 1.15 (t, *J* = 7.5 Hz, 3H), 1.47 (d, *J* = 6.0 Hz, 3H), 2.32-2.45 (m, 4H), 3.83 (q, *J* = 7.5 Hz, 2H),

4.54-4.62 (m, 1H), 7.25-7.96 (m, 7H); ^{13}C NMR (75 MHz, CDCl_3) d 11.89, 21.01, 27.82, 35.48, 41.17, 73.37, 119.63, 125.41, 126.93, 127.55, 128.18, 128.40, 129.18, 131.39, 133.75, 133.93, 134.90, 159.11, 166.13, 195.43; Elemental analysis: calculate C 70.56, H 5.92; found C 70.59, H 5.82;



IR: ? 1704 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.55 (t, $J = 6.0$ Hz, 2H), 3.68 (s, 2H), 4.46 (t, $J = 6.0$ Hz, 2H), 6.88 (t, $J = 4.5$ Hz, 1H), 7.43 (s, 5H); ^{13}C NMR (75 MHz, CDCl_3) d 25.06, 30.11, 44.87, 66.93, 129.65, 129.97, 134.98, 144.21, 164.44, 194.93;



IR: ? 1704 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) d 2.51 (t, $J = 6.0$ Hz, 2H), 3.63 (s, 2H), 4.42 (t, $J = 6.0$ Hz, 2H), 6.84 (t, $J = 4.5$ Hz, 1H), 7.25-7.39 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) d 20.74, 31.26, 121.50, 123.61, 132.29, 133.50, 135.27, 153.84, 164.76, 195.31;

References:

1. (a) M. Alami, F. Ferri, G. Linstrumelle, *Tetrahedron Lett.* **1993**, 34, 6403-6406
(b) B. Gabriele, G. Salerno, F. De Pascali, M. Costa, G. Chiusoli, *J. Org. Chem.* **1999**, 64, 7693-7699
2. K. Mori, M. Ohki, A. Sato, M. Matsui, *Tetrahedron*, **1972**, 28, 3739-3745
3. K. Marx, W. Eberbach, *Chemistry—A European Journal*, **2000**, 6, 2063-2068

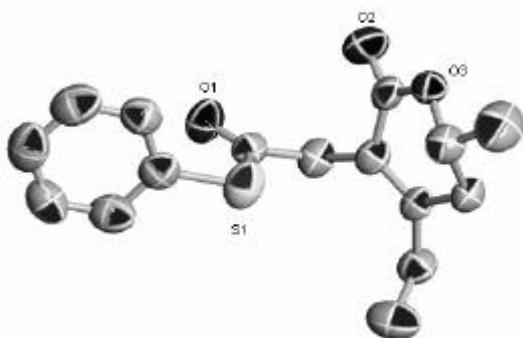


Table 1. Crystal data and structure refinement for ha05(**3h**).

Identification code	ha05
Empirical formula	C ₁₆ H ₁₈ O ₃ S
Formula weight	290.36
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.924(7) Å alpha = 90 deg. b = 9.996(6) Å beta = 98.094(11) deg. c = 13.988(9) Å gamma = 90 deg.
Volume	1512.3(16) Å ³
Z, Calculated density	4, 1.275 Mg/m ³
Absorption coefficient	0.218 mm ⁻¹
F(000)	616
Crystal size	0.40 x 0.30 x 0.25 mm
Theta range for data collection	2.51 to 24.81 deg.
Limiting indices	-12 ≤ h ≤ 12, -11 ≤ k ≤ 7, -14 ≤ l ≤ 16

Reflections collected / unique	6503 / 2449 [R(int) = 0.0311]
Completeness to theta = 24.81	93.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9475 and 0.9178
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2449 / 0 / 217
Goodness-of-fit on F ²	1.049
Final R indices [I > 2σ(I)]	R1 = 0.0511, wR2 = 0.1233
R indices (all data)	R1 = 0.0700, wR2 = 0.1334
Largest diff. peak and hole	0.277 and -0.232 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for ha05.

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

	x	y	z	U(eq)
S(1)	9220(1)	989(1)	6210(1)	69(1)
O(1)	9782(2)	990(2)	8105(1)	64(1)
O(2)	9462(2)	4609(2)	7491(2)	80(1)
O(3)	8737(2)	5237(2)	6028(1)	57(1)
C(1)	9098(2)	1413(3)	7437(2)	50(1)
C(2)	8029(2)	2347(3)	7530(2)	56(1)
C(3)	7795(2)	3348(3)	6731(2)	48(1)
C(4)	8729(2)	4413(3)	6775(2)	51(1)
C(5)	8025(2)	4855(3)	5118(2)	56(1)
C(6)	8052(3)	6017(4)	4443(3)	79(1)
C(7)	6712(8)	4522(9)	5310(7)	45(2)
C(8)	6746(4)	3493(5)	6096(3)	42(1)
C(9)	5607(4)	2673(4)	6097(3)	55(1)
C(10)	5397(7)	1683(6)	5293(4)	82(1)
C(7')	6930(30)	4160(30)	5170(30)	58(6)
C(8')	7061(13)	3087(15)	5923(12)	44(4)

C(9')	6151(12)	1923(13)	5757(11)	59(3)
C(10')	4827(12)	2292(16)	5579(13)	69(4)
C(11)	10199(3)	-1517(3)	6519(2)	62(1)
C(12)	11148(3)	-2413(3)	6694(2)	71(1)
C(13)	12343(3)	-1990(3)	6738(2)	68(1)
C(14)	12589(3)	-665(4)	6604(2)	67(1)
C(15)	11644(3)	240(3)	6443(2)	60(1)
C(16)	10440(2)	-189(3)	6405(2)	51(1)

Table 3. Bond lengths [Å] and angles [deg] for ha05.

S(1)-C(16)	1.771(3)
S(1)-C(1)	1.791(3)
O(1)-C(1)	1.189(3)
O(2)-C(4)	1.207(3)
O(3)-C(4)	1.330(3)
O(3)-C(5)	1.446(3)
C(1)-C(2)	1.515(4)
C(2)-C(3)	1.495(4)
C(3)-C(8')	1.316(17)
C(3)-C(8)	1.355(6)
C(3)-C(4)	1.470(4)
C(5)-C(7')	1.39(4)
C(5)-C(6)	1.501(4)
C(5)-C(7)	1.532(10)
C(7)-C(8)	1.502(12)
C(8)-C(9)	1.490(6)
C(9)-C(10)	1.491(7)
C(7')-C(8')	1.50(4)
C(8')-C(9')	1.53(2)
C(9')-C(10')	1.479(18)
C(11)-C(16)	1.367(4)
C(11)-C(12)	1.366(4)
C(12)-C(13)	1.366(4)
C(13)-C(14)	1.370(4)
C(14)-C(15)	1.367(4)
C(15)-C(16)	1.377(4)
C(16)-S(1)-C(1)	99.52(12)
C(4)-O(3)-C(5)	117.7(2)
O(1)-C(1)-C(2)	124.0(2)
O(1)-C(1)-S(1)	123.1(2)

C(2)-C(1)-S(1)	112.96(18)
C(3)-C(2)-C(1)	113.6(2)
C(8')-C(3)-C(8)	26.1(4)
C(8')-C(3)-C(4)	121.0(7)
C(8)-C(3)-C(4)	117.9(3)
C(8')-C(3)-C(2)	121.9(7)
C(8)-C(3)-C(2)	127.0(3)
C(4)-C(3)-C(2)	114.1(2)
O(2)-C(4)-O(3)	118.3(3)
O(2)-C(4)-C(3)	121.8(3)
O(3)-C(4)-C(3)	119.8(2)
C(7')-C(5)-O(3)	116.6(14)
C(7')-C(5)-C(6)	120.6(14)
O(3)-C(5)-C(6)	107.1(2)
C(7')-C(5)-C(7)	18.4(10)
O(3)-C(5)-C(7)	107.7(4)
C(6)-C(5)-C(7)	112.3(4)
C(8)-C(7)-C(5)	110.5(6)
C(3)-C(8)-C(7)	119.0(5)
C(3)-C(8)-C(9)	124.7(4)
C(7)-C(8)-C(9)	116.3(5)
C(10)-C(9)-C(8)	113.8(4)
C(5)-C(7')-C(8')	113(2)
C(3)-C(8')-C(9')	126.0(13)
C(3)-C(8')-C(7')	116.6(18)
C(9')-C(8')-C(7')	116.4(18)
C(10')-C(9')-C(8')	115.9(12)
C(16)-C(11)-C(12)	120.2(3)
C(11)-C(12)-C(13)	120.1(3)
C(12)-C(13)-C(14)	119.9(3)
C(15)-C(14)-C(13)	120.2(3)
C(14)-C(15)-C(16)	119.7(3)
C(11)-C(16)-C(15)	119.8(3)
C(11)-C(16)-S(1)	120.7(2)
C(15)-C(16)-S(1)	119.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ha05.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
S(1)	78(1)	88(1)	42(1)	3(1)	4(1)	25(1)
O(1)	67(1)	79(1)	43(1)	6(1)	-1(1)	16(1)
O(2)	72(1)	87(2)	72(1)	-4(1)	-19(1)	-7(1)
O(3)	48(1)	55(1)	67(1)	5(1)	6(1)	-6(1)
C(1)	52(1)	57(2)	41(1)	6(1)	5(1)	-3(1)
C(2)	53(1)	72(2)	45(2)	6(1)	12(1)	6(1)
C(3)	41(1)	60(2)	43(1)	4(1)	8(1)	4(1)
C(4)	40(1)	55(2)	55(2)	-6(1)	2(1)	10(1)
C(5)	57(2)	60(2)	52(2)	4(1)	14(1)	1(1)
C(6)	75(2)	89(2)	77(2)	29(2)	23(2)	0(2)
C(7)	40(3)	56(5)	41(3)	2(3)	5(2)	6(3)
C(8)	34(2)	54(3)	40(2)	-3(2)	12(2)	9(2)
C(9)	44(2)	64(2)	57(2)	4(2)	10(2)	-2(2)
C(10)	82(4)	80(4)	86(4)	-13(3)	21(3)	-27(3)
C(7')	52(11)	53(14)	70(14)	5(9)	12(9)	18(8)
C(8')	39(7)	43(9)	55(8)	-4(6)	29(6)	7(5)
C(9')	53(7)	48(7)	76(9)	-7(6)	8(7)	-4(6)
C(10')	45(7)	72(10)	89(10)	14(8)	-2(7)	-13(7)
C(11)	59(2)	66(2)	64(2)	-5(1)	19(1)	-11(1)
C(12)	89(2)	55(2)	74(2)	-2(2)	31(2)	1(2)
C(13)	72(2)	77(2)	56(2)	-2(2)	17(1)	22(2)
C(14)	54(2)	91(2)	57(2)	-6(2)	10(1)	-7(2)
C(15)	67(2)	59(2)	56(2)	-1(1)	12(1)	-8(1)
C(16)	57(2)	59(2)	37(1)	-2(1)	7(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ha05.

	x	y	z	U(eq)
H(2A)	7279	1813	7543	68
H(2B)	8199	2825	8146	68
H(5A)	8402	4060	4854	83
H(5B)	8546	4173	4857	83
H(6A)	8872	6409	4529	119

H(6B)	7455	6683	4580	119
H(6C)	7845	5710	3782	119
H(7A)	6310	5336	5502	54
H(7B)	6228	4180	4718	54
H(9A)	5661	2195	6713	66
H(9B)	4892	3273	6052	66
H(10A)	4642	1189	5336	123
H(10B)	6089	1066	5342	123
H(10C)	5324	2148	4680	123
H(7C)	6650	3760	4537	70
H(7D)	6298	4800	5306	70
H(9C)	6345	1406	5202	71
H(9D)	6283	1336	6323	71
H(10D)	4327	1487	5505	104
H(10E)	4667	2824	4995	104
H(10F)	4618	2808	6121	104
H(11A)	9376	-1814	6476	74
H(12A)	10978	-3322	6785	85
H(13A)	12996	-2607	6860	81
H(14A)	13411	-376	6623	80
H(15A)	11815	1150	6358	72

Table 6. Torsion angles [deg] for ha05.

C(16)-S(1)-C(1)-O(1)	4.3(3)
C(16)-S(1)-C(1)-C(2)	-175.09(19)
O(1)-C(1)-C(2)-C(3)	145.2(3)
S(1)-C(1)-C(2)-C(3)	-35.5(3)
C(1)-C(2)-C(3)-C(8')	88.3(7)
C(1)-C(2)-C(3)-C(8)	119.4(4)
C(1)-C(2)-C(3)-C(4)	-72.4(3)
C(5)-O(3)-C(4)-O(2)	168.7(2)
C(5)-O(3)-C(4)-C(3)	-14.8(3)
C(8')-C(3)-C(4)-O(2)	-175.1(7)
C(8)-C(3)-C(4)-O(2)	155.1(3)
C(2)-C(3)-C(4)-O(2)	-14.3(3)
C(8')-C(3)-C(4)-O(3)	8.4(7)
C(8)-C(3)-C(4)-O(3)	-21.4(4)
C(2)-C(3)-C(4)-O(3)	169.3(2)
C(4)-O(3)-C(5)-C(7')	34.2(11)
C(4)-O(3)-C(5)-C(6)	172.7(2)
C(4)-O(3)-C(5)-C(7)	51.7(4)

C(7')-C(5)-C(7)-C(8)	68(6)
O(3)-C(5)-C(7)-C(8)	-54.1(6)
C(6)-C(5)-C(7)-C(8)	-171.8(4)
C(8')-C(3)-C(8)-C(7)	-89.1(19)
C(4)-C(3)-C(8)-C(7)	15.1(6)
C(2)-C(3)-C(8)-C(7)	-177.1(4)
C(8')-C(3)-C(8)-C(9)	89(2)
C(4)-C(3)-C(8)-C(9)	-166.5(3)
C(2)-C(3)-C(8)-C(9)	1.2(6)
C(5)-C(7)-C(8)-C(3)	22.5(7)
C(5)-C(7)-C(8)-C(9)	-156.0(4)
C(3)-C(8)-C(9)-C(10)	-106.9(5)
C(7)-C(8)-C(9)-C(10)	71.5(6)
O(3)-C(5)-C(7')-C(8')	-43.9(17)
C(6)-C(5)-C(7')-C(8')	-176.5(10)
C(7)-C(5)-C(7')-C(8')	-109(7)
C(8)-C(3)-C(8')-C(9')	-96(2)
C(4)-C(3)-C(8')-C(9')	173.4(9)
C(2)-C(3)-C(8')-C(9')	14.0(14)
C(8)-C(3)-C(8')-C(7')	72(2)
C(4)-C(3)-C(8')-C(7')	-19.0(14)
C(2)-C(3)-C(8')-C(7')	-178.4(11)
C(5)-C(7')-C(8')-C(3)	37(2)
C(5)-C(7')-C(8')-C(9')	-154.3(14)
C(3)-C(8')-C(9')-C(10')	114.5(15)
C(7')-C(8')-C(9')-C(10')	-53(2)
C(16)-C(11)-C(12)-C(13)	-1.3(4)
C(11)-C(12)-C(13)-C(14)	-0.1(4)
C(12)-C(13)-C(14)-C(15)	1.1(4)
C(13)-C(14)-C(15)-C(16)	-0.7(4)
C(12)-C(11)-C(16)-C(15)	1.7(4)
C(12)-C(11)-C(16)-S(1)	-178.3(2)
C(14)-C(15)-C(16)-C(11)	-0.7(4)
C(14)-C(15)-C(16)-S(1)	179.3(2)
C(1)-S(1)-C(16)-C(11)	89.4(2)
C(1)-S(1)-C(16)-C(15)	-90.5(2)

Symmetry transformations used to generate equivalent atoms:

