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Products of Ozone Oxidation of Some Saturated Cyclic Hydrocarbons

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Abstract—Low-temperature ozone oxidation of a series of saturated carbocyclic hydrocarbons afforded the corresponding alcohols and/or ketones in high yield through intermediate trioxidanes. *exo,endo*-Tetracyclo-[6.2.1.0^{3,5}]undecane-2,7-dione and *exo,endo,endo*-hexacyclo[9.3.1.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane-2,10-dione were isolated, and *exo,endo,exo*-pentacyclo[6.3.1.0^{2,7}.0^{3,5}.0^{9,11}]dodecyl-, *exo,exo,exo*-heptacyclo-[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecyl, and 1-methylcyclohexyltrioxidanes were identified and characterized for the first time.

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Oxygen-containing derivatives of polycyclic hydrocarbons attract much interest as potential biologically active substances. Saturated polycyclic hydrocarbons have found wide application in the manufacture of multipurpose propellants [1] which undergo oxidation on storage; therefore, studies of their oxidative transformations by the action of various oxidants are also topical. Ozone is a popular oxidant which is widely used to obtain oxygen-containing organic compounds. However, room temperature ozonolysis is insufficiently selective. The selectivity of ozonolysis both in solution and on silica surface can be improved by reducing the reaction temperature to -30° C and lower. As a rule, low-temperature ozonation of cyclic hydrocarbons and alkanes on silica gel is characterized by high conversion, significant selectivity, and complete retention of configuration [2–6].

In this work we studied intermediates and products of low-temperature ozonation of *exo,endo*-tetracyclo- $[6.2.1.0^{2,7}.0^{3,5}]$ undecane (1a), *exo,endo,exo*-pentacyclo- $[6.3.1.0^{2,7}.0^{3,5}.0^{9,11}]$ dodecane (2a), *exo,endo,endo*-hexacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane (3 a), *e x o*, *e x o*, *e x o* - h e p t a c y c l o- $[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]$ pentadecane (4a), methylcyclohexane (5a), and bicyclo[4.1.0]heptane (6a) in solution and on silica surface, the corresponding alkyltrioxidanes (ROOOH) 1b–6b and alcohols and/or ketones.

The oxidation of compounds **1a–6a** with ozone was characterized by high yields (Table 1). The oxidation

was carried out on silica surface when the substrate solubility was low or the reaction in solution was slow. The oxidation of **1a** with ozone was selective only on silica surface, and the product was *exo,endo*-tetracyclo[$6.2.1.0^{2,7}.0^{3,5}$]undecan-2-ol (**1c**); in addition, *exo,endo*-tricyclo[$6.2.1.0^{3,5}$]undecane-2,7-dione (**1d**) was formed as a result of cleavage of the C²–C⁷ bond.

Compound **2a** was oxidized both in solution and on silica surface. Unlike low-temperature ozonation in methylene chloride, the oxidation on silica surface was fast and selective with formation of *exo*,*endo*,*exo*-pentacyclo[$6.3.1.0^{2,7}.0^{3,5}.0^{9,11}$]dodecan-2-ol (**2c**). The ozonation of **3a** both on silica surface and in solution gave the C²-C¹⁰ bond cleavage product, *exo*,*endo*,*endo*-hexacyclo[$9.3.1.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}$]-pentadecane-2,10-dione (**3c**). The structures of **2c** and **3c** were determined by X-ray analysis (Figs. 1, 2).

The oxidation of **4a** occurred at an appreciable rate only on silica surface at -35° C to afford *exo,exo,exo*heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2ol (**4c**). As reported in [1], the oxidation of **3a** and **4a** with dimethyl- and methyl(trifluoromethyl)dioxirane (CCl₄, 20°C) gave the corresponding alcohols in high yields [1]. The ozonation of methylcyclohexane (**5a**) on silica surface was described in [3]; therefore, we examined its oxidation in solution. In both cases, the final product was 1-methylcyclohexan-1-ol (**5c**). A mixture of the corresponding alcohol and ketone, bicyclo[4.1.0]heptan-2-ol (**7a**) and bicyclo[4.1.0]heptan-2-one (**7c**), was obtained in the oxidation of **6a**

15 10 Me 14 1a 2a 3a 4a 5a Comp. Ozonation Sorbent Conversion, % ROOOH Final product time, min or solvent no. **OOOH** QН 1b 1c 1a 50 SiO_2 100 0 ó 1d ОООН ŌН 2a 120 $CH_2Cl_2 \\$ 70 90 SiO₂ 80 120 SiO_2 98 2b 2c ооон 0 60 50 3a $CH_2Cl_2 \\$ 120 $CH_2Cl_2 \\$ 98 0 110 SiO_2 98 3b 3c **4a**^b 230 SiO_2 40 о́оон ÓН 4b 4c Ме Me -ооон юн

60

98

5b

Н

6b

ОН

7b

юоон

юоон



а Based on the reacted substrate.

60

75

 b At –35°C.

5a

6a

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t-BuOMe

t-BuOMe

6a

Yield,^a %

82

18

56

61

60

70

82

80

98

98

5 [7]

92 [7]

5c

7a

7c

.OH

-0



Fig. 1. Structure of the molecule of *exo,endo,exo-*pentacyclo- $[6.3.1.0^{2.7}.0^{3.5}.0^{9.11}]$ dodecan-2-ol (**2c**) according to the X-ray diffraction data.

with ozone in solution [7]. In all cases, the oxidation involved the weakest tertiary C–H bond (Table 2), which suggests a mechanism involving abstraction of

Table 2. Energies of dissociation of C–H bonds in molecules 1a-6a, calculated by the DFT/(U)B3PW91/6-31+G(d) method

Comp. no.	E_{C-H} , kcal/mol (atom number)		
1a	101.1 (1), 88.4 (2), 101.8 (3), 102.9 (4), 102.7 (5), 89.5 (6), 91.8 (7), 100.9 (8), 91.9 (9), 92.5 (10), 99.2 (11)		
2a	100.1 (1), 88.4 (2), 101.9 (3), 102.9 (4), 102.6 (5), 90.2 (6), 92.7 (7), 100.0 (8), 102.4 (9), 102.3 (10), 103.4(11), 97.6 (12)		
3 a	99.9 (1), 89.7 (2), 99.2 (3), 105.1 (4), 107.5 (5), 104.6 (8), 95.0 (9), 102.1 (13), 103.8 (14), 96.6 (15)		
4 a	100.6 (1), 93.0 (2), 99.4 (3), 106.4 (4), 107.5 (5), 103.2 (8), 95.1 (9), 101.9 (13), 103.7 (14), 94.0 (15)		
5a	90.1 (1), 93.3 (2), 93.0 (3), 93.1 (4), 96.8 (Me)		
6a	98.8 (1) 88.7 (2) 91.5 (3) 102.7 (7)		

Table 3. Chemical shifts of the OOOH proton in alkyltrioxidanes 2b, 4b, and 5b

Comp. no.	Solvent	δ _{000н} , ppm
2b	Acetone- d_6 -CFCl ₃ , 1:1	11.7–13.7 m
4b Acetone- d_6 -CFCl ₃ , 1		12.6–13.0 m
5b	Toluene- <i>d</i> ₈ –CFCl ₃ , 1:1	13.60 br.s



Fig. 2. Structure of the molecule of *exo,endo,endo*-hexa-cyclo[$9.3.1.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}$]pentadecane-2,10-dione (3c) according to the X-ray diffraction data.

hydrogen. Among carbocycles **1a–6a**, the reacting C^2 –H bond in **4a** is the strongest ($E_{CH} = 93.0 \text{ kcal} \times \text{mol}^{-1}$), which is responsible for the low reactivity of **4a**. Cleavage of the C^2 – C^{10} bond in **3a** and retention of the corresponding bond in *exo,exo,exo* isomer **4a** may be accounted for by the higher strength of that bond in the latter [by 6.4 kcal/mol according to B3PW91/ 6-31+G(*d*) calculations].

As a rule, ozonation of saturated organic compounds involves intermediate formation of trioxidanes. We were the first to identify by NMR spectroscopy three new trioxidanes **2b**, **4b**, and **5b**. The low-temperature ¹H NMR spectra (-40° C, CFCl₃-acetone-*d*₆) of the reaction mixtures displayed a multiplet in the region δ 11.5–14 ppm, which was assigned to the OOOH proton. The signal disappeared when the temperature rose to ambient (Table 3). Broadening of that signal in the spectra of **2b** and **4b** is likely to be related to specific solvation of trioxidanes with acetone to form stronger solvate shells which stabilize different trioxidane associates [8]. In the ozonation of **1a** and **3a**, diketones **1d** and **3c** may be formed via decomposition of bis-trioxidanes (Scheme 1).

It is known that many oxidation processes are accompanied by chemiluminescence which provides information on both emission source and reaction kinetics. We determined kinetic parameters of thermal decomposition of trioxidanes **5b** and **6b** in *tert*-butyl methyl ether by the IR chemiluminescence (IR-CL) method. Here, singlet oxygen acts as emitter. Compounds **1b–4b** showed no chemiluminescence in the IR region. The IR-CL decay curves for **5b** and **6b** are well described by first-order equations. The effective rates of decomposition (k_d) were calculated from the



semilog CL decay plots (Table 4), and the obtained data were used to calculate the activation parameters.

 $\log k_{5b} = (3.5 \pm 0.3) - (26.8 \pm 0.7)/2.3 RT;$ $\log k_{7b} = (11.9 \pm 0.9) - (81.7 \pm 1.9)/2.3 RT (kJ/mol).$

The IR-CL decay curve for the low-temperature ozonation of **6a** consists of two parts, which may be rationalized assuming the presence of two trioxidanes, **6b** (*endo*,*exo*) and **7b** (*endo*,*exo*), since the rate of ozonation of alcohols is much higher than the rate of ozonation of hydrocarbons [9] (Scheme 2). Comparison of the rate constants for the decomposition of **6b**, calculated from the IR-CL decay curve by the first-order equation (Table 4), with published data [7] led us to conclude that the first (fast) part of the IR-CL decay curve corresponds to the decomposition of alkyltrioxidane **6b**, and the second (slow), to the decomposition of trioxidanyl alcohol **7b**.

The observed chemiluminescence in the IR region suggests formation of singlet oxygen $(^{1}O_{2})$ in the decomposition of trioxidanes **5b** and **6b**. The yield of

singlet oxygen in the decomposition of **5b** does not exceed 1%, which is consistent with the data obtained previously for other alkyltrioxidanes. For example, the yield of ${}^{1}O_{2}$ from adamantyltrioxidane is 7.2%

Table 4. Effective rate constants (k_d) for the decomposition of trioxidanes **5b**-**7b** (*t*-BuOMe; $c_{5b} = 3.1 \times 10^{-2}$, $c_{6b} = c_{7b} = 3.36 \times 10^{-2}$ M)

Comp. no.	Temperature, °C	$k_{\rm d} \times 10^2$, s ⁻¹	$k_{\rm d} \times 10^2$, s ⁻¹ [7]
5b	-9.0	1.8 ± 0.2	_
	0.0	3.2 ± 0.3	_
	10.0	4.7 ± 0.4	_
	20.0	6.3 ± 0.6	_
6b	0.0	1.5 ± 0.2	$0.5 {\pm} 0.05$
	10.0	2.1 ± 0.2	1.5 ± 0.1
	20.0	3.5 ± 0.3	2.9 ± 0.2
7b	0.0	0.03 ± 0.003	$0.05 {\pm} 0.005$
	10.0	0.08 ± 0.008	$0.19 {\pm} 0.02$
	20.0	$0.24 {\pm} 0.02$	$0.75 {\pm} 0.07$

(-3.0°C, CH₂Cl₂), and from decahydronaphthalen-4ayltrioxidane, 1.2% (6.0°C, CH₂Cl₂) [8]. The overall yield of singlet oxygen in the decomposition of mixture **6b**/**7b** is 15.2% (20°C, *t*-BuOMe), and the major contribution is that of **7b**.

In summary, we have found conditions for efficient ozonation of cyclic hydrocarbons 1a-6a. The reaction involves the weakest C-H bond with intermediate formation of the corresponding trioxidanes. The oxidation of 1a and 3a with ozone is accompanied by decomposition of the carbon skeleton and formation of previously unknown diketones 1d and 3c.

EXPERIMENTAL

The spectral and analytical data were obtained at the *Khimiya* Joint Center, Ufa Institute of Chemistry, Russian Academy of Sciences. The ¹H and ¹³C NMR spectra were recorded on a Bruker AM-300 spectrometer at 300 and 75.47 MHz, respectively, using tetramethylsilane as internal standard. Chromatographic analysis was performed on a Chrom-5 gas chromatograph (5 m×3-mm column, stationary phase SE-30, oven temperature 50–270°C, carrier gas helium). The mass spectra were recorded on a Finnigan MAT GCQ GC/MS System (DB-5MS column, 30 m×0.25 m, film thickness 0.25 µm; carrier gas helium). The elemental compositions were determined on an EA-300 CHNSanalyzer (HEKA-Tech).

Quantum-chemical calculations were performed using a combination of the Becke three-parameter hybrid exchange functional (B3) [10, 11] and PW91 correlation functional [12] (B3PW91) and standard 6-31+G(d) basis set [13]. All geometric parameters of molecules and radical species were optimized at the B3PW91/6-31+G(d) level of theory without symmetry restrictions. The optimized structures were localized on the potential energy surface by analysis of the corresponding Hessian eigenvalues. The energies were corrected for zero-point vibration energy calculated by the DFT/B3PW91/6-31+G(d) method. The thermodynamic parameters were calculated for 298 K and 1 atm. All calculations were performed at the *Khimiya* Joint Center using NW Chem Ver. 5 software package [14].

General procedure for low-temperature ozonation. Ozone was generated in a conventional ozonizer [15]. Silica gel (Lancaster, 0.06–0.2 mm) was calcined at 300–350°C. All solvents were dried by standard procedures and distilled before use.

a. Ozonation in solution. A cold ozone/oxygen mixture was passed through a solution of 2a (0.2 mL, 1.4 mmol) or **3a** (0.13 g, 0.6 mmol) in 3 mL of methylene chloride or of **5a** (0.2 mL, 1.6 mmol) or **6a** (0.2 mL, 2 mmol) in 10 mL of *tert*-butyl methyl ether, maintained at -78° C.

b. Ozonation on silica surface. Compound 1a (0.15 mL, 1.1 mmol), 2a (0.2 mL, 1.4 mmol), 3a (0.26 g, 1.3 mmol), or 4a (0.12 g, 0.6 mmol), was dissolved in 15 mL of pentane, the solution was added to 3 g of freshly calcined silica gel under vigorous stirring, and the solvent was evaporated [16]. The sorbent was placed into a reactor, the reactor was cooled to a required temperature, and a cold ozone/oxygen mixture was supplied thereto.

Excess ozone was removed from the solution or silica surface by purging with oxygen. In both cases, the amount of absorbed ozone was determined by spectrophotometry [17]. The products were eluted from silica with cold acetone, and the concentration of trioxidanes **1b–6b** was determined as described in [18]. The solution was then allowed to warm up to room temperature to obtain final products.

The kinetics of decomposition of trioxidanes **1b–6b** were studied by the IR-CL method [17] in the temperature range from –9 to 20°C. A 10-mL reactor maintained at a constant temperature was charged with 1–2 mL of *tert*-butyl methyl ether, and 0.5–1.5 mL of a solution of ROOOH (0.012–0.049 M) was quickly added. After thermal equilibration, the kinetics of chemiluminescence decay were measured. The chemiluminescence setup was calibrated against triphenyl phosphite ozonide with a known yield of singlet oxygen (F = 1.0) [19]. The yield of singlet oxygen in the thermolysis of trioxidanes was calculated as described in [20].

exo,endo-Tetracyclo[6.2.1.0^{2,7}.0^{3,5}]undecan-2-ol (1c). Yield 82%. ¹³C NMR spectrum (CDCl₃), $\delta_{\rm C}$, ppm: 10.89 (C⁵), 21.38 (C⁶), 21.84 (C⁴), 22.87 (C⁹), 26.60 (C¹⁰), 28.73 (C³), 40.61 (C¹¹), 41.73 (C⁸), 49.00 (C¹), 55.80 (C⁷), 92.00 (C²). Found, %: C 80.42; H 9.88. C₁₁H₁₆O. Calculated, %: C 80.44; H 9.82.

exo,endo-Tetracyclo[6.2.1.0^{3,5}]undecane-2,7-dione (1d). Yield 18%. ¹³C NMR spectrum (CDCl₃), δ_{C} , ppm: 9.87 (C⁵), 17.10 (C⁴), 26.91 (C¹⁰), 28.05 (C⁹), 30.81 (C⁶), 36.66 (C³), 41.00 (C¹¹), 51.34 (C¹), 53.16 (C⁸), 212.4 (C⁷), 213.4 (C²). Found, %: C 74.15; H 7.93. C₁₁H₁₄O₂. Calculated, %: C 74.13; H 7.91.

exo,endo,exo-Pentacyclo[6.3.1.0^{2,7}.0^{3,5}.0^{9,11}]dodecan-2-ol (2c). ¹³C NMR spectrum (CDCl₃), $\delta_{\rm C}$, ppm: 3.32 (C¹⁰), 9.38 (C⁹), 10.36 (C¹¹), 10.41 (C⁴), 22.91 (C³), 25.92 (C⁵), 27.65 (C⁶), 28.28 (C¹²), 39.98 (C⁸), 47.85 (C¹), 57.08 (C⁷), 93.21 (C²). Mass spectrum, *m/z* (I_{rel} , %): 176 (0.3) [*M*]⁺, 158 (0.6), 147 (0.8), 133 (1.6), 121 (1.8), 117 (2.2), 115 (3.2), 107 (2.2), 97 (10.3), 96 (100), 95 (52.4), 91 (10.5), 81 (23.5), 80 (9.3), 79 (20.7), 78 (7.3), 77 (20.3), 67 (17.8), 55 (12.6), 53 (9.7). Found, %: C 81.76; H 9.17. C₁₂H₁₆O. Calculated, %: C 81.77; H 9.15. *M* 176.26.

exo,endo,endo-Hexacyclo[9.3.1.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane-2,10-dione (3c). ¹H NMR spectrum (acetone- d_6), δ , ppm: 0.20 d.t (1H, 13-H, J = 3.81, 3.77 Hz), 0.70 d.t (1H, 13-H, J = 8.22, 8.20 Hz), 1.30 d.t (1H, 6-H, J = 1.04, 5.54 Hz), 1.38 m (2H, 7-H), 1.42–1.50 m (1H, 15-H), 1.85–1.93 m (4H, 4-H, 5-H, 12-H, 14-H), 2.02–2.10 m (2H, 8-H, 15-H), 2.50– 2.55 m (2H, 3-H, 9-H), 2.90–3.00 m (2H, 1-H, 11-H). ¹³C NMR spectrum (acetone- d_6), δ_C , ppm: 7.13 (C¹³), 10.63 (C⁶), 15.18 (C⁴, C⁵), 21.63 (C¹², C¹⁴), 31.15 (C¹⁵), 36.80 (C⁷), 42.26 (C⁸), 54.39 (C¹, C¹¹), 58.92 (C³, C⁹), 213.18 (C², C¹⁰). Found, %: C 78.91; H 7.08. C₁₅H₁₆O₂. Calculated, %: C 78.92; H 7.06.

The spectral parameters of *exo,exo,exo*-heptacyclo- $[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]$ pentadecan-2-ol (4c), 1-methylcyclohexan-1-ol (5c), bicyclo[4.1.0]heptan-2-ol (7a), and bicyclo[4.1.0]heptan-2-one (7c) were consistent with published data [1, 7, 21–29].

The X-ray diffraction data for compounds 2c and 3c were obtained at the Institute of Organoelement Compounds, Russian Academy of Sciences, on a Bruker SMART diffractometer with a CCD detector (Mo K_{α} radiation, $\lambda 0.71073$ Å, ω -scanning, $2\theta_{max} = 58.24^{\circ}$). A correction for absorption was applied using SADABS program [30] ($T_{max} = 0.923$, $T_{min.} = 0.056$). The structures were solved by the direct method and were refined against F_{hkl}^2 by the full-matrix leastsquares procedure in anisotropic approximation for all non-hydrogen atoms and isotropic approximation for all localized hydrogen atoms. The positions of hydrogen atoms were calculated on the basis of geometry considerations and were refined according to the riding model: $U(H) = 1.5 U_{eq}(C)$, where $U_{eq}(C)$ is the equivalent temperature factor of the corresponding carbon atom. All calculations were performed using SHELXTL-Plus 5 software package [31].

Compound **2c**. $C_{12}H_{15}O$; *M* 175.24; monoclinic crystal system, space group *P*21/*c*; unit cell parameters [173(2) K]: a = 13.333(3), b = 17.160(3), c = 12.218(2) Å; V = 2793.7(10) Å³; Z = 4; $d_{calc} = 1.257$ g× cm⁻³. Total of 4898 reflection intensities were measured from a $0.2 \times 0.1 \times 0.1$ -mm colorless single crystal.

Final divergence factors: $wR_2 = 0.1913$ (all independent reflections), $R_1 = 0.0983$ [4653 reflections with $I > 2\sigma(I)$]; goodness of fit 0.902.

Compound **3c**. $C_{15}H_{16}O_2$; *M* 228.28; orthorhombic crystal system, space group *P*21/*mn*; unit cell parameters [293(2) K]: a = 9.218(5), b = 6.148(3), c = 9.907(5) Å; V = 561.4(5) Å³; Z = 2; $d_{calc} = 1.350$ g× cm⁻³. Total of 4017 reflection intensities were measured from a $0.4 \times 0.3 \times 0.2$ -mm colorless single crystal. Final divergence factors $wR_2 = 0.0962$ (all independent reflections), $R_1 = 0.0477$ [1226 reflections with $I > 2\sigma(I)$]; goodness of fit 0.960.

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