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Estimation of Enthalpies of Alkoxy Radical Formation and Bond Strengths in Alcohols and Ether

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Abstract—Kinetic data on the thermal decomposition of peroxides were analyzed, and energies of the O–O bond dissociation were calculated. Enthalpies of formation of various alkoxy radicals and peroxides were determined. The dissociation energies for the O–H bonds in alcohols and C–O bonds in ethers were estimated. Comparative analysis of literature and obtained data was performed.

INTRODUCTION

Alkoxy radicals participate in various radical chain reactions, such as oxidation, decomposition, chlorination, and so on. To calculate the enthalpies of reactions involving alkoxy radicals, one should know the enthalpies of their formation. However, these values are only known for few such radicals (according to [1], for 16 radicals). The scatter of the values of the O–H bond strength in alcohols is 8–12 kJ/mol [1]. Therefore, the accumulation of new thermochemical data and improvement of known data is a challenging task.

Data from kinetic measurements in the course of the unimolecular decomposition of symmetrical (ROOR) and nonsymmetrical (R^1OOR^2) peroxides provide a reliable base for the determination of enthalpies of alkoxy radical formation. The enthalpies, as well as the values of the strength of the O–H bond in alcohols and those of the C–O bond in ethers, may be calculated from the enthalpy of peroxide formation and the activation energy of its decomposition. This work is devoted to the above problem.

RESULTS AND DISCUSSION

The energy of the O–O bond dissociation ($D_{O–O}$) in thermal decomposition reactions of peroxides

$$R^1O–OR^2 \longrightarrow R^1O^\cdot + R^2O^\cdot \qquad (I)$$

assuming that the oscillatory model is true at high pressures in the liquid phase [2]) is equal to

$$D_{O–O} = E_a - 0.5RT. \qquad (1)$$

Here, E_a is the activation energy, R is the universal gas constant, and T is the temperature (K). The activation energy is calculated by the Arrhenius equation from the known rate constant k_d

$$E_a = RT\ln\left(\frac{A}{k_d}\right), \qquad (2)$$

where A is the average value of the preexponential factor for the group of reactions.

The bond dissociation energy of bonds relates to the enthalpies of formation of molecules and radicals as follows:

$$D_{O–O} = \Delta H(R^1O^\cdot) + \Delta H(R^2O^\cdot) - \Delta H(R^1OOR^2). \qquad (3)$$

The average values of the preexponential factor A for thermal decomposition of alkyl and alkylaromatic peroxides were estimated from experimental data and found equal to 2.4×10^{15} and 1.4×10^{15} s^{-1} for the gas and liquid phases, respectively. The activation energy values of the thermal unimolecular decomposition of peroxides were put into correspondence with the obtained value of A by formula (2).

Table 1 lists the values of the O–O bond strengths in symmetrical dialkyl peroxides and the enthalpies of formation of alkoxy radicals formed by peroxide decomposition. These values were calculated by formulas (1)–(3). Table 2 presents the results of calculation of the corresponding values for nonsymmetrical alkyl peroxides.

Data in Tables 1 and 2 show that the $D_{O–O}$ values for peroxides with different alkyl substituents are close in magnitude (151.8 ± 1.3 kJ/mol), except for bis(trifluoromethyl) peroxide ($D_{O–O}$ = 189.1 kJ/mol). In the latter case, there is a strong inductive effect of CF_3 groups. Markedly weaker O–O bonds ($D_{O–O}$ = 145.0 ± 4.0 kJ/mol) are inherent in peroxides of the $R^1R^2R^3COOCR^1R^2R^3$ type (except for $Me_3COOCMe_3$). Obviously, such a decrease in the O–O bond strength and, consequently, in the $D_{O–O}$ value is due to steric repulsion of two $CR^1R^2R^3$ groups in the peroxide. To avoid errors in the calculation of enthalpies of the alkoxy radical formation $\Delta H(RO^\cdot)$ for the above peroxides, this value was determined using the value $D_{O–O}$ = 151.8 kJ/mol (as for $Me_3COOCMe_3$, where steric repulsion appears to be insignificant).

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Table 1. Values of O–O bond strengths and enthalpies of formation of alkoxy radicals calculated from kinetic data on the thermal decomposition of peroxides (ROOR)

ROOR	T, K	k_α, s^{-1}	E, kJ/mol	D_{O-O}, kJ/mol	ΔH(ROOR), kJ/mol	$\Delta H(RO^{\cdot})$, kJ/mol	Reference
MeOOMe	400	2.80×10^{-5}	152.65	150.98	–125.9	12.54	[3]
	″	2.71×10^{-5}	152.76	151.09	–125.9	12.60	[4]
	″	2.05×10^{-5}	153.68	152.02	–125.9	13.06	[5]
	″	2.74×10^{-5}	152.72	151.06	–125.9	12.58	[6]
	″	2.71×10^{-5}	152.76	151.09	–125.9	12.60	[7]
	″	2.17×10^{-5}	153.49	151.83	–125.9	12.97	[8]
				151.35 ± 0.43		**12.73 ± 0.23**	
EtOOEt	400	5.06×10^{-5}	150.49	148.82	–192.8	–21.99	[9]
	″	9.65×10^{-5}	149.62	147.96	–192.8	–22.42	[10]
	″	1.17×10^{-4}	155.05	153.38	–192.8	–19.71	[11]
	″	5.36×10^{-5}	155.75	154.09	–192.8	–19.36	[12]
	″	3.35×10^{-5}	152.05	150.39	–192.8	–21.21	[13]
				150.93 ± 2.72		**–20.94 ± 1.36**	
PrOOPr	400	6.96×10^{-5}	149.62	147.96	–233.1	–42.57	[14]
	333	2.70×10^{-9}	152.68	151.30	–233.1	–40.90	[15]
				149.63		**–41.74**	
$Me_2CHOOCHMe_2$	400	1.36×10^{-5}	155.05	153.39	–272.0	–59.31	[12]
	″	1.10×10^{-5}	155.75	154.09	–272.0	–58.96	[16]
	″	7.92×10^{-6}	156.85	155.18	–272.0	–58.41	[17]
				154.22 ± 0.90		**–58.89 ± 0.45**	
BuOOBu	400	1.91×10^{-5}	153.92	152.26	–274.3	–61.02	[18]
	″	1.74×10^{-5}	154.23	152.57	–274.3	–60.87	[15]
				152.42		**–60.95**	
EtMeCHOOCHEtMe	400	3.84×10^{-5}	151.6	149.93	–304.0	–77.03	[19]
	″	9.50×10^{-6}	156.24	154.58	–304.0	–74.71	[20]
				152.26		**–75.87**	
$EtMe_2COOCEtMe_2$	400	8.17×10^{-5}	149.09	147.42	–374.76	–113.67	[21]
	″	3.83×10^{-5}	151.60	149.94	–374.76	–112.41	[22]
				148.68		**–113.04**	
$Me_3CMe_2COOCMe_2CMe_3$	398	4.84×10^{-4}	142.45	**140.80**	–470.54	**–159.47***	[23]
CF_3OOCF_3	400	9.08×10^{-11}	194.68	193.02	–1507.0	–656.99	[24]
	″	6.39×10^{-10}	188.19	186.53	–1507.0	–660.24	[25]
	″	4.55×10^{-10}	189.32	187.66	–1507.0	–659.67	[26]
				189.07 ± 3.46		**–658.97 ± 1.74**	
$Me_2CCH_2OOCH_2CMe_3$	400	2.93×10^{-4}	144.84	**143.17**	–349.82	**–99.11***	[15]
$Et_2MeCOOCEt_2Me$	400	6.12×10^{-5}	150.05	**148.38**	–416.02	**–132.21***	[22]
$Me_3COOCMe_3$	400	1.81×10^{-5}	154.10	152.43	–343.0	–95.28	[27]
	″	1.45×10^{-5}	154.83	153.17	–343.0	–94.91	[28]
	″	1.46×10^{-5}	154.81	153.15	–343.0	–94.93	[29]
	″	2.06×10^{-5}	153.67	152.00	–343.0	–95.50	[30]
	″	1.39×10^{-5}	154.98	153.31	–343.0	–94.84	[31]
	″	1.26×10^{-5}	155.30	153.64	–343.0	–94.68	[31]

Table 1. (Contd.)

ROOR	T, K	k_α, s^{-1}	E, kJ/mol	$D_{O–O}$, kJ/mol	ΔH(ROOR), kJ/mol	$\Delta H(RO^{\cdot})$, kJ/mol	Reference
$Me_3COOCMe_3$	″	1.37×10^{-5}	155.02	153.36	–343.0	–94.82	[32]
	″	4.09×10^{-5}	151.39	149.72	–343.0	–96.64	[33]
	″	1.46×10^{-5}	154.81	153.15	–343.0	–94.93	[21]
	″	4.33×10^{-5}	151.20	149.53	–343.0	–96.73	[34]
	″	4.29×10^{-5}	151.23	149.56	–343.0	–96.72	[34]
	″	2.31×10^{-5}	153.29	151.62	–343.0	–95.69	[34]
	″	2.41×10^{-5}	153.15	151.48	–343.0	–95.76	[34]
	393	9.00×10^{-6}	153.68	152.05	–343.0	–95.48	[35]
	400	1.76×10^{-5}	154.19	152.58	–343.0	–95.24	[34]
	393	8.30×10^{-6}	153.95	152.31	–343.0	–95.34	[35]
	400	1.80×10^{-5}	154.12	152.45	–343.0	–95.27	[34]
	383	2.63×10^{-6}	153.69	152.10	–343.0	–95.45	[36]
	400	3.13×10^{-5}	152.28	150.61	–343.0	–96.19	[34]
	″	5.23×10^{-5}	150.57	148.91	–343.0	–97.05	[37]
	″	2.58×10^{-5}	152.92	151.26	–343.0	–95.87	[37]
	″	3.73×10^{-5}	151.69	150.03	–343.0	–96.49	[37]
	″	2.44×10^{-5}	153.10	151.44	–343.0	–95.78	[37]
	″	4.86×10^{-5}	150.81	149.15	–343.0	–96.93	[37]
	″	2.88×10^{-5}	152.55	150.89	–343.0	–96.06	[37]
	″	3.33×10^{-5}	152.07	150.41	–343.0	–96.30	[34]
	″	2.98×10^{-5}	152.44	150.78	–343.0	–96.11	[34]
	″	1.80×10^{-5}	154.12	152.45	–343.0	–95.27	[34]
	″	2.63×10^{-5}	152.85	151.19	–343.0	–95.90	[34]
	393	1.34×10^{-5}	152.38	150.75	–343.0	–96.13	[38]
	400	2.14×10^{-5}	153.54	151.88	–343.0	–95.56	[34]
	″	2.72×10^{-5}	152.74	151.08	–343.0	–95.96	[39]
	″	3.33×10^{-5}	152.07	150.41	–343.0	–96.30	[40]
	″	2.15×10^{-5}	153.52	151.86	–343.0	–95.57	[41]
	″	1.32×10^{-5}	155.15	153.48	–343.0	–94.76	[20]
	″	2.08×10^{-5}	153.63	151.97	–343.0	–95.51	[22]
	″	1.01×10^{-5}	156.04	154.38	–343.0	–94.31	[42]
				151.61 ± 1.38		**–95.69 ± 0.69**	
$[PhMe_2CO]_2$	398	1.38×10^{-5}	144.82	143.17	–58.0	42.58	[38]
	400	6.12×10^{-5}	140.60	138.93	–58.0	40.47	[43]
	″	6.78×10^{-5}	140.25	138.59	–58.0	40.30	[34]
	″	7.28×10^{-5}	140.02	138.36	–58.0	40.18	[44]
	″	9.24×10^{-5}	139.22	137.56	–58.0	39.78	[43]
	″	4.31×10^{-5}	141.76	140.10	–58.0	41.05	[39]
	″	5.10×10^{-5}	141.20	139.54	–58.0	40.77	[45]
	″	6.35×10^{-5}	140.47	138.81	–58.0	40.41	[46]
	″	5.95×10^{-5}	140.69	139.03	–58.0	40.51	[47]
	″	2.53×10^{-5}	143.53	141.87	–58.0	41.94	[47]
	″	8.19×10^{-5}	139.63	137.96	–58.0	39.98	[48]
	″	3.71×10^{-5}	142.26	140.60	–58.0	41.30	[49]
	″	3.00×10^{-5}	142.97	141.30	–58.0	41.65	[50]
	388	8.10×10^{-6}	142.90	141.29	–58.0	41.64	[51]
				139.53 ± 1.38		**40.77 ± 0.69**	

* The enthalpy of radical formation is estimated assuming that $D_{C–O}$ = 151.6 kJ/mol.

Table 2. Values of O–O bond strengths and the enthalpies of formation of alkoxy radicals calculated from kinetic data on the thermal decomposition of nonsymmetrical peroxides (R^1OOR^2)

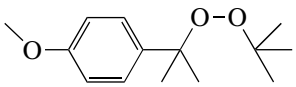
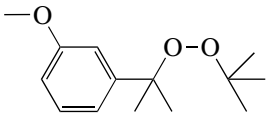
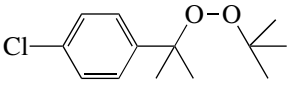
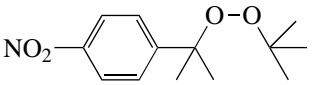
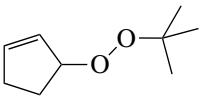
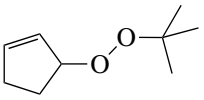
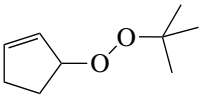
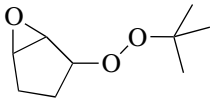
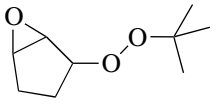
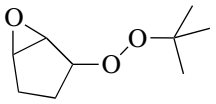
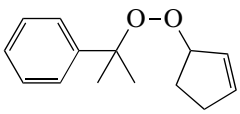
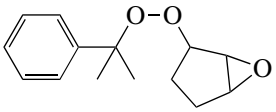
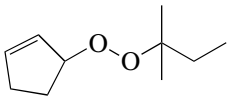
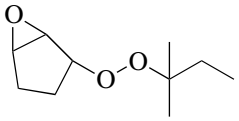
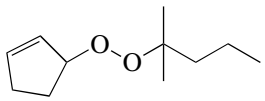
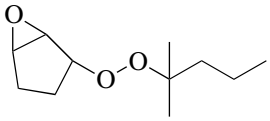
R^1OOR^2	T, K	k_α, s^{-1}	E, kJ/mol	D_{O-O}, kJ/mol	$\Delta H(R^1OOR^2)$, kJ/mol	$\Delta H(R^1O^\cdot)$, kJ/mol	$\Delta H(R^2O^\cdot)$, kJ/mol	Reference
$Me_3COOCMe_2Pr$	400	1.07×10^{-5}	155.85	154.18	**–384.11**	–95.69	**–134.24**	[52]
$Me_3COOC(Me)_2CHMe_2$	400	5.42×10^{-5}	150.45	148.79	**–385.97**	–95.69	**–141.49**	[52]
$Me_3COOCMe_2CH_2Cl$	400	3.73×10^{-5}	151.69	150.03	**–360.69**	–95.69	**–114.97**	[52]
$Me_3COOCMe_2CH_2Ph$	400	3.49×10^{-5}	151.91	150.25	**–214.12**	–95.69	**31.82**	[52]
	398	3.72×10^{-5}	150.94	149.29	**–353.76**	–95.69	**–108.78**	[23]
	398	3.22×10^{-5}	151.42	149.77	″	–95.69	″	[52]
	398	3.42×10^{-5}	151.22	149.57	**–231.33**	–95.69	**14.03**	[52]
	398	2.20×10^{-5}	152.68	151.03	**–215.65**	–95.69	**31.07**	[52]
	400	4.82×10^{-5}	150.84	149.18	**–157.77**	–95.69	**87.1**	[53]
	400	5.65×10^{-5}	150.31	148.64	″	–95.69	**86.56**	[53]
	400	3.93×10^{-5}	151.51	149.86	″	–95.69	**87.79**	[53]
							87.15 ± 0.62	
		1.04×10^{-4}	148.28	146.61	**–283.2**	–95.69	**–40.9**	[53]
		5.46×10^{-5}	150.43	148.76	″	–95.69	**–38.75**	[53]
		1.29×10^{-5}	155.22	153.56	″	–95.69	**–33.95**	[53]
							–37.87 ± 2.91	

Table 3. Enthalpies of formation of peroxides $\Delta H(R^1OOR^2)$ calculated from kinetic data on their thermal decomposition

R^1OOR^2	T, K	k_α, s^{-1}	E, kJ/mol	D_{O-O}, kJ/mol	$\Delta H(R^1OOR^2)$, kJ/mol	$\Delta H(R^1O^\cdot)$, kJ/mol	$\Delta H(R^2O^\cdot)$, kJ/mol	Reference
$Me_3COOCEtMe_2$	400	5.03×10^{-5}	150.70	149.04	–358.04	–95.69	–113.67	[36]
	″	3.30×10^{-5}	152.10	150.44	–359.80	–95.69	–113.67	[52]
				149.74	**–358.92**			
$Me_3COOCMe_2CMe_3$	400	8.28×10^{-5}	149.04	147.38	–414.84	–95.69	–171.77	[52]
$Me_3COOCMe_2Ph$	400	3.78×10^{-5}	151.65	149.99	–204.91	–95.69	40.77	[36]
	398	3.04×10^{-5}	151.61	149.96	–204.88	–95.69	40.77	[23]
				149.98	**–204.9**			
	400	2.16×10^{-4}	145.85	144.19	**–16.27**	40.77	87.15	[54]
	400	1.65×10^{-4}	146.75	145.08	**–142.18**	40.77	–37.87	[54]
	400	1.31×10^{-4}	147.52	145.85	**–171.74**	87.15	–113.04	[54]
	400	2.41×10^{-3}	137.83	136.17	**–287.08**	–37.87	–113.04	[54]
	400	5.10×10^{-4}	142.99	141.33	**–234.8**	40.77	–134.24	[54]
	400	9.13×10^{-4}	141.06	139.39	**–311.5**	–37.87	–134.24	[54]

The values of enthalpies of formation of some peroxides calculated from the experimental and above data are given in Table 3. As is seen from Table 3, the calculated value of the enthalpy of $Me_3COOCMe_2Ph$ formation agrees well with literature data [55].

Table 4 lists the calculated values of the O–H bond strengths in alcohols and enthalpies of formation of some alcohols. These data show that the obtained D_{O-H} values are close to the literature data. The error in the $\Delta H(RO^\cdot)$ determination is at most 2 kJ/mol. The energy of O–H bond dissociation in aliphatic alcohols is virtually constant in the limits of the above error and the error of ΔH(ROH) determination ΔH(ROH) (±2 kJ/mol).

The values of C–O bond strengths in ethers calculated from data reported here and elsewhere [56, 57] are presented in Table 5.

We used the values of enthalpies of peroxide and alcohol formation reported in [55] or estimated by the Benson increment method [58].

Thus, data obtained show that the O–H bond strength (D_{O-H}) in aliphatic alcohols (n = 15) is independent of the structure of an alkyl radical and equals 433.8 ± 1.7 kJ/mol. The D_{O-H} value for cumyl alcohol is lower at 395.0 kJ/mol, whereas that for CF_3OH is considerably higher (451.3 kJ/mol).

Table 4. The values of O–H bond strengths (D_{O-H}) in alcohols, the enthalpies of formation of alkoxy radicals $\Delta H(RO^{\cdot})$ and alcohols (ΔH(ROH))

Alcohol	D^{*}_{O-H}, kJ/mol	D_{O-H}, kJ/mol [1]	$\Delta H^{*}(RO^{\cdot})$, kJ/mol	ΔH(ROH), kJ/mol [55]
MeOH	431.73	436.2	12.73	–201.0
EtOH	432.36	432.8	–20.94	–235.3
PrOH	431.86	432.2	–41.74	–255.6
Me_2CHOH	431.91	438.5	–58.89	–272.8
BuOH	432.33	431.78	–60.95	–275.28
Me_3COH	434.91	439.8	–95.69	–312.6
EtCH(OH)Me	434.83	441.3	–75.87	–292.7
$EtCMe_2OH$	435.96	437.7	–113.04	–331.0
Me_3CCH_2OH	436.12		–99.11	–317.23*
Me_3CMe_2COH	433.56		–159.47	–375.03*
$MeEt_2COH$	431.12		–132.21	–345.43*
$PrCMe_2OH$	435.39		–134.24	–351.63*
Me_2CHCMe_2OH	434.41		–141.49	–357.9
Cyclopenten-1-ol	434.75		87.15	–129.6
$PhCMe_2OH$	394.65	391.88*	40.77	–135.88*
$PhCH_2CMe_2OH$	435.84		31.82	–186.02*
CF_3OH	451.26	453.33*	–658.27	–892.23*
$ClCH_2CMe_2OH$	445.59		–114.97	–342.56*

* This work.

Table 5. The values of C–O bond strengths (D_{C-O}, kJ/mol) in ethers and the enthalpies of formation of radicals and molecules (ΔH, kJ/mol) [54]

	$D_{C-O}(\Delta H(R^1OR))$				
$RO^{\cdot}$ / $^{\cdot}R^1$	$MeO^{\cdot}$ (12.73)	$EtO^{\cdot}$ (–20.94)	$PrO^{\cdot}$ (–41.74)	$Me_2CHO^{\cdot}$ (–58.89)	$Me_3CO^{\cdot}$ (–95.69)
Me (147.0)	**343.83** (–184.1)	**342.06** (–216.4)	**343.28** (–252.0)	**340.11** (–252.0)	**334.51** (–283.2)
Et (119.0)	**348.13** (–216.4)	**350.76** (–252.7)	**349.46** (–272.2)	**349.01** (–288.9)	**337.31** (–314.0)
Pr (100.0)	**350.75** (–238.02)	**351.26** (–272.2)	**351.26** (–293.0)		
$Me_2C^{\cdot}H$ (90.0)	**354.73** (–252.0)	**337.16** (–288.9)		**349.11** (–318.0)	**352.31** (–358.0)
$Me_3C^{\cdot}$ (48.0)	**343.93** (–283.2)	**341.06** (–314.0)		**347.11** (–358.0)	**313.31** (–316.1)

In ethers, the structure of an alkyl substituent significantly influences the D_{C-O} value. For instance, the branched substituents R lead to a decrease in the C–O bond strength.

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