

# The Role of Triplet Repulsion in Alkyl Radical Addition to a $\pi$ -C–O Bond and Alkoxy Radical Addition to a $\pi$ -C–C Bond

E. T. Denisov

Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow oblast, 142432 Russia

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**Abstract**—The experimental activation energies of the  $R^\cdot + O = CR^1R^2$  and  $RO^\cdot + CH_2 = CHR^1$  addition reactions are analyzed within the framework of the parabolic model of the bimolecular addition reaction. The activation energy also depends on the dissociation energy of the forming C–O bond and on the reaction enthalpy: the higher the dissociation energy, the higher the activation energy. The empirical relationship  $r_e/D_e = 0.97 \times 10^{-13} \text{ m kJ}^{-1} \text{ mol}$  is found for  $H^\cdot$ ,  $Cl^\cdot$ ,  $Br^\cdot$ ,  $R^\cdot$ , and  $RO^\cdot$  radical addition to multiple C=C and C=O bonds ( $r_e$  is the distance between the peaks of the intersecting parabolic curves). This is due to the effect of the triplet repulsion on radical addition. The interaction of polar groups and the steric effect also influence the activation energy.

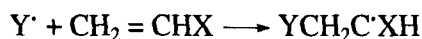
## INTRODUCTION

Analysis of the experimental data on the kinetics of alkyl radical addition to multiple C–C bonds performed within the framework of the parabolic model of bimolecular reactions showed that their activation energies strongly depend on triplet repulsion in the transition state [1, 2]. This was confirmed later [3] when analyzing the kinetics of atom addition to multiple C–C bonds. In  $X^\cdot + HY \rightarrow XH + Y^\cdot$  radical abstraction reactions, the electronegativity of the X and Y atoms plays a significant role along with triplet repulsion [4, 5]. The stronger the difference in the electronegativities of the X and Y atoms, the lower the activation energy.

This work focuses on the analysis of the experimental data on the addition of alkyl and alkoxy radicals to the  $\pi$ -C–O and  $\pi$ -C–C bonds, respectively. The reaction center of the transition state in these reactions contains oxygen and carbon atoms. Using these reactions as an example, we can answer the following three questions: (1) How does the triplet repulsion affect the activation energy of such reactions? (2) Does the heteroatomic structure of the reaction center influence the activation energy? and (3) Are there any other structural factors affecting the activation energy of these reactions? We use the parabolic model of bimolecular reactions to answer these questions [1–5].

## CALCULATION PROCEDURE

Within the framework of the parabolic model [1], the addition of the  $Y^\cdot (R^\cdot, RO^\cdot)$  radical



is considered as a result of the intersection of two potential curves that describe the energies of the stretching vibrations of the atoms of the breaking C=C

(i) and forming Y–C (C–O or O–C) (f) bonds, respectively, in the coordinates of the amplitude of atomic stretching vibration vs. its potential energy coordinates. It is assumed that the atomic stretching vibration is harmonic and its potential energy is proportional to the square of the vibration amplitude. In terms of this model, the radical addition reaction is characterized by the following parameters: the enthalpy  $\Delta H_e$ , the activation energy  $E_e$ , the distance  $r_e$  between the peaks of the two parabolic curves corresponding to the potential energy of the vibration of the reacting bonds, and the dynamic characteristics of the vibration of these bonds  $b_i$  and  $b_f$  ( $2b_i^2$  is the force constant of the  $i$ th bond).

$$\Delta H_e = D_i - D_f + 0.5hN(v_i - v_f), \quad (1)$$

where  $D_i$  and  $D_f$  are the dissociation energies of the breaking and forming bonds, respectively;  $h$  and  $N$  are the Plank and Avogadro constants, respectively; and  $v_i$  and  $v_f$  are the frequencies of the stretching vibration of the breaking and forming bonds, respectively. The activation energy  $E_e$  used in the parabolic model is related to the activation energy  $E$  determined from the experimental data by the equation

$$E_e = E + 0.5(hNv_i - RT). \quad (2)$$

Given the experimental rate constant of the reaction  $k$  at a given temperature, the activation energy may be calculated by the Arrhenius equation using the preexponential factor  $A$  typical of the reaction series of the same structural type:

$$E = RT \ln(A/k). \quad (3)$$

For alkyl radical addition to  $CH_2=CHX$  in a hydrocarbon solution,  $A = 5 \times 10^8 \text{ l mol}^{-1} \text{ s}^{-2}$ . In accordance with

the collision theory, the  $A$  factor for the addition of other  $Y\cdot$  radicals to the  $C=C$  bond is calculated by the equation  $A(Y\cdot) = A(CH_3\cdot) \times (r_{C-Y}/r_{C-C})^2$ . Within the framework of the parabolic model, the  $\Delta H_e$ ,  $E_e$ ,  $b = b_i$ , and  $\alpha = b_i/b_f$  parameters are related to each other by the following equation [1]:

$$br_e = a\sqrt{E_e - \Delta H_e} + \sqrt{E_e}. \quad (4)$$

Given the  $br_e$  parameter for each reaction group with  $br_e = \text{const}$ , the activation energy of its thermoneutral analog  $E_{e,0}$  ( $E_{e,0} = E_e$  at  $\Delta H_e = 0$ ) may be calculated as follows:

$$E_{e,0} = (br_e)^2(1 + \alpha)^{-2}. \quad (5)$$

The  $br_e$  values were calculated using the following parameters:

Reaction	$\alpha$	$b \times 10^{11}$ , (kJ/mol) <sup>1/2</sup>	$0.5hNv_i$ , kJ/mol	$0.5hN(v_i - v_f)$ , kJ/mol
$RO\cdot + CH_2=CHX \rightarrow ROCH_2C\cdot HX$	1.413	5.389	9.9	3.3
$R\cdot + O=CR^1R^2 \rightarrow RR^1R^2CO\cdot$	1.336	5.991	10.3	2.1
$R\cdot + O=CR^1R^2 \rightarrow ROC\cdot R^1R^2$	1.570	5.991	10.3	3.7

To determine the reaction enthalpy, I first calculated the enthalpies of the formation of the corresponding  $R\cdot$  radicals in the gas phase under standard conditions using the enthalpy of the RH molecule and the dissociation energy of the R-H bond. The enthalpies of molecule formation given in the tables in [6] and the bond dissociation energies taken from [7-9] were used in the calculations. The activation energy was calculated from the rate constant of the reaction by the Arrhenius equation  $E = RT \times \ln(A/k)$  using the preexponential factor  $A = 5 \times 10^{11} \text{ l mol}^{-1} \text{ s}^{-1}$ , which is typical of  $R\cdot$  and  $RO\cdot$  radical additions.

## RESULTS AND DISCUSSION

The results of calculation are summarized in Tables 1 and 2. Table 1 shows that all of the reactions of alkoxy radical addition to olefins (the first seven reactions) are characterized by virtually the same  $br_e$  parameter. The least-squares averaging gives  $br_e = 19.49 \pm 0.33 \text{ (kJ/mol)}^{1/2}$ . The addition of the  $RO\cdot$ , carboxyl, nitroxyl, and sterically hindered phenoxyl radicals to styrene is characterized by a somewhat higher  $br_e$  parameter. For methyl radical addition to the carbonyl group of acetone

(Table 2), the  $br_e$  parameter is  $19.67 \text{ (kJ/mol)}^{1/2}$ . The  $br_e$  values are also higher for the addition of the methyl radical to  $PhC(O)Me$  ( $br_e = 20.52 \text{ (kJ/mol)}^{1/2}$ ),  $Ph_2C(O)$  (the average  $br_e$  value,  $21.56 \pm 0.38 \text{ (kJ/mol)}^{1/2}$ ), and benzoquinone, as well as for the addition of the ethyl radical to  $Ph_2CO$ . A still higher  $br_e$  value is observed for the addition of the polystyrene radical to benzoquinone ( $br_e = 25.03 \text{ (kJ/mol)}^{1/2}$ ).

All the above reactions may be subdivided into seven groups. Table 3 compares the parameters specifying each group with those corresponding to the  $H\cdot$  and  $CH_3\cdot$  addition to the  $\pi$ -C-C bond. The linear correlation was found earlier [2, 3] between the  $r_e$  parameter and the dissociation energy  $D_e$  of the  $R-CH_2CH_2X$  forming bond in the  $R\cdot + CH_2=CHX$  addition:  $r_e/D_e = 0.97 \times 10^{-13} \text{ m kJ}^{-1} \text{ mol}$ . Is there any correlation between the  $r_e$  and  $D_e$  values in the case of the  $RO\cdot$  and  $R\cdot$  radical addition to  $CH_2=CHX$  and the carbonyl group, respectively? The results of such a comparison are given below:

Reaction	Bond	$D_e$ , kJ/mol	$r_e \times 10^{11}$ , m	$(r_e/D_e) \times 10^{13}$ , m kJ <sup>-1</sup> mol
$RO\cdot + CH_2=CHX$	EtO-Et	359	3.62	1.01
$RCO_2\cdot + CH_2=CHX$	MeCOO-Et	350	3.82	1.09
$R\cdot + O=CR^1R^2$	Me <sub>2</sub> C(OH)-Me	364.4	3.28	0.90
$H\cdot + O=CR^1R^2$	Me <sub>2</sub> HCO-H	460	4.40	0.96
$CH_3\cdot + CH_2=CHX$	Et-Et	384	3.71	0.97

The  $r_e/D_e$  values are nearly the same for all addition reactions ( $r_e/D_e \times 10^{13} = 0.96 \pm 0.06$  m kJ<sup>-1</sup> mol) independently of the nature and strength of the forming bond. The fact that the activation energy of the thermo-neutral addition reaction  $E_{e,0}$  correlates with the dissociation energy of the forming bond provides empirical evidence for the importance of the triplet repulsion in radical addition reactions. Obviously, in the transition state with the reaction centers  $C(\uparrow) \cdots C(\downarrow) \cdots C(\uparrow)$ ,  $C(\uparrow) \cdots O(\downarrow) \cdots C(\uparrow)$ , and  $O(\uparrow) \cdots C(\downarrow) \cdots C(\uparrow)$ , the interaction between the electrons of the terminal atoms with the parallel spins contributes significantly to the activation energy of the reaction. The stronger the forming bond (C–C, C–O, or O–H), the higher the energy of its nonbonding orbital and the higher the activation energy (i.e., the higher the  $r_e$  parameter and  $E_{e,0} \sim r_e^2$ ).

Comparison of the parameters of the addition of the alkyl radicals to the  $\pi$ -C–C and  $\pi$ -C–O bonds leads to another important conclusion. In the  $X^\cdot + HY \rightarrow XH + Y^\cdot$  radical abstraction reactions, the electron affinity of the X and Y atoms (groups) play a significant role. The stronger the difference in the electron affinities of the X and Y atoms, the lower the activation energy [4, 5].

For example, in the  $RO^\cdot + R'H \rightarrow ROH + R'^\cdot$  reaction, the activation energy decreases by 20 kJ/mol because of the different electron affinities of the O and C atoms [5]. Does this factor affect the activation energy of the addition reactions? The comparison of the  $r_e/D_e$  values for the addition with the reaction centers  $C(\uparrow) \cdots C(\downarrow) \cdots C(\uparrow)$

on the one hand and  $O(\uparrow) \cdots C(\downarrow) \cdots C(\uparrow)$  and  $C(\uparrow) \cdots O(\downarrow) \cdots C(\uparrow)$  on the other shows that  $r_e/D_e = \text{const}$  for these three reaction groups. Therefore, their activation energies depend only on the force constants of the reacting bonds, the reaction enthalpies, and the strength of the forming bond (the triplet repulsion). The same conclusion follows from the comparison of the  $H^\cdot + CH_2=CHX$  and  $H^\cdot + O=CR^1R^2$  reactions, for which  $r_e/D_e = \text{const}$  as well.

The  $br_e$  values observed for the reactions involving styrene, *p*-benzoquinone, and the aromatic nitroxyl radical (see Tables 1, 2) are higher than those expected from the relationship  $r_e/D_e = 0.96 \times 10^{-13}$  m kJ<sup>-1</sup> (see above):

Reaction	$br_e$ , (kJ/mol) <sup>1/2</sup>	$E_{e,0}$ , kJ/mol	$\Delta E_\pi$ , kJ/mol
$RO^\cdot + CH_2=CHX$	19.49	65.2	0
$RO^\cdot + CH_2=CHXPh$	20.57	76.4	11.2
$R^\cdot + PhC(O)Me$	20.52	63.7	0
$R^\cdot + OC_6H_4O$	23.15	81.1	17.4
$R^\cdot + OC_6H_4O$	25.03	94.8	31.1

A similar effect of the aromatic ring in the  $\alpha$  position to the reaction center is also observed in the radical abstraction reactions [4]. This may be explained as follows. In the  $O(\uparrow) \cdots C(\downarrow) \cdots C(\uparrow)Ph$  reaction center, the unpaired electron of the  $\alpha$  carbon atom interacts with

**Table 1.** Kinetic parameters of the addition of oxygen-centered radicals to olefins

Reaction*	$-\Delta H_e$ , kJ/mol	$E$ , kJ/mol	$br_e$ , (kJ/mol) <sup>1/2</sup>	Reference
$CH_3O^\cdot + cis\text{-MeCH=CHMe}$	88.0	12.1	19.23	[10]
$Me_3CO^\cdot + cis\text{-MeCH=CHMe}$	86.0	15.1	19.67	[11]
$Me_3CO^\cdot + CH_2=CHEt$	74.3	18.0	19.36	[11]
$Me_3CO^\cdot + CH_2=CHCHMe_2$	74.3	17.8	19.33	[11]
$Me_3CO^\cdot + CH_2=CMe_2$	77.4	14.8	19.02	[11]
$Me_3CO^\cdot + \text{cyclo-C}_5\text{H}_8$	79.8	18.0	19.75	[12]
$Me_3CO^\cdot + \text{cyclo-C}_6\text{H}_{10}$	83.9	18.1	20.05	[13]
$Me_3CO^\cdot + CH_2=CHPh$	123.3	9.7	21.09	[11]
$PhO^\cdot + CH_2=CHPh$	13.5	81.6	23.89	[14]
$PhO^\cdot + CH_2=CMeCOOMe$	-1.2	86.2	23.41	[14]
$R_2NO^\cdot + CH_2=CHPh$	-26.7	94.6	22.52	[14]
$RCO_2^\cdot + CH_2=CHPh$	128.4	5.1	20.57	[15]

\*  $PhO^\cdot$  is 2,4,6-tri-*tert*-butylphenoxyl and  $R_2NO^\cdot$  is di(methoxyphenyl)nitroxyl

**Table 2.** Kinetic parameters of the addition of alkyl radicals to the C=O group

Reaction	$-\Delta H_e$ , kJ/mol	$E$ , kJ/mol	$br_e$ , (kJ/mol) <sup>1/2</sup>	Reference
$C^\bullet H_3 + Me_2C(O) \longrightarrow Me_3CO^\bullet$	18.6	51.5	19.67	[16]
$C^\bullet H_3 + PhC(O)Me \longrightarrow PhMeC^\bullet OMe$	40.4	31.9	20.52	[17]
$C^\bullet H_3 + Ph_2C(O) \longrightarrow Ph_2C^\bullet OMe$	53.4	28.2	21.03	[18]
$CH_3C^\bullet H_2 + Ph_2C(O) \longrightarrow Ph_2C^\bullet OEt$	57.6	30.3	21.71	[19]
$CH_3C^\bullet H_2 + Ph_2C(O) \longrightarrow Ph_2C^\bullet OEt$	57.6	31.7	21.93	[19]
$C^\bullet H_3 + OC_6H_4O \longrightarrow MeOC_6H_4O^\bullet$	140.6	5.3	23.28	[18]
$C^\bullet H_3 + OC_6H_4O \longrightarrow MeOC_6H_4O^\bullet$	140.6	6.4	23.50	[20]
$-CH_2C^\bullet HPh + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	113.3	$24.5 \pm 1.4$	25.03	[21]
$-CH_2C^\bullet HCOOMe + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	132.7	35.9	27.61	[21]
$-CH_2C^\bullet HMeCOOMe + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	128.4	$34.5 \pm 0.5$	27.17	[21]
$-CH_2C^\bullet HCN + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	128.1	37.3	27.52	[21]

**Table 3.** Kinetic parameters of different reaction groups of radical addition to the C=C and C=O bonds

Reaction	$br_e$ , (kJ/mol) <sup>1/2</sup>	$E_{e,0}$ , kJ/mol	$r_e \times 10^{11}$ , m	Reference
$H^\bullet + CH_2=CHX \longrightarrow CH_3C^\bullet HX$	24.59	101.6	4.56	[3]
$Me^\bullet + CH_2=CHX \longrightarrow MeCH_2C^\bullet HX$	20.01	82.6	3.71	[2]
$RO^\bullet + CH_2=CHX \longrightarrow ROCH_2C^\bullet HX$	19.49	65.2	3.62	This work
$RO^\bullet + CH_2=CHPh \longrightarrow ROCH_2C^\bullet HPh$	21.09	76.4	3.91	"
$RCO_2^\bullet + CH_2=CHPh \longrightarrow RCO_2CH_2C^\bullet HPh$	20.57	72.7	3.82	"
$H^\bullet + O=CR^1R^2 \longrightarrow R^1R^2C^\bullet OH$	26.37	102.9	4.40	[3]
$R^\bullet + O=CR^1R^2 \longrightarrow RR^1R^2C^\bullet O$	19.67	70.9	3.28	This work
$R^\bullet + PhC(O)Me \longrightarrow PhMeC^\bullet OR$	20.52	63.7	3.42	"
$R^\bullet + Ph_2C(O) \longrightarrow Ph_2C^\bullet OR$	21.56	70.4	3.60	"
$R^\bullet + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	23.15	81.1	3.86	"
$R^\bullet + OC_6H_4O \longrightarrow ROC_6H_4O^\bullet$	25.03	94.8	4.18	"

the  $\pi$  electrons of the aromatic ring. This interaction (the delocalization of the reaction center electrons) increases the energy of the  $O\cdots C\cdots C$  reaction center, which, in turn, favors an increase in the energy of the nonbonding orbital of the  $O\cdots C$  bond and, hence, the triplet repulsion in the transition state. Using the above experimental  $br_e$  parameters, one can calculate the contribution of the  $\pi$ -electron interaction to the activation energy  $\Delta E_\pi$  by the equation [5]

$$\Delta E_\pi = \frac{(br_e)_\pi^2 - (br_e)^2}{(1 + \alpha)^2} \quad (6)$$

As shown above, this contribution ranges from 11 to 31 kJ/mol. Similarly, the  $\Delta E_\pi$  value for the reaction of *p*-benzoquinone with the radicals of polymerizing styrene is higher than that for the  $Me^\bullet + OC_6H_4O$  reaction, because the delocalization of the  $\pi$  electrons involves two benzene rings of the  $OC_6H_4O\cdots C\cdots CPh$  reaction center.

For the reaction of 2,4,6-tri-*tert*-butylphenoxy radical with styrene, the  $E_{e,0}$  value is 98 kJ/mol, which is by 22 kJ/mol higher than that for the reaction of the  $RO^\bullet$  radical with styrene. Obviously, the effect of the  $\pi$  electrons of the aromatic ring in this case is combined with the steric hindrances caused by two *o-tert*-butyl groups.

The  $br_e$  parameters for the reactions of macroradicals containing polar groups with *p*-benzoquinone are also higher than those for the  $R' + OC_6H_4O$  reaction (see Table 2). This may be attributed to the dipole-dipole interaction of the polar groups with the polar reaction center that takes place in these reactions. This interaction is also observed in the radical abstraction

reactions, and its contribution to the activation energy may be estimated by the equation [5]:

$$\Delta E_\mu = \frac{br_e^2 - 23.03^2}{(1 + \alpha)^2} \quad (7)$$

The calculation results are given below.

Radical	$\sim CH_2C^{\cdot}HCOOMe$	$\sim CH_2C^{\cdot}MeCOOMe$	$\sim CH_2C^{\cdot}HCN$
$br_e, (kJ/mol)^{1/2}$	27.61	27.17	27.52
$\Delta E_\mu, kJ/mol$	35.1	31.5	34.4

As can be seen, the contribution of the polar (or, more precisely, multidipole) interaction [22] to the activation energy is rather significant. This is also observed in other radical addition reactions.

### CONCLUSION

Thus, the activation energy of the addition of alkoxy and alkyl radicals to the  $\pi$ -C-C and  $\pi$ -C-O bonds, respectively, substantially depends on the triplet repulsion along with the reaction enthalpy. This manifests itself in that the  $r_e$  parameter is directly proportional to the dissociation energy of the forming bond. Note that the proportionality coefficient (the  $r_e/D_e$  ratio) is the same for these reactions and for the addition of H, D, Cl, and Br atoms and alkyl radicals to the  $\pi$ -C-C bond [2, 3]. This also suggests that the electronegativity of the atoms in the  $X\cdots C\cdots C$  and  $C\cdots O\cdots C$  reaction centers has no effect on the activation energy, that is, plays a minor role in the addition reactions. An increase in the triplet repulsion also causes an increase in the  $r_e$  parameter in the presence of the aromatic ring in the  $\alpha$  position with respect to the reaction center. In the addition of the polar macroradicals to benzoquinone, the effect of the polar interaction is also observed, which increases the activation energy of the addition.

In the addition of the 2,4,6-tri-*tert*-butylphenoxy radical to monomers, the steric effect is clearly observed, which also favors an increase in the activation energy. Therefore, the addition of the carbon-centered and oxygen-centered radicals to the carbonyl group and double C-C bond, respectively, depends on the following factors: the reaction enthalpy, the triplet repulsion in the transition state, the polar interaction, and the steric effect. The parabolic model allows us to calculate an increment that characterizes the contribution of this interaction to the activation energy in each particular case.

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