Enthalpies of formation of organic free radicals of alcohol and ether derivatives

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Numerical values of the enthalpies of formation of oxygen-containing organic radicals of alcohol and ether derivatives ($\Delta_f H°$) were analyzed. For seven out of 25 compounds the corresponding $\Delta_f H°$ values were determined more accurately. For 35 radicals, the $\Delta_f H°$ values were determined for the first time based on the published values of bond dissociation energies in molecules and on the corresponding enthalpies of their formation. Based on the analysis of the $\Delta_f H°$ values for 60 radicals studied, a structure—property (enthalpy of formation) correlation was established, described in the framework of the group additivity scheme. The parameters for calculations of $\Delta_f H°$ values for the title radicals were recommended.

Key words: enthalpy of formation, phenomenological calculation, thermodynamic functions, structure—property correlation, group additivity scheme.

The discovery of free radicals (R·) and the establishment of their leading role in many natural and technological processes belongs to the fundamental achievements of chemistry in the XXth century. Experimental studies of the most important physicochemical (including spectral and thermodynamic) characteristics of free radicals face severe difficulties due to the instability of R·.[1]

The available qualitative and quantitative data[1,2] on the energies of formation ($\Delta_f H°$) of organic free radicals are scarce compared with the corresponding data array for organic molecules.[3] In this connection, the development of methods for calculations of $\Delta_f H°(R·)$ values becomes topical.

Currently, quantum chemical methods cannot always serve as sources of reliable quantitative data on $\Delta_f H°(R·)$ values for large molecules. The state of the art in quantum chemical methods of determination of thermodynamic properties of organic compounds is such that the CBS-n, G-n, W-n, HEAT, BAC-MP4 methods as well as the methods of isodesmic, homodesmic, isogyric, and desmotic reactions allow one to obtain the enthalpies of formation with the accuracy to 4 kJ mol^{-1} (so-called chemical accuracy)[4—9] only for molecules comprising from two to ten atoms and for some radicals containing at most five to seven atoms. As the number of atoms increases or if atoms of other periods of periodic table are included, the predictive power of these methods abruptly decreases and some methods become so resource-intensive that their practical implementation virtually impossible. Mass calculations of compounds built of more than ten atoms with the chemical accuracy are problematic.

The development of phenomenological methods[1] is restrained by the lack of reference data. In this connection, an approach used earlier (see Refs 10—16) seems to be efficient. It allows one to obtain new $\Delta_f H°(R·)$ values starting with the known bond dissociation energies (D) based on analysis of the structure—property correlations, thus developing the phenomenological methods of calculations by determining new parameters and refining the known values.

This approach is used in the present work devoted to acyclic radicals containing alkyl fragments and the —OH and —O— functional groups. A full list of compounds studied is presented in Table 1.

Practical implementation of this approach includes analysis of the available data and selection of reference values as the most important step. The $\Delta_f H°$ values for 25 free radicals are known from the literature (see Table 1); for 13 radicals, they were analyzed in Ref. 1, while the data for other radicals were presented only in compilations[2,17,18] and cannot be classified as reference ones. In some cases, the $\Delta_f H°(R·)$ values for the same compound are different. All of them are included in further consideration. The final choice of particular values was done on the basis of analysis of the previously determined and new $\Delta_f H°(R·)$ values performed in the framework of the group additivity scheme and using a quantitative structure—property (enthalpy of formation) correlation.

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Table 1. The enthalpies of formation of free radicals R$^{\cdot}$ ($\Delta_f H^\circ(R^{\cdot})$) and corresponding molecules RH ($\Delta_f H^\circ(RH)$), and the R—H bond dissociation energies (D(R—H)) (kJ mol^{-1})

Radical R$^{\cdot}$	$-\Delta_f H^\circ(R^{\cdot})^a$	D(R—H)^b	$-\Delta_f H^\circ(RH)$	$-\Delta_f H^\circ(R^{\cdot})^c$	$-\Delta_f H^\circ(R^{\cdot})_{rec}{}^d$	$-\Delta_f H^\circ(R^{\cdot})_{calc}{}^e$	δ^f
C$^{\cdot}$H$_2$OH	21.0[1] 17.0[2] 9[3]	402.5±1.3	205.0±10[3]	20.5	21.0±5	21.23	0.23
C$^{\cdot}$H$_2$CH$_2$OH	56.2[1] 31.0[2]	410.0±8.4	234.0±2.0[3]	42.0	42.0	45.79	3.79
CH$_3$C$^{\cdot}$HOH	63.6[1] 55.6[2] 52.9[17]	400.3	234.0±2.0[3]	51.7	51.7	52.04	0.34
C$^{\cdot}$H$_2$OCH$_3$	11.7[1] 0[2] −9.8[18]	405.0	184.1±0.5[3]	−2.9	−2.9	3.6	6.5
OHCH$_2$C$^{\cdot}$HOH	220.0[1] 220.1[2] 203.9[12]	400	394.4±2.8[3]	212.4	212.4	205.26	−7.14
OHCH$_3$C$^{\cdot}$OH	—	385	425[g]	258	258	258.63	0.63
C$^{\cdot}$H$_2$(CH$_2$)$_2$OH	66.9[1,2]	406.3±8.4	256.0±3[3]	67.7	66.9	67.55	0.65
CH$_3$C$^{\cdot}$HCH$_2$OH	78.6[1] 78.7[2]	394.6±8.4	256.0±3[3]	79.4	78.6	80.7	2.1
CH$_3$CH$_2$C$^{\cdot}$HOH	81[2] 73.3[17]	399.5	256.0±3[3]	74.5	74.5	73.8	−0.7
C$^{\cdot}$H$_2$CH(OH)CH$_3$	96.2[1,2]	394.6±8.4	272.8[3]	96.2	96.2	84.53	−11.67
(CH$_3$)$_2$C$^{\cdot}$OH	107.1[1] 96.4[2] 99.9[17]	390.5	272.8[3]	100.3	96.4	95.64	−0.76
C$^{\cdot}$H$_2$OCH$_2$CH$_3$	44.3[1] 45.2[2]	389.1	216.4±0.64[3]	45.3	44.3	37.8	−6.5
CH$_3$OC$^{\cdot}$HOCH$_3$	—	391.0	348.2±0.79[3]	175.2	175.2	174.67	−0.53
CH$_3$(CH$_2$)$_2$C$^{\cdot}$HOH	95.7[17]	397.2	277.0±5.0[3]	97.8	97.8	95.56	−2.24
CH$_3$C$^{\cdot}$(OH)CH$_2$CH$_3$	123.3[17]	389.7	293.1[3]	121.4	121.4	117.4	−4.0
C$^{\cdot}$H$_2$C(CH$_3$)$_2$OH	112.1[2] 113.1[17]	417.4	312.6±0.88[3]	113.2	112.1	105.35	−6.75
CH$_3$C$^{\cdot}$HOCH$_2$CH$_3$	84.5[1] 81.2[2] 70.0[18]	399.5	252.7±2.0[3]	71.2	71.2	68.61	−2.59
OH(CH$_2$)$_3$C$^{\cdot}$HOH	255.2[1] 239.7[18]	404.2	426.0±5.7[3]	239.8	239.8	248.78	8.98
OH(CH$_2$)$_2$C$^{\cdot}$(OH)CH$_3$	—	387.7	433.0±3.0[3]	263.3	263.3	270.62	7.32
OHCH(CH$_3$)C$^{\cdot}$(CH$_3$)OH	—	383.1	461.0[g]	295.9	295.9	287.6	−8.3
(CH$_3$O)$_2$C$^{\cdot}$CH$_3$	220.3[18]	381.2	389.7±0.84[3]	226.5	226.5	223.37	−3.13
(CH$_3$)$_3$CC$^{\cdot}$HOH	147.3[1] 141.0[17]	395.2	318.3[g]	141.1	141.1	135.81	−5.29
OHCH$_2$C(CH$_3$)$_2$C$^{\cdot}$HOH	—	408.3	469.0[g]	278.7	278.7	289.03	10.33
(CH$_3$CH$_2$O)$_2$C$^{\cdot}$H	200.3[18]	390.1	413.1[3]	241.0	241.0	243.07	2.07
CH$_3$(CH$_2$)$_4$C$^{\cdot}$HOH	123.2[17]	391.4	316.0±10[3]	142.6	142.6	139.08	−3.52
(CH$_3$)$_2$C$^{\cdot}$OCH(CH$_3$)$_2$	146.0[18]	390.8	318.0±3.0[3]	145.2	145.2	150.95	5.75
CH$_3$C$^{\cdot}$HOC(CH$_3$)$_3$	—	405.4	317.8[3]	130.4	130.4	128.17	−2.23
(CH$_3$O)$_2$C$^{\cdot}$(CH$_2$)$_2$CH$_3$	—	378.8	426.0±2.0[3]	265.2	265.2	266.89	1.69
(CH$_3$O)$_2$C$^{\cdot}$CH(CH$_3$)$_2$	—	381.4	442.5[g]	279.1	279.1	277.8	−1.3
(CH$_3$CH$_2$O)$_2$C$^{\cdot}$CH$_3$	—	380.2	453.6±3.1[3]	291.4	291.4	291.77	0.37
(CH$_3$(CH$_2$)$_2$O)$_2$C$^{\cdot}$H	239.9[18]	391.8	461.4[g]	287.6	287.6	286.59	−1.01
((CH$_3$)$_2$CHO)$_2$C$^{\cdot}$H	—	390.5	495.6[g]	323.1	323.1	320.55	−2.55
CH$_3$(CH$_2$)$_3$OC$^{\cdot}$H(CH$_2$)$_2$CH$_3$	160.5[18]	392.2	334.0±2.0[3]	159.8	159.8	155.65	−4.15
(CH$_3$)$_3$COC(CH$_3$)$_2$C$^{\cdot}$H$_2$	179.9[18]	402.1	361.1±0.8[3]	177.0	177.0	181.48	4.48
(CH$_3$CH$_2$O)$_2$C$^{\cdot}$(CH$_2$)$_2$CH$_3$	—	378.3	500.3[g]	340.0	340.0	335.29	−4.71
(CH$_3$CH$_2$O)$_2$C$^{\cdot}$CH(CH$_3$)$_2$	—	380.5	510.3[g]	347.8	347.8	346.2	−1.6

(*to be continued*)

Table 1 (*continued*)

Radical R·	$-\Delta_f H°(R·)^a$	$D(R—H)^b$	$-\Delta_f H°(RH)$	$-\Delta_f H°(R·)^c$	$-\Delta_f H°(R·)_{rec}{}^d$	$-\Delta_f H°(R·)_{calc}{}^e$	δ^f
$(CH_3(CH_2)_2O)_2C·CH_3$	—	379.6	500.3[g]	338.7	338.7	335.29	−3.41
$((CH_3)_2CHO)_2C·CH_3$	—	380.7	525.9±4.8[3]	363.2	363.2	369.25	6.05
$CH_3(CH_2)_7C·HOH$	—	395.8	377.0±9.0[3]	199.2	199.2	204.36	5.16
$(CH_3(CH_2)_3O)_2C·H$	282.7[18]	389.1	501.0±3.0[3]	329.9	329.9	330.11	0.21
$((CH_3)_2CHCH_2O)_2C·H$	—	389.5	523.2[g]	351.7	351.7	351.93	0.23
$(CH_3CH_2CH(CH_3)O)_2C·H$	—	391.5	537.4[g]	363.9	363.9	364.07	0.17
$CH_3(CH_2)_8C·HOH$	—	395.5	395.0±10.0[3]	217.5	217.5	226.12	8.62
$(CH_3(CH_2)_3O)_2C·CH_3$	—	379.0	542.1[g]	381.1	381.1	378.81	−2.29
$(CH_3(CH_2)_2O)_2C·CH(CH_3)_2$	—	379.5	552.1[g]	390.6	390.6	389.72	−0.88
$((CH_3)_2CHCH_2O)_2C·CH_3$	—	379.1	562.1[g]	401.0	401.0	400.63	−0.37
$((CH_3)_2CHO)_2C·(CH_2)_2CH_3$	—	379.6	576.3[g]	414.7	414.7	412.77	−1.93
$((CH_3)_2CHO)_2C·CH(CH_3)_2$	—	381.4	586.3[g]	422.9	422.9	423.68	0.78
$(CH_3(CH_2)_2CH(CH_3)O)_2C·H$	—	390.2	579.2[g]	407.0	407.0	407.59	0.59
$((CH_3)_2CHCH_2CH_2O)C·H$	—	388.4	565.0[g]	394.6	394.6	395.45	0.85
$(CH_3)_3C(CH_2)_7C·HOH$	—	391.9[h]	464.4[g]	290.5	290.5	288.13	−2.37
$(CH_3(CH_2)_4O)_2C·CH_3$	—	378.3	583.9[g]	423.6	423.6	422.33	−1.27
$(CH_3(CH_2)_3O)_2C·CH(CH_3)_2$	—	379.0	593.3[g]	432.3	432.3	433.24	0.94
$((CH_3)_2CHCH_2CH_2O)_2C·CH_3$	—	378.3	603.9[g]	443.6	443.6	444.15	0.55
$((CH_3)_2CHCH_2O)_2C·CH(CH_3)_2$	—	380.5	613.9[g]	451.4	451.4	455.06	3.66
$(CH_3CH_2CH(CH_3)O)_2C·CH(CH_3)_2$	—	380.5	628.1[g]	465.6	465.6	467.2	1.6
$(CH_3)_3C(CH_2)_8C·HOH$	—	390.8[h]	485.5[g]	312.7	312.7	309.89	2.81
$(CH_3(CH_2)_4O)_2C·CH(CH_3)_2$	—	378.3	635.7[g]	475.4	475.4	476.76	1.36
$((CH_3)_2CH(CH_2)_2O)_2C·CH(CH_3)_2$	—	379.6	655.7[g]	494.1	494.1	498.58	4.48
$(CH_3(CH_2)_2CH(CH_3)O)_2C·CH(CH_3)_2$	—	379.6	669.9[g]	508.3	508.3	510.72	2.42

[a] According to published data.
[b] According to Ref. 2.
[c] Calculated from Eq. (1).
[d] Recommended values.
[e] Calculated using the parameters listed in Table 2.
[f] $\delta = \Delta_f H°(R·)_{rec} - \Delta_f H°(R·)_{calc}$.
[g] Calculated using the parameters of the group additivity scheme.[19]
[h] According to Ref. 20.

In respect to $\Delta_f H°(R·)$ calculations, the group additivity scheme was implemented for the largest class of organic radicals.[1] Also, it is rigorously substantiated theoretically[21] studies of the effect of free valence and group transferability.

The structure—property (enthalpy of formation) correlation for oxygen-containing organic free radicals was studied in the framework of the group additivity approach with substantiation of possible approximations earlier.[1,22,23] In the present paper, the radicals are simulated by a larger set of groups; this enables detalization of the approach developed previously.[1,22,23] An attempt to establish a quantitative correlation between the structure and enthalpies of formation for radicals considered in the framework of the group additivity scheme was also reported.[24] Based on the group fragmentations for radicals,[25] seven new groups were introduced into consideration (two of them, as assumed, are similar). The increments of these groups (contributions to $\Delta_f H°$) were determined using six reference values. Such a method of determination of parameter ignoring commonly accepted methods[26] of solution of inverse problems of the phenomenological approach casts some doubt about the validity of the results (first of all, numerical values) obtained in Ref. 24.

The $\Delta_f H°(R·)$ values for 35 free radicals of the studied class were determined for the first time; for seven radicals, they were defined more exactly (see Table 1) using the published values of the C—H bond dissociation energies (see Ref. 2) and the $\Delta_f H°$ values of the corresponding RH molecules and the fundamental thermochemical relation

$$D(R—H) = \Delta_f H°(R·) + \Delta_f H°(H) - \Delta_f H°(R—H). \qquad (1)$$

The quantitative data necessary for the determination of $\Delta_f H°$ values of the given radicals are listed in Table 1. The lack of the reference data on $\Delta_f H°(RH)$ of the corresponding molecules usually prevents expansion of the $\Delta_f H°(R·)$ data array (see Ref. 1). In this case, it seems reasonable[1,10,16] to use the reliable calculated values. In the present work, the $\Delta_f H°(RH)$ values for 29 compounds were also calculated using the parameters of the group additivity model[19] (see Table 1).

The $\Delta_f H°(R·)$ values determined in this work along with the published data were used to construct a struc-

ture—property correlation in the framework of the group additivity scheme.[1] In the present work, such a correlation was considered in the framework of the first approximation[1] of the group additivity model for calculations of $\Delta_f H°(R^{\cdot})$ values. The set of fragments (groups) used for simulation of $R^{\cdot}$ is shown in Table 2.

The group contributions to $\Delta_f H°(R^{\cdot})$ were calculated using the solutions of overdetermined systems of linear equations by the least squares method using the Maple software. All primary $\Delta_f H°(R^{\cdot})$ values (see Table 1, second column) were considered. From the set of solutions obtained using alternative literature data on $\Delta_f H°(R^{\cdot})$ for some compounds (see Table 1), we selected the most appropriate values, *i.e.*, those which provide the best agreement with the initial data array.

Thus, particular experimental data were chosen as the recommended ones (if different values for the same compound were available) on the basis of the best agreement with the quantitative structure—property (enthalpy of formation) correlation established in the framework of the group additivity scheme.

All solutions were additionally substantiated following Ref. 26. The results of comparison of the $\Delta_f H°(R^{\cdot})$ values calculated using the parameters listed in Table 2 with the recommended values are presented in Table 1. Taking into account the error of determination of $\Delta_f H°(R^{\cdot})$ values (6—8 kJ mol^{-1}; maximum error is 13 kJ mol^{-1}),[1] the agreement between the calculated and recommended experimental data is quite satisfactory. The deviations larger than 8 kJ mol^{-1} were obtained for five out of 60 radicals. According to the criteria from Ref. 1, the $\Delta_f H°(R^{\cdot})$ values for these compounds can be considered as preliminary ones.

Thus, the enthalpies of formation of 35 oxygen-containing organic radicals of alcohol and ether derivatives were determined for the first time. Parameters for calculations of $\Delta_f H°$ values of the radicals belonging to this homologous series were found and a novel, ~2.5 times larger set of $\Delta_f H°$ values of radicals of the studied class was recommended. These results extend the quantitative and methodological basis of thermochemistry of organic free radicals.

Table 2. Contributions of different groups to the enthalpies of formation of radicals

Group	Contribution to $\Delta_f H°(R^{\cdot})$ /kJ mol^{-1}	Group	Contribution to $\Delta_f H°(R^{\cdot})$ /kJ mol^{-1}
$C^{\cdot}—(H)_2(C)$	148.47[1]	O—(H)(C)	−160.06*
$C^{\cdot}—(H)(C)_2$	154.60[1]	$C—(H)_3(C)$	−41.04[1]
$C^{\cdot}—(C)_3$	161.00[1]	$C—(H)_2(C)_2$	−21.76[1]
$C^{\cdot}—(C)_2(O)$	146.5*	$C—(H)(C)_3$	−13.39[1]
$C^{\cdot}—(H)(C)(O)$	149.06*	$C—(C)_4$	−1.69[1]
$C^{\cdot}—(H)_2(O)$	138.83*	$C—(H)_3(O)$	−41.04*
$C^{\cdot}—(H)(O)_2$	110.19*	$C—(H)_2(C)(O)$	−34.2*
$C^{\cdot}—(C)(O)_2$	102.53*	$C—(C)_2(H)(O)$	−31.9*
$O—(C)_2$	−101.39*	$C—(C)_3(O)$	−11.68*

* Present work.

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