ESTIMATION OF THE STANDARD *G*-FUNCTIONS OF SUBSTANCES IN THE IDEAL-GAS STATE BY THE BENSON METHOD

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Received May 3, 1988
Accepted June 17, 1988

The Benson method used to estimate thermodynamic properties of substances in the ideal-gas state is modified for calculating the standard G functions $(G^0 - H^0_{298})/T$. The estimation method is verified using a set of 342 organic compounds.

To estimate thermodynamic properties of substances in the ideal-gas state, the Benson method[1,2] is widely used. This method makes it possible to determine standard entropy and standard enthalpy of formation of substance at the temperature of 298 K and standard molar heat capacity within the range of temperatures of 300–1 000 K or 300–1 500 K. The aim of this work is the extension of the Benson method for estimating the standard G-functions $(G^0 - H^0_{298})/T$.

Calculation of the Standard G-Function

For the standard G-function related to the temperature of 298 K, the relation holds

$$\frac{G^0 - H^0_{298}}{T} = \frac{1}{T}\int_{298}^{T} C^0_{pm}\,dT - S^0_{298} - \int_{298}^{T} \frac{C^0_{pm}}{T}\,dT, \qquad (1)$$

where C^0_{pm} denotes the standard molar heat capacity and S^0 the standard entropy of substance in the ideal-gas state. The quantities on the right-hand side of Eq. (1) can be estimated by means of the Benson method. The standard molar heat capacity is given in this method by the relation

$$C^0_{pm} = \sum_i n_i [C_p]_i\,, \qquad (2)$$

where $[C_p]_i$ is the value of the i-th contribution and n_i is its multiplicity. For the standard entropy holds the equation

$$S^0_{298} = \sum_i n_i [S]_i - R \ln \frac{\sigma_{ext}\,\sigma_{int}}{n_{opt}}\,, \qquad (3)$$

TABLE I

Values of contributions to the standard *G*-functions $(G^0 - H^0_{298})/T$ (J/K mol). The indices have the meaning as follows: C_d double-bonded carbon, C_t triple-bonded carbon, C_B carbon in the aromatic ring, C_a allenic carbon, N_i nitrogen in the imines, N_a nitrogen in the azo compounds

Group	*T*, K						
	300	400	500	600	800	1 000	1 500
$C-(C)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(C_2)(H)_2$	−39·41	−40·39	−42·43	−44·94	−50·48	−56·12	−69·37
$C-(C)_3H$	50·50	49·68	47·94	45·77	41·01	36·21	25·17
$C-(C)_4$	146·86	146·04	144·28	142·09	137·29	132·57	122·36
$C-(C_d)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(C_d)(C)(H)_2$	−41·00	−41·94	−43·93	−46·41	−51·95	−57·63	−70·98
$C-(C_d)(C)_2(H)$	46·82	46·04	44·34	42·19	37·41	32·56	21·40
$C-(C_d)(C)_3$	145·27	144·50	142·79	140·61	135·81	131·05	120·72
$C-(C_d)_2(H)_2$	−42·68	−43·56	−45·51	−47·97	−53·51	−59·21	−72·63
$C-(C_t)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(C_t)(C)(H)_2$	−43·10	−43·99	−45·90	−48·28	−53·58	−59·03	−71·98
$C-(C_t)(C)_2(H)$	46·82	46·08	44·47	42·44	37·91	33·30	22·56
$C-(C_B)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(C_B)(C)(H)_2$	−39·08	−40·14	−42·36	−45·09	−51·06	−57·06	−70·81
$C-(C_B)(C)_2(H)$	50·84	49·94	48·02	45·63	40·43	35·27	23·72
$C-(C_B)(C)_3$	147·19	146·33	144·41	142·01	136·80	131·74	121·04
$C-(C_B)(C_d)(H)_3$	−42·68	−43·56	−45·51	−47·97	−53·51	−59·21	−72·63
$C_d-(H)_2$	−115·52	−116·42	−118·29	−120·59	−125·64	−130·78	−142·88
$C_d-(C)(H)$	−33·35	−34·08	−35·57	−37·37	−41·30	−45·25	−54·44
$C_d-(C)_2$	53·14	52·43	51·04	49·42	46·05	42·82	35·72
$C_d-(C_d)(H)$	−26·69	−27·50	−29·19	−31·26	−35·73	−40·17	−50·22
$C_d-(C_d)(C)$	61·09	60·31	58·71	56·83	52·91	49·19	41·23
$C_d-(C_t)(H)$	−26·69	−27·50	−29·19	−31·26	−35·73	−40·17	−50·22
$C_d-(C_B)(H)$	−26·69	−27·50	−29·19	−31·26	−35·73	−40·17	−50·22
$C_d-(C_B)(C)$	61·09	60·31	58·71	56·83	52·91	49·19	41·23
$C_t-(H)$	−103·35	−104·25	−106·05	−108·16	−112·54	−116·73	−126·00
$C_t-(C)$	−22·94	−25·30	−27·45	−29·42	−32·92	−35·99	−42·34
$C_t-(C_d)$	−26·90	−27·36	−28·33	−29·52	−32·20	−34·91	−41·08
$C_t-(C_B)$	−26·90	−27·36	−28·33	−29·52	−32·20	−34·91	−41·08
$C_B-(H)$	−48·24	−48·84	−50·12	−51·73	−55·37	−59·13	−68·05
$C_B-(C)$	32·17	31·71	30·78	29·65	27·15	24·62	18·75
$C_B-(C_d)$	32·63	31·02	30·82	29·40	26·43	23·55	17·13
$C_B-(C_t)$	32·63	32·02	30·82	29·40	26·43	23·55	17·13
$C_B-(C_B)$	36·15	35·55	34·31	32·81	29·59	26·44	19·56
C_a	−25·10	−25·77	−27·10	−28·64	−31·83	−34·85	−41·39
Ortho	6·74	6·54	6·14	5·70	4·85	4·15	2·98
Cyclopropane	−134·31	−133·83	−133·02	−132·17	−130·63	−129·34	−126·90

TABLE I
(*Continued*)

Group	*T*, K						
	300	400	500	600	800	1 000	1 500
Cyclobutane	−124·68	−123·96	−122·70	−121·41	−119·17	−117·42	−114·51
Cyclobutene	−121·34	−120·94	−120·23	−119·49	−118·16	−117·04	−114·96
Cyclopentane	−114·22	−113·03	−110·94	−108·78	−105·04	−102·15	−97·55
Cyclopentene	−107·95	−106·99	−105·27	−103·44	−100·17	−97·55	−93·15
Cyclohexane	−78·66	−77·69	−76·07	−74·55	−72·33	−71·11	−70·52
Cyclohexene	−89·68	−78·80	−71·61	−66·52	−59·86	−55·78	−50·42
Cis-2-butene	−4·95	−2·04	−0·06	1·37	3·31	4·56	
Cis-3-enes	2·58	5·50	7·47	8·90	10·84	12·09	
Alkene *cis*	0·07	2·99	4·96	6·39	8·33	9·58	
$C-(O)(H)_3$	−127·25	−128·34	−130·64	−133·48	−139·81	−146·34	−161·94
$C-(O)(C)(H)_2$	−43·10	−44·01	−45·99	−48·47	−53·97	−59·61	
$C-(O)(C)_2(H)$	46·02	45·13	43·20	40·81	35·58	30·38	
$C-(O)(C)_3$	140·41	139·59	137·81	135·63	130·94	126·40	
$C-(O)(C_B)(H)_2$	−40·59	−41·33	−43·07	−45·38	−50·78	−56·49	
$C_d-(O)(H)$	−33·47	−34·20	−35·69	−37·50	−41·42	−45·38	−54·57
$C_B-(O)$	42·68	41·96	40·43	38·54	34·53	30·67	
$(O)-(C)(H)$	−121·63	−122·34	−123·72	−125·31	−128·63	−131·89	−139·28
$O-(C)_2$	36·32	−36·89	−38·00	−39·26	−41·82	−44·26	
$O-(C_d)(C)$	−40·59	−41·16	−42·26	−43·52	−46·09	−48·53	
$O-(C_d)_2$	−33·89	−34·46	−35·57	−36·83	−39·39	−41·83	
$O-(C_B)(H)$	−121·75	−122·47	−123·85	−125·44	−128·77	−132·01	−139·40
$O-(O)(H)$	−116·52	−117·41	−119·15	−121·20	−125·43	−129·48	−138·32
$O-(O)(C)$	−39·33	−39·94	−41·08	−42·36	−44·92	−47·31	−52·48
$C-(CO)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(CO)(C)(H)_2$	−40·17	−41·27	−43·55	−46·27	−52·13	−57·95	
$C-(CO)(C)_2H)$	50·21	49·11	46·89	44·30	38·94	33·81	
$CO-(H)_2$	−224·56	−225·99	−228·83	−232·19	−239·33	−246·41	
$CO-(C)(H)$	−146·15	−147·34	−149·72	−152·54	−158·53	−164·47	
$CO-(C)_2$	−62·80	−63·76	−65·66	−67·92	−72·73	−77·48	
$CO-(O)(H)$	−146·15	−147·34	−149·72	−152·54	−158·53	−164·47	
$CO-(O)(C)$	−61·84	−62·86	−64·88	−67·26	−72·27	−77·14	
$O-(CO)(H)$	−102·59	−103·28	−104·74	−106·51	−110·35	−114·16	
$O-(CO)(C)$	−35·10	−35·72	−36·88	−38·24	−41·09	−43·85	
Oxirane	−127·61	−127·22	−126·40	−125·45	−123·60	−122·01	
Oxetane	−109·05	−102·75	−98·00	−94·24	−88·62	−84·74	
$C-(N)(H)_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
$C-(N)(C)(H)_2$	−41·00	−41·95	−43·96	−46·45	−51·98	−57·62	−70·86
$C-(N)(C)_2(H)$	48·95	48·09	46·26	43·98	38·98	33·98	22·61
$C-(N)(C)_3$	142·67	141·86	140·08	137·89	133·15	128·52	118·55
$C_B-(N)$	40·54	39·82	38·31	36·47	32·59	28·88	

TABLE I
(Continued)

Group	*T*, K						
	300	400	500	600	800	1 000	1 500
N-(C)(H)$_2$	−124·31	−125·29	−127·24	−129·57	−134·55	−139·50	−150·99
N-(C)$_2$(H)	−37·41	−38·15	−39·69	−41·56	−45·66	−49·78	−59·24
N-(C)$_3$	56·32	55·69	54·36	52·72	49·15	45·64	37·95
N-(C$_B$)(H)$_2$	−124·31	−125·29	−127·24	−129·57	−134·55	−139·50	−150·99
N-(N)(H)$_2$	−121·88	−122·95	−125·14	−127·77	−133·43	−139·03	−151·95
N-(N)(C)(H)	−40·21	−41·06	−42·78	−44·83	−49·19	−53·43	−62·90
N-(N)(C)$_2$	57·74	57·43	56·73	55·81	53·66	52·40	
CO-(N)(H)	−146·15	−147·34	−149·72	−152·54	−158·53	−164·47	
CO-(N)(C)	−67·78	−68·71	−70·57	−72·79	−77·56	−82·43	
N-(CO)(H)$_2$	−103·21	−100·59	−100·21	−100·95	−104·00	−107·92	
N-(CO)(C)(H)	−16·32	−17·01	−18·48	−20·30	−24·25	−28·07	
N$_a$-(H)	−112·13	−112·88	−114·35	−116·10	−119·79	−123·43	−131·72
N$_a$-(C)	−33·47	−34·00	−35·16	−36·62	−39·79	−42·88	
N$_i$-(H)	−51·46	−52·03	−53·33	−55·09	−59·25	−63·68	
C-(CN)(C)(H)$_2$	−168·20	−170·14	−174·11	−178·93	−189·33	−199·71	−223·33
C-(CN)(C)$_2$(H)	−82·84	−84·74	−88·55	−93·06	−102·62	−111·98	−133·00
C-(CN)(C)$_3$	11·71	10·15	6·89	2·92	−5·61	−13·98	
C$_d$-(CN)(H)	−153·10	−156·50	−160·99	−165·84	−175·59	−184·87	
C$_d$(CN)(C)	−66·57	−68·26	−71·64	−75·64	−84·00	−92·05	
C$_t$-(CN)	−148·11	−149·86	−153·29	−157·27	−165·45	−173·22	−190·12
C$_B$-(CN)	−85·77	−87·46	−90·82	−94·79	−103·05	−111·00	
C-(NO$_2$)(C)(H)$_2$	−202·51	−204·74	−209·40	−215·08	−227·46	−239·88	
C-(NO$_2$)(C)$_2$(H)	−112·55	−114·69	−119·16	−124·60	−136·41	−148·14	
O-(NO)(C)	−175·43	−181·55	−187·38	−192·84	−202·72	−211·42	−229·37
O-(NO$_2$)(C)	−202·93	−204·58	−207·99	−212·16	−221·20	−230·14	
Aziridine	−132·21	−131·86	−131·19	−130·45	−129·00	−127·72	
Azetidine	−122·59	−121·82	−114·96	−118·89	−116·12	−111·15	
Azolidine	−111·71	−110·72	−108·94	−107·08	−103·79	−101·20	
C-(F)$_3$(C)	−177·82	−180·04	−184·50	−189·79	−200·89	−211·62	
C-(F)$_2$(H)(C)	−163·60	−165·33	−168·89	−173·17	−182·35	−191·38	
C-(F)$_2$(C)$_2$	−74·48	−76·21	−79·74	−83·95	−92·91	−101·65	
C-(F)(H)$_2$(C)	−148·11	−149·55	−152·52	−156·15	−164·04	−171·95	
C-(F)(C)$_2$(H)	−58·58	−59·87	−62·54	−65·77	−72·77	−79·71	
C-(F)$_2$(Cl)(C)	−169·45	−171·85	−176·65	−182·31	−194·06	−205·29	
C-(Cl)$_3$(C)	−210·88	−213·65	−219·10	−225·41	−238·27	−250·33	
C-(Cl)$_2$(H)(C)	−182·84	−184·94	−189·13	−194·08	−204·43	−214·41	
C-(Cl)$_2$(C)$_2$	−93·72	−95·90	−100·30	−105·47	−116·07	−126·00	
C-(Cl)(H)$_2$(C)	−158·16	−159·71	−162·90	−166·73	−174·94	−183·08	
C-(Cl)(H)(C)$_2$	−73·64	−75·2	−78·12	−81·55	−88·79	−96·00	
C-(Cl)(C)$_3$	22·59	20·99	17·85	14·21	6·77	−0·27	

TABLE I
(*Continued*)

Group	*T*, K						
	300	400	500	600	800	1 000	1 500
C–(Br)(H)$_2$(C)	−170·71	−172·31	−175·57	−179·50	−187·91	−196·21	
C–(Br)(C)$_3$	8·37	6·75	3·52	−0·27	−8·13	−15·62	
C–(I)$_2$(C)(H)	−228·45	−230·65	−235·07	−240·28	−251·12	−261·48	
C–(I)(H)$_2$(C)	−177·82	−179·43	−182·72	−186·69	−195·21	−203·64	
C–(I)(H)(C)$_2$	−92·89	−94·49	−97·74	−101·61	−109·74	−117·60	
C–(I)(C)$_3$	0·00	−1·73	−5·22	−9·35	−17·89	−25·93	
C–(C$_B$)(F)$_3$	−179·08	−181·29	−185·81	−191·23	−202·68	−213·78	
C$_d$–(F)$_2$	−156·06	−157·73	−161·04	−164·93	−173·00	−180·74	
C$_d$–(F)(H)	−137·24	−138·44	−140·92	−143·91	−150·30	−156·62	
C$_d$–(Cl)*a*	−176·31	−184·45	−191·97	−198·84	−210·93	−221·26	
C$_d$–(Cl(H)	−148·11	−149·48	−152·23	−155·51	−162·43	−169·18	
C$_d$–(C)(Cl)	−62·76	−64·10	−66·65	−69·57	−75·45	−80·93	
C$_d$–(Br)(H)	−160·25	−161·65	−164·49	−167·86	−174·96	−181·83	
C$_d$–(I)(H)	−169·45	−170·97	−173·97	−177·50	−184·85	−191·91	
C$_B$–(F)	−67·36	−68·47	−70·73	−73·42	−79·08	−84·54	
C$_B$–(Cl)	−79·08	−80·35	−82·87	−85·84	−92·00	−97·84	
C$_B$–(Br)	−90·38	−91·70	−94·33	−97·40	−103·72	−109·68	
C$_B$–(I)	−99·16	−100·53	−103·22	−106·36	−112·77	−118·79	
C–(Cl)(C)(O)(H)	−81·78	−90·39	−97·62	−103.92	−114·64	−123·68	
C–(I)(O)(H)$_2$	−170·29	−171·76	−174·84	−178·59	−186·73	−194·84	
C–(H)$_3$(S)	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	
C–(C)(H)$_2$S	−41·31	−41·20	−42·62	−44·76	−50·01	−55·73	
C–(C)$_2$(H)(S)	47·36	46·48	44·59	42·25	37·10	31·94	
C–(C)$_3$(S)	143·97	143·13	141·31	139·07	134·20	129·46	
C$_d$–(H)(S)	−33·47	−34·20	−35·69	−37·50	−41·42	−45·38	
C$_d$–(C)(S)	51·84	48·25	45·32	42·83	38·70	35·29	
C$_B$–(S)	−42·68	−43·40	−44·93	−46·81	−50·83	−54·69	
S–(C)(H)	−136·94	−137·93	−139·82	−142·00	−146·43	−150·63	
S–(C)$_2$	−55·02	−55·84	−57·38	−59·12	−62·56	−65·77	
S–(C$_d$)$_2$	−68·95	−69·78	−71·40	−73·29	−77·27	−81·32	
S–(C$_B$)(H)	−52·97	−53·82	−55·44	−57·30	−61·17	−64·96	
S–(S)(C)	−51·76	−52·63	−54·30	−56·18	−59·91	−63·28	
S–(S)$_2$	−56·07	−56·86	−58·38	−60·12	−63·59	−66·79	
CO–(S)(C)	−64·56	−65·52	−67·42	−69·68	−74·49	−79·23	
S–(H)(CO)	−130·54	−131·82	−134·27	−137·05	−142·60	−147·70	
N–(C)(S)(H)$_2$	−122·13	−123·20	−125·36	−127·94	−133·45	−138·87	
S–(C)(CN)	−171·80	−173·41	−176·58	−180·26	−187·86	−195·13	
C–(S)O(H)$_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93
SO–(C)$_2$	−75·73	−77·26	−80·29	−83·78	−90·84	−97·39	
C–(SO$_2$)(H)$_3$	−127·24	−128·34	−130·64	−133·48	−139·81	−146·34	−161·93

TABLE I
(*Continued*)

Group	*T*, K						
	300	400	500	600	800	1 000	1 500
SO_2–$(C)_3$	−87·45	−89·21	−92·73	−96·88	−105·56	−113·95	
CS–$(N)_2$	−64·56	−65·52	−67·42	−69·68	−74·49	−79·23	
Thiirane	−123·12	−115·79	−110·85	−107·17	−101·78	−97·64	
Thietane	−113·50	−104·36	−98·00	−93·21	−86·21	−81·04	
Thiolane	−98·31	−87·59	−80·24	−74·79	−67·02	−61·44	
Thiane	−73·05	−72·12	−70·64	−69·32	−67·56	−66·66	
Thiophene	−98·31	−87·59	−80·24	−74·79	−67·02	−61·44	

where $[S]_i$ denotes the value of the i-th contribution with its multiplicity n_i, σ_{ext} the number of external and σ_{int} the number of internal symmetry, n_{opt} the number of optical isomers of the substance, and $\boldsymbol{R}$ the gas constant. From Eqs (*1*)–(*3*) follows for the standard *G*-function the relation

$$\frac{G^0 - H^0_{298}}{T} = \sum_i n_i [G]_i + \boldsymbol{R} \ln \frac{\sigma_{ext}\, \sigma_{int}}{n_{opt}}, \tag{4}$$

where $[G]_i$ is the value of the i-th contribution to the *G*-function and n_i is the respective multiplicity.

The value of contribution $[G]_i$ can be calculated by means of Eq. (*1*) from the contributions to entropy and to molar heat capacity. The temperature dependence of molar heat capacity has been expressed by the equation[3]

$$[C_p]_i = a + b_1 \left(\frac{c_1}{T}\right)^2 \frac{e^{-c_1/T}}{(1 - e^{-c_1/T})^2} + b_2 \left(\frac{c_2}{T}\right)^2 \frac{e^{-c_2/T}}{(1 - e^{-c_2/T})^2}, \tag{5}$$

where $a - c_2$ are empirical constants. The integrals in Eq. (*1*) are, on using relation (*5*), given by the relations

$$\int [C_p]_i \, dT = aT + \frac{b_1 c_1}{1 - e^{-c_1/T}} + \frac{b_2 c_2}{1 - e^{-c_2/T}}, \tag{6}$$

$$\int \frac{[C_p]_i}{T} = a \ln T + \frac{1}{T} \frac{b_1 c_1}{1 - e^{-c_1/T}} + \frac{1}{T} \frac{b_2 c_2}{1 - e^{-c_2/T}} - b_1 \ln (e^{c_1/T} - 1) - b_2 \ln (e^{c_2/T} - 1). \tag{7}$$

RESULTS AND DISCUSSION

The values of contributions to the standard *G*-function, as calculated from Eqs (*1*) and (*5*)–(*7*), are given in Table I.

The calculation of the standard *G*-function by means of relation (*4*) was verified on using a set of 342 organic substances. For single groups of compounds studied, the average and maximum percent deviations of tabulated and estimated values

TABLE II

Deviations of tabulated and estimated values of the standard *G*-function (%)

Group of substances	Number	Ref.	δ_{av}	δ_{max}
Alkanes	38	6	0·78	1·45
Alkenes	27	6, 7	1·01	1·90
Alkynes	10	6, 8	0·66	1·41
Dienes	10	6	1·36	3·80
Cyclopentanes	9	6, 9	0·89	2·38
Cyclohexanes	12	6, 9	0·32	1·26
Benzenes	14	6, 7, 10	0·30	0·94
Styrenes	8	6	0·88	2·43
Naphthalenes	16	4	5·19	7·02
Alcohols	11	7, 8, 11, 12	0·94	4·41
Ethers	11	7, 11	2·48	4·73
Aldehydes	5	7, 11	0·14	0·28
Ketones	5	7, 11, 13, 14	0·72	1·33
Acids, esters	5	7, 8, 11	2·85	4·46
Phenols	7	10, 15, 16	0·76	1·65
Amines	14	7, 18–20	1·27	3·15
Cyclic amines	2	7	1·70	1·81
Nitrocompounds	5	7	1·52	2·58
Amides	3	21	1·35	1·75
Nitriles	5	7	2·04	3·32
Nitrates	3	7	2·94	3·55
Haloalkanes	36	7, 8, 22–24	1·29	3·83
Haloalkenes	12	7, 25	1·09	3·56
Halobenzenes	17	7, 17, 26–29	1·78	4·69
Halonaphthalenes	8	5	7·65	8·52
Thiols	12	7	0·81	2·31
Sulfides	17	7	0·82	2·29
Cyclic sufides	3	7	3·13	3·91
Disulfides	5	7	0·49	0·75

TABLE III

Deviations of tabulated and estimated values of entropy and molar heat capacity (%)

Substance	$\delta(S)$	$\delta_{av}(C_{pm})$	$\delta_{max}(C_{pm})$
Naphthalene	9·99	1·66	2·64
1-Methylnaphthalene	6·92	0·32	0·47
1-Ethylnaphthalene	6·64	0·26	0·59
1,2-Dimethylnaphthalene	6·03	0·41	1·08
1,3-Dimethylnaphthalene	4·99	1·23	1·72
1,4-Dimethylnaphthalene	4·45	1·61	2·13
1-Bromonaphthalene	8·55	0·98	2·66
1-Chloronaphthalene	6·39	0·71	1·05
1-Fluoronaphthalene	8·59	1·00	1·40
1-Iodonaphthalene	8·41	0·49	0·87
1,4-Dibromonaphthalene	6·30	1·18	1·71
1,4-Dichloronaphthalene	6·76	1·42	1·99

were evaluated according to the equation

$$\delta = \frac{G_{tab} - G_{est}}{G_{tab}} \cdot 100 . \qquad (8)$$

The results of comparison of the tabulated and estimated values of the standard *G*-function are given in Table II.

It is apparent from the table that the highest deviations in estimation of the standard *G*-functions in terms of the given method exhibit the naphthalene derivatives. Therefore, the values of entropy and molar heat capacity were calculated by means of the Benson method and compared with the values reported in the literature for naphthalenes[4] and halogen derivatives of naphthalene[5]. The percent deviations of the estimated and tabulated values calculated according to Eq. (*8*) are given in Table III. It can be seen from the table that the Benson method does not enable one to reliably estimate the entropy for the given compounds. This fact is evidently the reason of errors when estimating the standard *G*-functions of the naphthalene derivatives.

For the other studied types of organic substances it is possible to consider the errors of estimation of the *G*-functions as satisfactory and in agreement with the accuracy of estimation of the other thermodynamic quantities by means of the Benson method.

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Translated by J. Linek.