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Enthalpies of Formation of Six-Membered Nitrogen-Containing Aromatic Heterocyclic Compounds

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Abstract—Good correlation was revealed between experimental and PM3-calculated heats of formation of polycyclic six-membered nitrogen-containing compounds. The correlation is described by linear regression equation that can be further used to predict enthalpy of formation of similar compounds. Using the equation, we calculated enthalpy of formation of 63 compounds of the studied class.

Keywords: heat of formation, nitrogen-containing heterocyclic compound, semiempirical quantum-chemical simulation

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Development and implementation of highly efficient production of new organic compounds is essentially based on the information on their physicochemical properties. Thermochemical data including enthalpy of formation is among the most important properties of the compounds.

Experiment has remained the major source of thermochemical data. However, direct determination of thermochemical properties of many organic (and especially organoelement) compounds is complicated, being even impossible in certain cases. In view of that, importance of theoretical determination of thermochemical properties of organic compounds has become a topical issue of modern chemistry. Semiempirical quantum-chemical simulation methods have been widely applied to compute enthalpy of formation of various compounds, primarily due to simplicity and availability of the simulation software and their relatively low system requirements for the hardware used. Moreover, semiempirical methods can be used to reveal anomalies in the general trends of enthalpy of formation of similar organic compounds [1].

Fairly good correlation between experimental and the computed values of enthalpy of formation has been revealed in the cases of adamantane derivatives [2–4], polycyclic aromatic hydrocarbons [5], and heterocyclic compounds containing sulfur [6, 7] or oxygen [8]. That allowed theoretical prediction of enthalpy of formation of compounds belonging to those classes.

This work investigated similar behavior of polycyclic six-membered nitrogen-containing aromatic compounds. Modern chemistry of heterocyclic compounds has become a rapidly developing field of organic chemistry. Diversity of properties of nitrogen-containing heterocycles opens vast possibilities of their applications in practice. In particular, quinoline and isoquinoline cyclic systems are frequently found in natural compounds. Quinoline nucleus is a building block of quinoline alkaloids [9]. Quinoline derivatives are used to produce cyanine dyes and many drugs. For instance, substituted 2-methyl-3-alkylquinolines have been recently marked as a novel class of psychoactive pharmaceuticals [10]. Alkylquinolines are used as additives enhancing wearproof properties of oils. 2-Alkylquinolines with the alkyl substituent longer than C_6 are patented as surfactants [11].

Quinoxaline derivatives have revealed wide range of biological activity including anticancer, antimicobacterial, anti-inflammatory, antiviral, anti-protozoal, and antibacterial, and are thus promising objects of pharmaceutical studies. Photo- and electroluminescent properties of these compounds are used in development of organic light diodes and optoelectronic devices [12, 13].

Phenylpyridines are important intermediates of synthesis of drugs, agrochemicals, herbicides, insecticides, dehydrators, surfactants, and anti-inflammatory agents

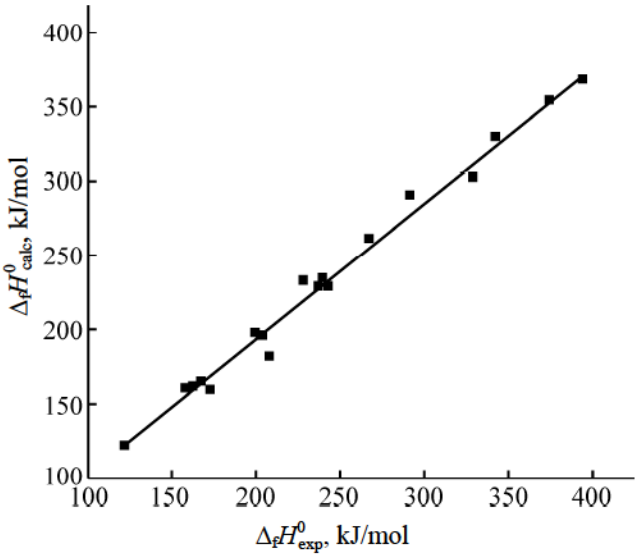
[14]. 2-Phenylpyridine and its derivatives have been widely used as ligands [14]. Many of heterocyclic nitrogen compounds have been recognized as efficient inhibitors of steel corrosion in acidic media [15].

In order to estimate the possibility of application of semiempirical quantum-chemical simulation methods to predict enthalpy of formation of polycyclic six-membered nitrogen-containing heterocycles, we selected 28 compounds (**I**–**XXVIII**) with experimentally determined gas-phase formation enthalpy [16–36]. Those compounds included polycyclic annealed [benzo- (**I**–**VIII**) and dibenzoannealed (**IX**–**XIII**) pyridines, benzoannealed diazines (**XIV**–**XIX**), 2,2'-biquinoline (**XX**)] as well as non-annealed heterocyclic compounds [isomeric bipyridines (**XXI**–**XXIV**) and phenylpyridines (**XXV**–**XXVII**) and 2,2':6',2"-terpyridine (**XXVIII**)].

Analysis of the reference data (Table 1) revealed that for the majority of those compounds accuracy of experimental determination of formation enthalpy was below 3–5 kJ/mol. However, in the cases of several compounds the scatter of the available data was of 7–18 kJ/mol; those compounds were 5,6-benzoquinoline (**X**), 6,7-benzoquinoline (**XI**), quinazoline (**XVI**), and phthalazine (**XVII**). Moreover, the discrepancy of experimental data from different authors reached 15–26 kJ/mol in the cases of 7,8-benzoquinoline (**XII**), acridine (XIII), quinazoline (**XVI**), phthalazine (**XVII**), 9,10-diazaanthracene (**XVIII**), benzo[*c*]cinnoline (**XIX**), and 2,2'-bipyridine (**XXI**).

For each of those compounds we performed full geometry optimization of the molecules and computed their formation enthalpy using the PM3, MINDO, AM1, and MNDO semiempirical quantum-chemical methods implemented in MOPAC software package.

In the cases of three nitrogen-containing phenanthrene analogs (**IX**, **X**, and **XII**), a nitrogen-containing anthracene analog (**XI**), 2,2'-biquinoline (**XX**), and two isomeric bipyridines (**XXII** and **XXIII**), the quantum-chemical simulation gave the computed $\Delta_f H^0_{calc}$ values significantly differing from the available experimental ones $\Delta_f H^0_{exp}$. The deviation between the experimental and the theoretical values of formation enthalpy reached 11–57 kJ/mol for those compounds. The discrepancy between the computed (*ab initio*) and the experimental data for bipyridine isomers was earlier noted in [37]. In the case of 4,4'-bipyridine (**XXIII**), the deviation was assigned to the enhanced hygroscopicity resulting in partial formation of the corresponding hydrate in the calorimeter prior to combustion. The deviation with the experiment in the case of 2,2'-biquinoline (**XX**) was of 78.0 kJ/mol [1]; similarly, large deviation between the experiment and the G3MP2 simulation was found for benzo[*c*]cinnoline (**XIX**) [31]. In view of inaccuracy of the experimental data and extremely large deviation from the computed values, the seven above-mentioned compounds were excluded from calculation of the $\Delta_f H^0_{calc} = f(\Delta_f H^0_{exp})$ correlation model.



Dependence of $\Delta_f H^0_{calc}$ on $\Delta_f H^0_{exp}$.

The calculated correlation coefficients between the experimental and the computed values were of 0.9948 (the PM3 method), 0.9747 (AM1), 0.9806 (MNDO), and 0.7436 (MINDO). Hence, only PM3 method gave the computed values well correlated with the available experimental data for the studied series of six-membered nitrogen-containing aromatic compounds. The AM1 and MNDO methods provided for moderate correlation with the experiment, whereas the correlation was below acceptable for the MINDO method. Mean absolute deviation between the experimental and the computed values of formation enthalpy (Δ) was of 9.4 kJ/mol in the case of the PM3 method, 2.6 times lower than that in the case of the AM1 simulation.

The linear correlation between $\Delta_f H^0_{calc}$ and $\Delta_f H^0_{exp}$values (see figure) may be described by the first order equation:

$$\Delta_f H^0_{calc} = 0.9152\Delta_f H^0_{exp} + 10.902.$$

Using the above equation, we recalculated the PM3-computed values of formation enthalpy; the

Table 1. Results of quantum-chemical computation of enthalpy of formation of six-membered nitrogen-containing heterocyclic compounds by PM3 method[a]

Comp. no.	Compound name	Enthalpy of formation, kJ/mol		Δ, kJ/mol	Comp. no.	Compound name	Enthalpy of formation, kJ/mol		Δ, kJ/mol
		$\Delta_f H^0_{calc}$	$\Delta_f H^0_{exp}$				$\Delta_f H^0_{calc}$	$\Delta_f H^0_{exp}$	
I	Quinoline	198.91	200.52±1.36 [17]	1.59	**XII**	7,8-Benzoquinoline	261.74	**250.4±2.3** [20] 230.5±5.0 [21]	11.34 31.24
II	Isoquinoline	197.42	204.61±1.33[17] 204.0 [16]	7.19 6.58	**XIII**	Acridine (2,3-benzo-quinoline)	290.35	273.9±2.3 [20] **292.47±4.2** [28]	16.45 2.10
III	2-Methyl-quinoline	160.69	159.1±3.1 [22]	1.59	**XIV**	Quinoxaline	235.02	**240.3±3.3** [30] 262.3±4.2 [28]	5.28 27.28
IV	4-Methyl-quinoline	161.56	162.1±3.2 [22]	0.54	**XV**	2,3-Dimethyl-quinoxaline	159.92	172.9±3.0 [22]	12.98
V	6-Methyl-quinoline	160.09	161.0±3.0 [18]	0.91	**XVI**	Quinazoline	228.11	**243.1±2.7** [30] 258.6±8.8 [23]	14.90 30.49
VI	8-Methyl-quinoline	165.08	167.7±3.1 [18]	2.62	**XVII**	Phthalazine	302.34	**329.9±3.3** [30] 345±18 [23]	27.60 42.66
VII	2,6-Dimethyl-quinoline	121.31	120.9±2.9 [19]	0.41	**XVIII**	Phenazine (9,10-diazaantracene)	330.15	338.3±3.4 [24] 328.8±2.9 [25] **343.6±2.8** [26] 337.6±6.3 [28] 331.7±1.3 [29]	8.15 1.35 13.45 7.5 1.55
VIII	2,7-Dimethyl-quinoline	121.42	121.8±3.0 [19]	0.38	**XIX**	5,6-Phenan-throline (benzo[*c*]-cinnoline)	354.53	**376.0±4.9** [23] 391.7 [27] 402.5±2.8 [31]	21.47 37.17 47.97
IX	6-Phenantridine (3,4-benzo-quinoline)	255.72	240.5±4.2 [20] 243.5±5.5 [19]	15.22 12.22	**XX**	2,2'-Biquinoline	405.67	347.9±7.9 [32]	57.77
X	5,6-Benzo-quinoline	259.81	233.7±7.4 [21]	26.11	**XXI**	2,2'-Bipyridine	261.81	**267.9±3.0** [34] 289.0±5.2 [32]	6.09 27.19
XI	6,7-Benzo-quinoline	285.36	243.5±5.5 [21]	41.86	**XXII**	2,4'-Bipyridine	261.98	284.2±2.7 [34]	22.22

Table 1. (Contd.)

Comp. no.	Compound name	Enthalpy of formation, kJ/mol		Δ, kJ/mol	Comp. no.	Compound name	Enthalpy of formation, kJ/mol		Δ, kJ/mol
		$\Delta_f H^0_{calc}$	$\Delta_f H^0_{exp}$				$\Delta_f H^0_{calc}$	$\Delta_f H^0_{exp}$	
XXIII	4,4'-Bipyridine	260.45	293.1±3.6 [34]	32.65	**XXVI**	3-Phenyl-pyridine	229.63	240.9±5.5 [35]	11.27
XXIV	4,4'-Dimethyl-2,2'-bipyridine	181.72	209.3±4.1 [36]	27.58	**XXVII**	4-Phenyl-pyridine	231.77	240.0±3.3 [35]	8.23
XXV	2-Phenyl-pyridine	232.57	228.3±5.8 [35]	4.27	**XXVIII**	2,2':6',2''-Terpyridine	367.97	394.6±4.6 [23]	26.63

[a] Data used to obtain the linear regression equation are given in bold.

results are given in Table 2. From the tabulated data one can see that substitution of the simulated values $\Delta_f H^\circ_{calc}$ with the correlation-corrected ones $\Delta_f H^{0*}_{calc}$ decreased the mean absolute deviation between the experimental and the computed values (Δ*) to 5.6 kJ/mol (about 1.7 times lower than that in the case of uncorrected values); that was already comparable to the accuracy of experimental determination of the formation enthalpy for majority of compounds under consideration.

Table 2. Recalculation of enthalpy of formation ($\Delta_f H^{0*}_{calc}$) using the linear regression equation and comparison with

Comp. no.	Enthalpy of formation, kJ/mol		Δ*, kJ/mol	Comp. no.	Enthalpy of formation, kJ/mol		Δ*, kJ/mol
	$\Delta_f H^0_{exp}$	$\Delta_f H^{0*}_{calc}$			$\Delta_f H^0_{exp}$	$\Delta_f H^{0*}_{calc}$	
I	200.5 [17]	205.4	4.9	**XV**	172.9 [22]	162.8	10.1
II	204.6 [17]	203.8	0.8	**XVI**	243.1 [30]	237.3	5.8
III	159.1 [22]	163.7	4.6	**XVII**	329.9 [30]	318.4	11.5
IV	162.1 [22]	164.6	2.5	**XVIII**	343.6 [26]	348.8	5.2
V	161.0 [18]	163.0	2.0	**XIX**	376.0 [23]	375.5	0.5
VI	167.7 [18]	168.5	0.8	**XX**	347.9 [32]	431.3	83.4
VII	120.9 [19]	120.6	0.3	**XXI**	267.9 [34]	274.2	6.3
VIII	121.8 [19]	120.8	1.0	**XXII**	284.2 [34]	274.3	9.9
IX	243.5 [19]	267.5	24.0	**XXIII**	293.1 [34]	272.7	20.4
X	233.7 [21]	272.0	38.3	**XXIV**	209.3 [34]	186.6	22.7
XI	243.5 [21]	299.9	56.4	**XXV**	228.3 [35]	242.2	13.9
XII	250.4 [20]	274.1	23.7	**XXVI**	240.9 [35]	239.0	1.9
XIII	292.5 [28]	305.3	12.8	**XXVII**	240.0 [35]	241.3	1.3
XIV	240.3 [30]	244.9	4.6	**XXVIII**	394.6 [23]	390.2	4.4
Mean absolute deviation, kJ/mol	with compounds **IX–XII, XX, XXII, XXIII**		13.4	Mean absolute deviation, kJ/mol	without compounds **IX–XII, XX, XXII, XXIII**		5.6

Table 3. Comparison of the deviation (Δ) between experimental and calculated enthalpies of formation of the compounds using Parameter Model 7, 6, and 3 methods

Comp. no.	$\Delta_f H^\circ_{exp}$, kJ/mol (kcal/mol[a])	Absolute deviation Δ, kJ/mol (kcal/mol[a])			
		PM6	PM7	PM3	
				before correction	after correction
I	200.50 (47.92)	11.63 (2.78)	7.41 (1.77)	1.59	4.93
II	204.60 (48.90)	4.85 (1.16)	1.30 (0.31)	7.19	0.81
III	159.12 (38.03)	7.49 (1.79)	6.86 (1.64)	1.59	4.57
IV	162.09 (38.74)	8.41 (2.01)	4.31 (1.03)	0.54	2.52
V	161.00 (38.48)	8.91 (2.13)	6.19 (1.48)	0.91	2.01
VI	167.70 (40.08)	6.40 (1.53)	1.67 (0.40)	2.62	0.76
VII	120.92 (28.90)	4.39 (1.05)	4.69 (1.12)	0.41	0.26
VIII	121.80 (29.11)	1.46 (0.35)	2.85 (0.68)	0.38	1.04
IX	240.50 (57.48)	30.67 (7.33)	27.95 (6.68)	15.22	27.00
X	233.89 (55.90)	36.82 (8.80)	36.23 (8.66)	26.11	38.27
XI	243.51 (58.20)	27.66 (6.61)	24.94 (5.96)	41.86	56.39
XII	250.42 (59.85)	18.91 (4.52)	17.20 (4.11)	11.34	23.68
XIII	273.89 (65.46)	22.80 (5.45)	26.11 (6.24)	16.45	31.4
XIV	240.29 (57.43)	30.79 (7.36)	23.64 (5.65)	5.28	4.58
XV	172.89 (41.32)	16.19 (3.87)	10.96 (2.62)	12.98	10.07
XVI	243.10 (58.10)	15.65 (3.74)	0.38 (0.09)	14.99	5.77
XVII	329.92 (78.85)	32.26 (7.71)	39.50 (9.44)	27.6	11.46
XVIII	338.49 (80.90)	19.83 (4.74)	22.26 (5.32)	8.15	10.5
XIX	376.15 (89.90)	16.11 (3.85)	15.31 (3.66)	21.47	0.53
XX	425.94[b] (101.80)	1.59 (0.38)	3.26 (0.78)	19.33	6.35
XXI	289.12 (69.10)	3.89 (0.93)	11.09 (2.65)	27.19	14.8
XXII	284.22 (67.93)	3.43 (0.82)	5.56 (1.33)	22.22	9.86
XXIII	293.10 (70.05)	12.34 (2.95)	25.31 (6.05)	32.65	12.22
XXIV	209.29 (50.02)	14.02 (3.35)	17.53 (4.19)	27.58	22.65
XXVIII	394.56 (94.30)	34.90 (8.34)	27.20 (6.50)	26.63	4.45
Mean absolute deviation, kJ/mol	with compounds **IX–XII, XX, XXII, XXIII**	15.66 (3.74)	14.79 (3.53)	14.89	12.28
	without compounds **IX–XII, XX, XXII, XXIII**	14.44 (3.45)	12.74 (3.04)	11.31	7.40

[a] Data (in kcal) taken from [38]. [b] The value is not experimentally determined; it is a result of semi-empirical simulation [1, 33].

Comparison of the discrepancies between the experimental data and the results of simulation performed in later versions of the method, Parameter Model PM6 and PM7 [38] (Table 3) revealed that, similarly to the PM3 simulation, the deviation was quite high (16–36 kJ/mol) for 4,4'-bipyridine **XXIII** and for benzoquinoline isomers (**IX–XIII**). Mean absolute deviation between the experimental and the PM7-computed data

Table 4. Results of computation of enthalpy of formation of polycyclic six-membered nitrogen-containing aromatic compounds

Comp. no.	Compound name	Enthalpy of formation, kJ/mol		Comp. no.	Compound name	Enthalpy of formation, kJ/mol	
		$\Delta_f H^\circ_{calc}$	$\Delta_f H^\circ_{calc}$			$\Delta_f H^\circ_{calc}$	$\Delta_f H^\circ_{calc}$
XXIX	3-Methylquinoline	158.61	161.39	**LXI**	α-Naphthoquinoline	384.98	408.74
XXX	7-Methylquinoline	159.32	162.17	**LXII**	Naphtho(2,1-*f*)quinoline	325.72	343.99
XXXI	1-Methylisoquinoline	162.08	165.19	**LXIII**	Benzo[*c*]acridine	345.16	365.23
XXXII	3-Methylisoquinoline	158.37	161.13	**LXIV**	Naphtho(2,3-*h*)quinoline	342.72	362.56
XXXIII	2,3-Dimethylquinoline	124.23	123.83	**LXV**	1,10-Dimethylbenz[*a*]acridine	291.31	306.39
XXXIV	2,4-Dimethylquinoline	123.67	123.22	**LXVI**	10-Azabenzo[*a*]pyrene	372.99	395.64
XXXV	2,8-Dimethylquinoline	127.25	127.13	**LXVII**	2-Azachrysene	324.05	342.16
XXXVI	3,6-Dimethylquinoline	119.72	118.90	**LXVIII**	Benzo[*a*]acridine	343.51	363.43
XXXVII	3,5-Dimethylquinoline	122.99	122.47	**LXIX**	7,9-Dimethylbenz[*c*]acridine	273.05	286.44
XXXVIII	4,8-Dimethylquinoline	129.96	130.09	**LXX**	Dibenzo[*a*,*j*]acridine	400.05	425.21
XXXIX	5,8-Dimethylquinoline	129.03	129.07	**LXXI**	Dibenzo[*c*,*h*]acridine	403.28	428.73
XL	2-Ethylquinoline	141.57	142.78	**LXXII**	Dibenzo[*a*,*h*]acridine	401.71	427.02
XLI	3-Ethylquinoline	141.38	142.57	**LXXIII**	Dibenzo[*a*,*i*]acridine	434.39	462.73
XLII	4-Ethylquinoline	142.59	143.89	**LXXIV**	Cinnoline	301.29	317.29
XLIII	4,6-Dimethylquinoline	123.87	123.43	**LXXV**	2-Methylquinoxaline	195.66	201.88
XLIV	8-Ethylquinoline	148.13	149.94	**LXXVI**	6-Methylquinoxaline	195.42	201.61
XLV	2-Vinylquinoline	269.18	282.21	**LXXVII**	4-Methylquinazoline	192.41	198.33
XLVI	3-Vinylquinoline	263.69	276.21	**LXXVIII**	3,3'-Bipyridine	258.92	271.00
XLVII	4-Vinylquinoline	274.00	287.48	**LXXIX**	2-Phenylpyrimidine	265.46	278.1
XLVIII	6-Ethylquinoline	140.04	141.10	**LXXX**	4-Phenylpyrimidine	263.60	276.11
XLIX	2,4,6-Trimethylquinoline	85.80	81.84	**LXXXI**	5-Phenylpyrimidine	264.99	277.63
L	2-Methyl-5-phenylpyridine	190.94	196.72	**LXXXII**	2.3'-Bipyridine	260.41	272.63
LI	2-Benzylpyridine	208.34	215.74	**LXXXIII**	1,7-Phenanthroline	290.24	305.22
LII	3-Benzylpyridine	208.57	215.98	**LXXXIV**	1,10-Phenanthroline	299.59	315.44
LIII	4-Benzylpyridine	207.56	214.88	**LXXXV**	5-Methyl-1,10-phenanthroline	265.92	278.65
LIV	2-Propylquinoline	123.38	122.90	**LXXXVI**	4,7-Phenanthroline	290.51	305.52
LV	2-(4-Methylphenyl)pyridine	193.23	199.22	**LXXXVII**	Pyrido(3,2-g)quinoline	314.66	331.90
LVI	3-Methyl-2-phenylpyridine	199.59	206.17	**LXXXVIII**	Benzo[*a*]phenazine	383.97	407.64
LVII	7-Ethyl-2-methylquinoline	103.64	101.33	**LXXXIX**	1,3-Diazapyrene	333.28	352.82
LVIII	6-Isopropylquinoline	127.78	127.71	**XC**	2,7-Diazapyrene	326.90	345.28
LIX	1-Phenylisoquinoline	338.68	358.15	**XCI**	2,3-Diphenylpiperazine	385.54	409.35
LX	6-Phenylquinoline	300.25	316.15				

(14.79 kJ/mol) was slightly higher than that attained in this work (12.28 kJ/mol) after the correction using the linear regression. Omitting the compounds with extremely large deviation between the experimental and the theoretical data (**IX**–**XII**, **XX**, **XXII**, and **XXIII**) somewhat reduced the PM7-simulated mean absolute deviation (12.74 kJ/mol) but it was still 1.7 times higher than that reached in this work (7.40 kJ/mol for the PM3-computed corrected values).

That comparison concluded that the PM3 method can be used in combination with the derived correlation equation to predict enthalpy of formation of the studied class of compounds. Table 4 shows the simulation results (gas-phase formation enthalpy) for 63 six-membered nitrogen-containing heterocycles **XXIX**–**XCI** without experimental data available; the simulation was performed using the PM3 method followed by the correction using the regression equation.

To conclude, this work has revealed a good correlation between the experimentally determined gas-phase formation enthalpy of a number of six-membered nitrogen-containing heterocyclic compounds and the similar values simulated using the PM3 method. This method can be therefore recommended for computation of thermochemical data of this class of compounds. The derived equation of linear regression between the computed and the experimental values has allowed for further correction of the computed data, reducing the discrepancy between the simulated and the experimental data. The described method has been finally applied to compute the gas-phase formation enthalpy of the compounds not characterized experimentally.

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