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FULL PAPER

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Accurate prediction of standard enthalpy of formation based on semiempirical quantum chemistry methods with artificial neural network and molecular descriptors

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Abstract

This work investigates possible improvements in the accuracy of semiempirical quantum chemistry (SQC) methods for the prediction of standard enthalpy of formation ($\Delta_f H^o$) through the use of an artificial neural network (ANN) with molecular descriptors. A total of 142 organic compounds with enough structural diversity has been considered in the training set. Standard enthalpy of formation for the selected compounds at the semiempirical PM3 and PM6 quantum chemistry methods is collected from literature and is calculated by using the semiempirical PM7 method in this work. The multiple stepwise regression is first used to screen effective molecular descriptors, which are highly correlated with the error terms of the standard enthalpy of formation compared with experimental values. The obtained seven effective molecular descriptors are then used as input set to establish three 7-11-1 neural network-based correction models to improve the accuracy of SQC methods. By using the developed correction models, the mean absolute errors for $\Delta_f H^o$ of PM3, PM6, and PM7 methods are reduced from 22.36, 18.60, and 17.27 to 9.86, 9.83, and 8.95, respectively, in kJ/mol. Meanwhile, the results of the test set show that the neural network does not have the problem of overfitting. Detailed analysis of the seven effective molecular descriptors indicates that the major source of the correction models is the electron-withdrawing effect. The developed ANN models for the three selected SQC methods provide an efficient method for the quick and accurate prediction of thermodynamic properties.

KEYWORDS

artificial neural network, enthalpy of formation, molecular descriptors, semiempirical quantum chemistry methods

1 | INTRODUCTION

Thermodynamic properties are critical in almost all branches of chemistry and chemical engineering, such as chemical kinetics, combustion processing, and petroleum industry.[1,2] They are used to determine heat of reaction, equilibrium constant, reaction rate constants, and so on. Thus, accurate prediction of thermodynamic properties is one of the major focuses for both experimental and theoretical researchers.[3,4] Among the various thermodynamic properties, standard enthalpy of formation ($\Delta_f H^o$) is a key parameter of species. Generally, experimental measurements of thermodynamic properties are reliable but become difficult and expensive as the research systems become larger. Hence, empirical methods were developed. Among the empirical methods, the group additivity (GA) method developed by Benson et al[5] is one of the quickest

and most convenient methods to determine the thermodynamic properties of molecules and has been widely used in the development of chemical kinetic models. However, the performance and the scope of applicability of the GA method strongly depend on the accuracy of group contribution values and the proper treatment of group interactions to consider the overall molecular structures.[6,7]

With the development of advanced ab initio quantum chemistry methods and the increasing computational ability, computational methods have become a major method to obtain thermodynamic properties of molecules. The use of accurate CCSD(T)with the complete basis set (CBS) method or composite G4, CBS-QB3, W1 methods can attain "chemical accuracy" (≈ 4.18 kJ/mol) in the prediction of enthalpy of formation.[3,8] However, theoretical studies conducted using these methods are still limited to small-molecule systems. Recent advances in the development of various functionals in density functional theory (DFT) have facilitated theoretical studies on large molecules with reduced computational resources.[9] However, the accuracy of DFT results strongly depend on the selection of functional and basis sets. A series of research work indicates that the errors from the DFT method for $\Delta_f H^o$ are in fact systematic, and the least-square method and artificial neural network (ANN) were used to correct the errors.[10–12] Although the accuracy in the prediction of $\Delta_f H^o$ has been increased, large-scale computations by using DFT with or without correction are still limited, such as in the development of detailed combustion kinetic models, which consists of hundreds/thousands of species.[2,13]

On the other hand, semiempirical quantum chemistry (SQC) methods are much faster than DFT, and the computational cost can also compete with the empirical GA method.[14,15] Consequently, the errors are also larger than that of DFT methods. As the molecular system increases, the resources consumed by DFT calculations will increase explosively.[13] On the contrary, the SQC method still has faster calculation speed and considerable accuracy when calculating larger molecular systems. However, in combination with machine learning (ML) methods, SQC methods may become viable alternatives to DFT or GA methods for the large-scale estimation of thermodynamic properties.[16] In fact, simple corrections for some SQC methods have already been developed.[17,18] However, previous studies may often not be general enough to derive a general scheme for such purposes. To facilitate large-scale estimation of $\Delta_f H^o$, this work intends to develop a general correction scheme based on PM3,[19,20] PM6, and PM7[21] SQC methods in combination with ANN and molecular descriptors.

The paper is organized as follows: First, the computational details including the data sources, descriptions of molecular descriptors, and ANN method are provided in Section 2. Section 3 first presents the selection of molecular descriptors via multiple stepwise regression method. After that, the results from the ANN model are analyzed and validated. The details of the selected molecular descriptors are discussed. Major conclusions are presented in Section 4.

2 | COMPUTATIONAL DETAILS

2.1 | Data sources

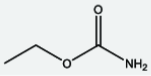
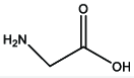
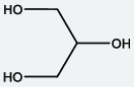
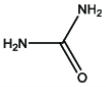
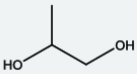
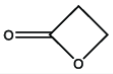
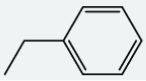
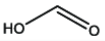
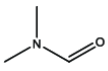
In order to ensure the generality of the ANN model, 142 compounds with different functional groups and chemical bonds are selected in the training set. Among the most widely used SQC methods, the PMx methods (PM3, PM6, PM7), in an attempt to improve the accuracy via adding modifications to the core repulsion functions and performing a more thorough and extensive parametrization, have been shown to be great improvements in predicting a wide range of molecular properties.[19–21] The PM7 method with explicit dispersion corrections in its definition and reparameterized via large set of experimental and high-level ab initio reference data especially demonstrated high accuracy among various SQC methods. Hence, to ensure that the developed ANN model has wide applicability, $\Delta_f H^o$ of the selected 142 compounds via the three PMx (PM3, PM6, PM7) methods are all included in this work. Specifically, the experimental values as reference data and the results computed using the PM3 and PM6 methods are derived from the Computational Chemistry Comparison and Benchmark DataBase (CCCBDB).[22] The $\Delta_f H^o$ at the PM7 level of theory are calculated in this work by using the MOPAC 2016 software.[23] All data can be seen in Table 1.

2.2 | Molecular descriptors

A molecular descriptor is the numerical representation of a molecular structure,[24] which is suitable for use in the ANN model to improve the prediction of molecular properties. However, the number of molecular descriptors must be very large to describe a wide range of molecule training sets. Thus, it is critical to select appropriate molecular descriptors for interested molecular properties. First, to comprehensively describe the molecules, 1444 descriptors are calculated for each molecule by using the PaDEL software.[24] These descriptors are diverse and can represent various structures of the selected molecules. Taking the molecular information index as an example, an atom is composed of protons, neutrons, and extra nuclear electrons. The information index I_{at} of an atom is defined as[24]:

$$I_{at} = (N_n + N_p + N_{el})\log_2(N_n + N_p + N_{el}) - N_{el}\log_2 N_{el} - (N_n + N_p)\log_2(N_n + N_p) \quad (1)$$

TABLE 1 Standard enthalpy of formation ($\Delta_f H^o$) from experiments, PM*x* methods, and ANN model-corrected values

No.	Structure	Name	$\Delta_f H^o$						
			Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
1		Formaldehyde	−108.7	−142.7	−86.4	−106.9	−126.4	−102.8	−109.6
2		Urethane	−446.3	−383.6	−391.9	−417.7	−439.7	−445.2	−437.6
3		Glycine	−390.5	−401.3	−389.3	−366.8	−401.6	−398.1	−386.1
4		1,2,3-Propanetriol	−577.9	−591.2	−600.4	−584.2	−576.7	−599.6	−586.5
5		Urea	−237.1	−196.3	−205.8	−214.5	−234.6	−234.9	−241.3
6		Propylene glycol	−429.8	−436.6	−429.7	−430.1	−425.4	−440.1	−428.9
7		β-Propiolactone	−297.1	−260.5	−275.4	−254.3	−284.4	−297.3	−295.3
8		Ethoxy ethane	−250.8	−240.6	−244.5	−235.6	−255.7	−263.3	−249.3
9		Acetamide	−238.5	−213.3	−230.3	−236.0	−246.7	−235.4	−246.3
10		Ethanol	−234.8	−237.9	−229.3	−233.8	−229.4	−219.1	−228.0
11		Formic acid	−378.8	−394.9	−367.3	−338.1	−412.2	−372.8	−376.6
12		Methyl alcohol	−201	−217	−202	−204.8	−211.3	−199.5	−196.6
13		Isopropyl alcohol	−272.7	−267.6	−271.3	−280.8	−278.0	−270.1	−278.2
14		Acetone	−217.1	−223.2	−227.4	−232.1	−225.3	−206.9	−236.5
15		Dimethyl sulfoxide	−150.5	−162.6	−136.9	−157.3	−166.0	−140.5	−157.2
16		Dimethyl sulfone	−372.8	−319.5	−393.5	−383.9	−333.2	−365.4	−390.2
17		dimethylformamide	−191.6	−182.1	−171.3	−183.5	−165.7	−189.1	−188.7

(Continues)

TABLE 1 (Continued)

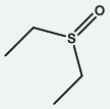
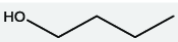
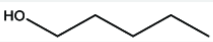
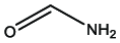
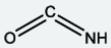
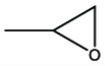
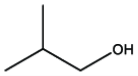
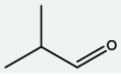
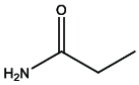
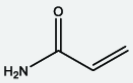
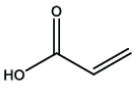
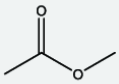
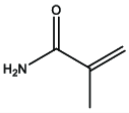
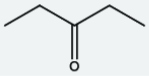
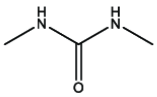
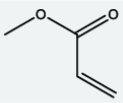
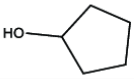
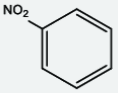
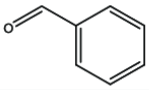
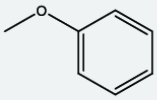
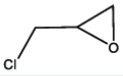
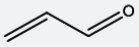
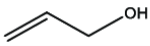
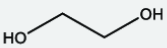
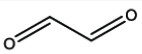
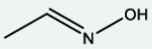
No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
18		Diethyl sulfoxide	−205.2	−192.3	−180.8	−197.1	−209.9	−174.1	−200.3
19		1-Propanol	−255.2	−260.3	−251.1	−259.0	−256.6	−238.4	−254.5
20		1-Butanol	−274.6	−282.8	−271.2	−274.5	−273.4	−264.8	−270.4
21		1-Pentanol	−295.6	−305.5	−292.2	−272.4	−300.3	−282.7	−293.7
22		Acetaldehyde	−170.7	−185.1	−159.6	−171.3	−173.9	−140.0	−170.9
23		formamide	−186	−169.4	−169.8	−184.5	−184.9	−176.0	−185.5
24		Isocyanic acid	−101.7	−64	−87.7	−97.8	−95.6	−108.6	−103.1
25		Ethylene oxide	−52.6	−34.2	−41.8	−47.1	−52.5	−54.0	−50.0
26		Acetyl Chloride	−242.8	−222.6	−243	−244.6	−231.5	−212.7	−251.6
27		Phosgene	−220.4	−205.4	−210.9	−200.2	−223.2	−230.0	−221.9
28		Methane, nitro-	−74.7	−66.9	−68	−106.0	−65.2	−62.1	−97.0
29		Propylene oxide	−93.7	−69.6	−81.4	−141.3	−93.3	−85.6	−94.6
30		Ethanol, 1,1-dimethyl-	−312.4	−298.2	−313.8	−266.7	−317.1	−321.5	−267.5
31		1-Propanol, 2-methyl-	−283.8	−292.3	−284	−286.2	−296.2	−285.3	−283.0
32		Propanal, 2-methyl-	−215.8	−229.3	−198.8	−213.3	−212.0	−223.5	−215.8
33		Propanamide	−258.9	−233.2	−245.6	−248.5	−254.6	−258.4	−253.1
34		Acrylamide	−130.2	−103.8	−117.1	−126.3	−130.0	−128.0	−136.0
35		2-Propenoic acid	−323.5	−311.4	−307.3	−316.8	−328.9	−326.7	−325.1

TABLE 1 (Continued)

No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
36		methyl acetate	−408.8	−393.8	−406.6	−402.8	−408.8	−400.7	−414.9
37		Methacrylamide	−157.7	−140.7	−157.5	−148.4	−151.4	−163.5	−152.6
38		3-Pentanone	−253.4	−257.6	−252	−264.9	−251.7	−251.5	−270.9
39		Urea, N,N′-dimethyl-	−221.6	−200.9	−201.7	−210.5	−217.9	−220.4	−236.5
40		2-Propenoic acid, methyl ester	−333	−282.1	−294	−302.3	−293.9	−299.7	−314.5
41		Cyclopentanol	−242.6	−270.3	−267.1	−261.5	−239.1	−224.8	−243.9
42		Nitrobenzene	68.5	60.5	78.7	35.1	63.5	35.2	52.2
43		benzaldehyde	−37.2	−44.8	−11.2	−25.6	−55.7	−39.9	−20.7
44		Anisole	−76.7	−61.2	−69.7	−71.4	−88.2	−88.5	−83.4
45		Oxirane, (chloromethyl)-	−107.9	−79.7	−101.1	−105.1	−108.0	−97.5	−108.3
46		Acrolein	−84	−76.6	−48.9	−62.7	−67.5	−67.4	−65.7
47		2-Propen-1-ol	−123.6	−130.8	−132	−138.9	−127.5	−114.2	−134.7
48		1,2-Ethanediol	−387.5	−398.3	−386.6	−386.5	−377.2	−386.6	−384.8
49		Ethanedial	−212	−269.3	−191.4	−219.8	−229.4	−215.5	−221.7
50		Acetaldoxime	−22.5	−12.3	−30.4	−31.4	−24.7	−14.1	−10.3
51		methyl formate	−352.4	−364.2	−352.7	−351.3	−360.9	−355.2	−367.7

(Continues)

TABLE 1 (Continued)

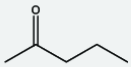
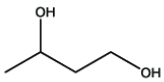
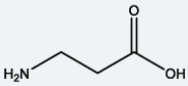
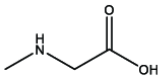
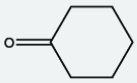
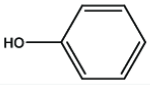
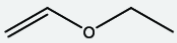
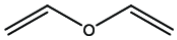
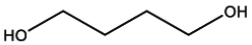
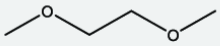
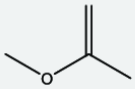
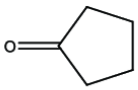
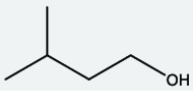
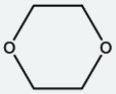
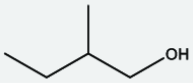
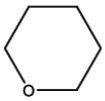
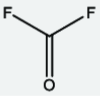
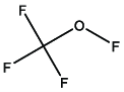
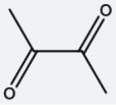
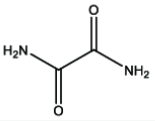
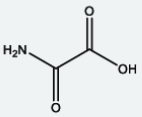
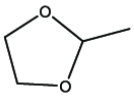
No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
52		2-Pentanone	−259	−263.5	−262.9	−271.2	−274.4	−263.1	−276.5
53		1,3-Butanediol	−433	−448.2	−469	−460.7	−452.3	−431.3	−459.9
54		β-alanine	−424	−412.5	−397.5	−408.5	−425.6	−413.9	−414.8
55		Sarcosine	−367.2	−397.5	−371.6	−293.8	−390.4	−365.7	−321.3
56		cyclohexanone	−231.1	−251.9	−249.7	−200.6	−281.7	−242.7	−232.2
57		phenol	−96.4	−90.7	−87.4	−92.7	−104.4	−93.6	−103.7
58		Ethene, ethoxy-	−140.2	−118.8	−136.8	−138.6	−125.0	−132.9	−139.7
59		Vinyl ether	−12.7	3	−21	−23.7	−12.0	−1.1	−28.4
60		Furan	−34.7	−17	−34	−23.7	−0.1	−48.4	−17.6
61		1,4-Butanediol	−426.8	−444.1	−433.7	−414.4	−438.9	−432.7	−424.8
62		Ethane, 1,2-dimethoxy-	−342.8	−365	−363.6	−354.7	−344.3	−326.3	−352.1
63		2H-Pyran, 3,4-dihydro-	−112.8	−139.5	−153.3	−124.0	−116.2	−128.3	−130.1
64		1,3,5-Trioxane	−465.8	−512.3	−521.6	−460.7	−466.2	−483.2	−473.2
65		Dimethyl ether	−184.1	−202.3	−191.3	−178.1	−192.4	−186.5	−183.5
66		1-Propene, 2-methoxy-	−148.6	−132.2	−152.8	−154.9	−144.3	−154.7	−156.5
67		Cyclopentanone	−192.1	−231	−225.1	−223.7	−193.8	−191.4	−191.6
68		1-Butanol, 3-methyl-	−301.3	−300.8	−294.3	−296.5	−298.0	−289.1	−293.0

TABLE 1 (Continued)

No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
69		Butanal	−206.1	−226.4	−195	−212.2	−204.7	−186.1	−213.6
70		1,4-Dioxane	−315.3	−348.1	−357.7	−290.0	−312.1	−322.4	−299.3
71		Carbon dioxide	−393.5	−355.8	−354.5	−331.9	−377.1	−397.8	−393.1
72		1-Butanol, 2-methyl-	−302	−302.8	−293	−325.8	−299.3	−285.7	−323.3
73		2H-Pyran, tetrahydro-	−223.8	−240.4	−243.6	−173.5	−213.3	−212.5	−219.1
74		Isoxazole	78.6	146.5	98.1	114.9	84.0	98.1	78.9
75		Oxazole	−15.5	−6.3	−6.5	35.0	−68.9	−20.8	−15.7
76		Carbonic difluoride	−623.8	−591.8	−583.9	−580.9	−606.6	−618.8	−623.4
77		Trifluoromethylhypofluorite	−764.8	−782.8	−755.7	−754.1	−783.2	−766.3	−764.6
78		2,3-Butanedione	−326.8	−340.7	−325	−343.2	−345.3	−349.3	−351.7
79		Ketene	−47.7	−38.6	−77	−53.4	−47.3	−46.2	−59.8
80		Carbonyl sulfide	−141.7	−99.5	−107.3	−103.0	−120.5	−120.9	−138.5
81		Oxalamide	−387.1	−327.8	−344.4	−364.8	−341.5	−385.0	−390.6
82		Oxamic acid	−552.3	−525.8	−503.8	−523.0	−514.0	−492.4	−549.4
83		1,3-Dioxolane, 2-methyl-	−350.2	−374.6	−392.5	−342.4	−350.5	−360.9	−352.8

(Continues)

TABLE 1 (Continued)

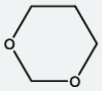
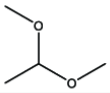
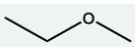
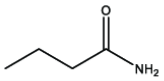
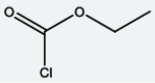
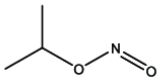
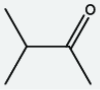
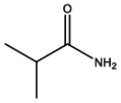
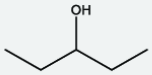
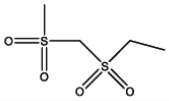
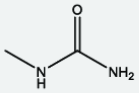
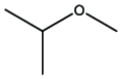
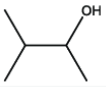
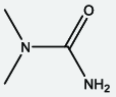
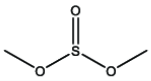
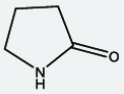
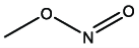
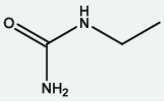
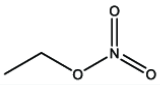
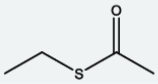
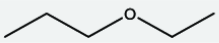
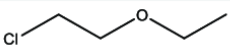
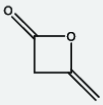
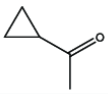
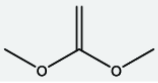
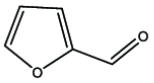
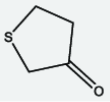
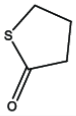
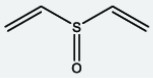
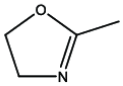
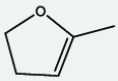
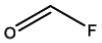
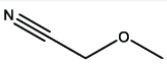
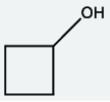
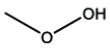
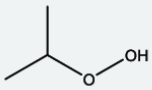
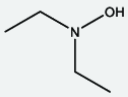
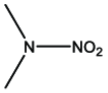
No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
84		Oxetane	−80.5	−112	−121.3	−106.2	−99.3	−117.2	−79.8
85		Carbon suboxide	−97.6	−100.8	−178.7	−106.5	−103.0	−97.8	−118.1
86		1,3-Dioxane	−338.4	−367.5	−381.7	−314.4	−339.5	−335.5	−333.4
87		1,1-Dimethoxyethane	−389.7	−393.7	−401.2	−404.8	−390.2	−393.8	−406.2
88		Ethane, methoxy-	−216.5	−221.7	−218.1	−217.3	−225.1	−203.0	−218.8
89		Butanamide	−279.2	−250.7	−267.1	−275.5	−280.9	−284.4	−277.1
90		Carbonochloridic acid, ethyl ester	−459.4	−397.8	−418.7	−431.1	−459.9	−453.0	−453.8
91		Isopropyl nitrite	−133.5	−81.9	−136.8	−172.0	−132.7	−129.7	−133.3
92		ethanol	−128	−132.1	−138.6	−141.2	−125.5	−118.3	−134.7
93		Acetyl fluoride	−442.1	−412.7	−420.9	−422.3	−421.0	−433.3	−430.6
94		2-Butanone, 3-methyl-	−262.6	−263.2	−261.4	−245.3	−275.9	−262.8	−251.3
95		Propanamide, 2-methyl-	−282.6	−252	−265.3	−274.2	−273.5	−270.3	−275.6
96		3-Pentanol	−314.7	−308.9	−306.5	−312.5	−311.8	−298.9	−313.2
97		(Methylsulfonyl)ethane	−408.4	−330.5	−407.8	−397.3	−407.9	−408.3	−397.9
98		Urea, methyl-	−233.5	−199.2	−203.3	−212.9	−240.5	−233.1	−246.4
99		Propane, 2-methoxy-	−252	−249.3	−259.8	−251.7	−258.0	−252.0	−250.4
100		Methyl nitrate	−122	−135.6	−153.5	−110.0	−124.2	−126.5	−127.4

TABLE 1 (Continued)

No.	Structure	Name	$\Delta_f H^\circ$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
101		2-Butanol, 3-methyl-	−316.4	−306	−311	−346.8	−316.9	−318.6	−347.2
102		Urea, N,N-dimethyl-	−220	−198.8	−201.1	−211.9	−226.6	−217.3	−231.6
103		Sulfurous acid, dimethyl ester	−483.3	−542.4	−519.9	−496.7	−481.2	−495.0	−508.8
104		2-Pyrrolidinone	−197.4	−209.9	−213.7	−207.9	−203.8	−198.1	−199.7
105		Methyl nitrite	−65.4	−26.7	−94.2	−80.3	−65.4	−90.5	−64.0
106		Urea, ethyl-	−257.5	−224.2	−232.1	−237.1	−262.1	−254.9	−265.8
107		Nitric acid, ethyl ester	−154.8	−152.3	−182.7	−162.4	−152.4	−155.5	−176.1
108		s-Ethyl thioacetate	−227.8	−180.5	−227	−219.9	−235.5	−223.8	−231.1
109		Butane, 1-methoxy-	−258.1	−266.5	−259.8	−228.3	−268.5	−233.3	−230.0
110		Propane, 1-ethoxy-	−272.2	−262.9	−266.1	−265.5	−269.9	−264.2	−265.8
111		1-Chloro-2-ethoxyethane	−297.1	−253.5	−272	−257.9	−295.2	−288.9	−297.3
112		Carbon monoxide	−110.5	−82.7	−57.2	−106.9	−66.4	−103.6	−99.6
113		1,3-Dioxolane	−298	−344.6	−345.6	−327.9	−298.6	−297.6	−353.0
114		2-Oxetanone, 4-methylene-	−190.2	−155.3	−185.8	−163.5	−179.7	−184.9	−205.8
115		Methyl cyclopropyl ketone	−115.3	−104.9	−129.8	−119.5	−101.3	−106.3	−104.4
116		Ethene, 1,1-dimethoxy-	−280.7	−285.1	−280.8	−263.1	−273.4	−286.1	−268.3
117		furfural	−149.6	−153.9	−127	−138.5	−154.3	−170.4	−138.1

(Continues)

TABLE 1 (Continued)

No.	Structure	Name	$\Delta_f H°$ Exp.[a]	PM3	PM6	PM7	PM3-ANN	PM6-ANN	PM7-ANN
118		Dihydro-3-(2H)-thiophenone	−135.3	−164.6	−180.3	−172.4	−138.9	−139.4	−145.3
119		Dihydro-2-(3H)-thiophenone	−196.2	−160.5	−200.4	−179.3	−193.5	−162.5	−187.0
120		Vinyl sulfoxide	25	48	56.1	30.0	43.1	31.8	23.5
121		Oxazole, 4,5-dihydro-2-methyl-	−130.5	−134.5	−136.7	−97.6	−183.8	−99.9	−130.6
122		Cyclobutanone	−91.6	−136	−89.5	−126.6	−95.7	−79.5	−94.2
123		Furan, 2,3-dihydro-	−75	−104	−113.5	−105.0	−85.4	−82.9	−91.3
124		Furan, 2,3-dihydro-5-methyl-	−130.2	−140.8	−157.8	−150.3	−143.2	−139.8	−129.2
125		formyl fluoride	−376.6	−371.5	−352.9	−353.6	−365.5	−371.8	−362.6
126		Propane, 2-methoxy-2-methyl-	−283.2	−268.7	−291.5	−290.8	−284.3	−282.8	−287.2
127		Methoxyacetonitrile	−35.7	−42.8	−36.3	−41.0	−29.3	−39.4	−46.9
128		Cyclobutanol	−144.8	−200.2	−204.1	−182.6	−154.3	−176.8	−144.1
129		Methyl peroxide	−131	−155.4	−99.2	−91.6	−125.9	−131.5	−106.6
130		Hydroperoxide, 1-methylethyl	−197.1	−193.8	−163	−183.9	−186.9	−188.5	−195.7
131		Acetyl radical	−10.3	−86.1	−85.2	−17.8	−74.9	−65.6	−17.3
132		Diethylhydroxylamine	−121.8	−95.1	−116.2	−147.8	−114.2	−117.7	−146.2
133		Dimethylnitroamine	−5	5.2	−32.2	6.5	2.8	−13.8	10.3