Prediction of Thermochemical Properties for Gaseous Ammonia Oxide

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Ammonia oxide (NH_3O), a zwitterionic tautomer of hydroxylamine (NH_2OH), has been identified to explain the high reactivity of NH_2OH. Recent evidence has shown that ammonia oxide exists in the condense phase and aqueous solution. However, neither experimental nor theoretical data of its thermochemical properties are presently available. In this work, thermochemical parameters of ammonia oxide are calculated, under standard conditions, using isodesmic reactions at several theoretical methods (HF, MP2, B3LYP, G2, G2MP2, G3, G3B3, and CBS-Q) and several basis sets (Dunning correlation-consistent and Pople-style). To monitor the computed values, the values of hydrogen peroxide are calculated by the same methods and compared with the experimental data. The quantum chemistry calculations predict the value of molar enthalpy of formation to be $(55.7 \pm 2.9)\ \mathrm{kJ \cdot mol^{-1}}$ and molar Gibbs energy of formation to be $(103.8 \pm 2.9)\ \mathrm{kJ \cdot mol^{-1}}$, for gaseous ammonia oxide at 1 atm and 298.15 K. The determined molar entropy and molar heat capacity at constant volume, also at 1 atm and 298.15 K, are $(221.1 \pm 0.1)\ \mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ and $(28.9 \pm 0.3)\ \mathrm{J \cdot mol^{-1} \cdot K^{-1}}$, respectively. We have demonstrated that molecular simulation is a powerful tool to obtain thermodynamic properties of unstable compounds, such as ammonia oxide.

Introduction

Hydroxylamine (NH_2OH) is a unique ambident α-nucleophile and plays an important role in the semiconductor, chemical, and pharmaceutical industries.[1] It is used as a solvent in microchip production to remove organic and inorganic impurities from wafers and also as an important feedstock for dyes, rust inhibitors, and products, such as painkillers, antibiotics, and tranquillizers.[2] It is always challenging to handle hydroxylamine and its aqueous solution due to their high reactivity, which has led to two tragic incidents in the chemical industry.[3,4] Since then, thermal decomposition hazards of hydroxylamine + water solutions have been investigated extensively using calorimeters.[5,6] On the basis of our current theoretical investigation on the initial thermal decomposition of hydroxylamine, ammonia oxide (NH_3O) has been identified and proposed to explain the exceptional reactivity of hydroxylamine. The most favorable initial decomposition pathway has been determined as a bimolecular isomerization of hydroxylamine into ammonia oxide.[7]

Ammonia oxide, the zwitterionic tautomer of hydroxylamine, has been discussed since the 19th century and has attracted the interest of both experimentalists and theoreticians, as one of the last remaining small elusive molecules to be characterized.[8−11] Ammonia oxide is not a typical oxyanion, because the nitrogen atom bears up to three hydrogen atoms which are adequately located to facilitate a thermodynamically favorable proton transfer. Experimental mass spectrometric studies together with electronic structure calculations by Bronstrup et al. strongly suggested the existence of the elusive ammonia oxide molecule and its radical cation.[8] Kirby et al. have shown solid evidence for its existence in the condensed phase, in the shape of a crystal structure containing equal amounts of the neutral and the conjugate acid (NH_3OH^+).[12] More recently, Kirby et al. have reported that ammonia oxide is presented in substantial amounts (some 20 %) in ordinary aqueous solutions of hydroxylamine under normal conditions (25 °C and ionic strength $1.0\ \mathrm{mol \cdot L^{-1}}$).[13]

It is well-known that theoretical methods are always necessary to predict properties for reactive chemicals when sufficient experimental data are not available. For this highly reactive compound, ammonia oxide, theoretical studies are of prime importance and have been conducted by several research groups. For example, ab initio molecular orbital (MO) theory has been explored to determine the molecular structure of ammonia oxide, especially the N−O bond length.[14] Hart also investigated its basic molecular properties, including geometry, stability, and bonding, using ab initio calculations.[15,16] This structure information provides the experimental benchmark for theoretical work and a possible explanation for the exceptional reactivity of hydroxylamine. Most recently, Fernández et al. carried out theoretical calculations to study the tautomeric equilibrium between hydroxylamine and ammonia oxide and to estimate the equilibrium constant.[17] The calculated results also indicated that although hydroxylamine is favored, there should be enough ammonia oxide in aqueous solution to be a kinetically active species.[17]

Reliable thermochemical data for quantitative predictions of chemical reactivity and potential runaway reactions are required to design a safer and economical process. To the best of our knowledge, thermochemical data of ammonia oxide have been so far impossible to be experimentally measured, and no attempt has been made to evaluate them. From this point, we decided to carry out a theoretical study to estimate its thermochemical properties. As part of our ongoing interest in evaluating chemical reactivity for different reactive chemicals,[18−20] here we sought to elucidate the thermochemical properties of gaseous ammonia oxide using quantum mechanical calculations. Density functional

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Table 1. Standard Molar Enthalpies of Formation and Molar Gibbs Energies of Formation at 1 atm and 298.15 K[a]

compound	ΔH_f kJ·mol^{-1}	ΔG_f kJ·mol^{-1}
H_2	0	0
H_2O	−241.8	−228.6
NH_3	−45.9	−16.4
H_2O_2	−136.3	−105.6

[a] The data are derived from the *CRC Handbook of Chemistry and Physics*, Standard Thermodynamic Properties of Chemical Substances.

theory (DFT) and ab initio wave function theory (WFT) were employed to determine molar enthalpy of formation, molar Gibbs energy of formation, molar entropy, and molar heat capacity at constant volume for ammonia oxide in the gas phase. The results can provide a better understanding of the thermal stability of hydroxylamine and ammonia oxide and provide practical guidance on the manufacturing, storage, and transportation of hydroxylamine and its aqueous solution.

Theoretical Calculations. A variety of theoretical methods, ab initio (HF, MP2),[21] DFT (B3LYP),[22] and composite (G2,[23] G3,[24] G3B3,[25] and CBS-Q[26]), as implemented in the Gaussian 03 suite of programs were used for geometry optimizations and frequency calculations.[27] The calculations were performed with Dunning correlation consistent polarized valence basis sets (cc-pVDZ, cc-pVTZ, where D and T refer to the number of contracted functions in each valence subshell).[28,29] Pople-style basis sets (6-31+G(d), 6-311+G(2df,p))[30,31] with diffuse functions (denoted by “+”) and polarization functions (denoted by “d”, “p”, “f”, for angular flexibility to represent regions of high electron density among bonded atoms) were also employed.

Errors in absolute quantities from quantum chemical calculations are often systematic. To compensate for some of the systematic errors, isodesmic reactions, which conserve the number of each type of bond in reactants and products, are used to obtain more accurate thermochemical data.[32] The choice of an isodesmic reaction is very important, because a better bond balance can result in a more effective cancelation of the systematic errors.[33,34] The following isodesmic reactions, 1 and 2, were used to calculate the thermochemical data for ammonia oxide in this work.

$$NH_3O + H_2 \rightarrow H_2O + NH_3 \tag{1}$$

$$NH_3O + H_2O \rightarrow H_2O_2 + NH_3 \tag{2}$$

To gauge the computed thermochemical values of ammonia oxide, the thermochemical data for hydrogen peroxide, which reliable experimental data are available, were also calculated by the same methods (same basis sets) and with another isodesmic reaction, 3. The experimental thermochemical data for hydrogen peroxide are known to have high accuracy from the literature, making it an ideal and important test case for the calculation procedures.

$$H_2O_2 + H_2 \rightarrow 2H_2O \tag{3}$$

The experimental values of enthalpy of formation and Gibbs energy of formation in the gas phase at 1 atm and 298.15 K for hydrogen gas, ammonia, water, and hydrogen peroxide were collected from *CRC Handbook of Chemistry and Physics* and listed in Table 1.[35] Therefore, the enthalpy of formation or Gibbs energy of formation for ammonia oxide can be calculated by combining the enthalpy of reaction or Gibbs energy of reaction obtained from an isodesmic reaction with the experimental values of the known compounds. Significant progress in both computer technology and development of the quantum chemical method has made it feasible to use electronic structure calculations, that is, ab initio and DFT, to predict thermochemical properties accurately.[36] Here two isodesmic reactions were employed because agreement between values obtained from reactions 1 and 2 can serve as an indicator that the theory is adequate to model the system. The molar entropy and molar heat capacity at constant volume of gaseous ammonia oxide can be easily obtained from the frequency calculations of the target molecule by using the *Gaussian 03* suite of programs.

Results and Discussion

Enthalpy of Formation. The molar enthalpy of formation of ammonia oxide, ΔH_f, was determined using isodesmic reactions 1 and 2. The enthalpy of reaction (ΔH_{Rxn}) can be calculated from thermochemistry calculations via the *Gaussian 03* suite of programs. On the basis of the calculated enthalpy of reaction and the experimental values of other known compounds, the molar enthalpy of formation of ammonia oxide can be obtained according to eqs 4 and 5.

$$\Delta H_{f,NH_3O} = \Delta H^{exp}_{f,NH_3} + \Delta H^{exp}_{f,H_2O} - \Delta H^{exp}_{f,H_2} - \Delta H^{cal}_{Rxn1} \tag{4}$$

$$\Delta H_{f,NH_3O} = \Delta H^{exp}_{f,NH_3} + \Delta H^{exp}_{f,H_2O_2} - \Delta H^{exp}_{f,H_2O} - \Delta H^{cal}_{Rxn2} \tag{5}$$

$$\Delta H_{f,H_2O_2} = 2\Delta H^{exp}_{f,H_2O} - \Delta H^{exp}_{f,H_2} - \Delta H^{cal}_{Rxn3} \tag{6}$$

where ΔH^{exp}_{f} is the experimental enthalpy of formation of the known compound and ΔH^{cal}_{Rxn} is the calculated enthalpy of reaction (enthalpy change) using molecular simulation.

Equation 6 was used to calculate the enthalpy of formation for hydrogen peroxide, which would be used to compare with the experimental data of hydrogen peroxide, to monitor the accuracy of the computed values for ammonia oxide. The difference between the values calculated using reactions 1 and 2 can be taken as a guide for selecting theories performing well for the system. Values for the molar enthalpy of formation calculated under standard conditions using the various levels of theory and basis sets are summarized in Table 2.

Hartree−Fock (HF) is the lowest level ab initio theory employed in this work. We expected the HF method to yield fairly good results, despite the fact that it does not include a full treatment of electron correlation, because errors can be canceled by the use of isodesmic reactions. The calculated data show that molar enthalpies of formation calculated with the HF method did not exhibit consistent improvement with increasing basis sets. The HF/cc-pVDZ level of theory produced a small difference between reactions 1 and 2 and also predicted a reasonable enthalpy of formation for hydrogen peroxide with reaction 3. However, the enthalpy of formation value was significantly different from the value obtained via the composite methods (see the discussion later). The MP2, a post SCF method using second-order Moller−Plesset perturbation theory, is one of the least expensive ways to improve on HF. The data calculated with the MP2 method exhibited improvement with

Table 2. Summary of Calculated Molar Enthalpies of Formation at 1 atm and 298.15 K

		ΔH_{f} ($\mathrm{H_2O_2}$)	ΔH_{f} ($\mathrm{NH_3O}$)	
		kJ·mol^{-1}	kJ·mol^{-1}	
method	basis set	Rxn 3	Rxn 1	Rxn 2
HF	6-31G(d,p)	−122.9	88.3	74.7
	6-311+G(2df,p)	−118.4	67.1	49.0
	cc-pVDZ	−136.2	74.4	74.2
	cc-pVTZ	−123.1	73.2	59.9
MP2	6-31G(d,p)	−160.3	69.3	93.2
	6-311+G(2df,p)	−130.1	61.2	54.9
	cc-pVDZ	−155.6	76.7	95.9
	cc-pVTZ	−131.5	58.6	53.7
B3LYP	6-31G(d, p)	−190.5	36.0	90.1
	6-311+G(2df,p)	−152.0	40.9	56.5
	cc-pVDZ	−192.6	33.4	89.6
	cc-pVTZ	−162.4	45.7	71.7
G1		−144.3	51.8	59.7
G2		−135.3	53.1	52.0
G2MP2		−134.3	54.2	52.1
G3		−134.1	59.3	57.0
G3B3		−134.9	58.0	56.4
CBS-Q		−139.2	53.4	56.2

Table 3. Summary of Calculated Molar Gibbs Energies of Formation at 1 atm and 298.15 K

		ΔG_{f} ($\mathrm{H_2O_2}$)	ΔG_{f} ($\mathrm{NH_3O}$)	
		kJ·mol^{-1}	kJ·mol^{-1}	
method	basis set	Rxn 3	Rxn 1	Rxn 2
HF	6-31G(d,p)	−89.1	139.6	123.1
	6-311+G(2df,p)	−84.7	118.4	97.5
	cc-pVDZ	−102.5	125.6	122.6
	cc-pVTZ	−89.4	124.5	108.3
MP2	6-31G(d,p)	−126.7	120.9	142.0
	6-311+G(2df,p)	−96.5	112.8	103.6
	cc-pVDZ	−122.0	128.2	144.6
	cc-pVTZ	−97.9	113.0	105.3
B3LYP	6-31G(d,p)	−156.9	87.6	138.8
	6-311+G(2df,p)	−118.4	92.4	105.2
	cc-pVDZ	−159.1	84.9	138.3
	cc-pVTZ	−128.8	97.2	120.4
G1		−110.6	103.0	108.0
G2		−101.6	104.3	100.3
G2MP2		−100.6	105.5	100.4
G3		−100.4	110.5	105.3
G3B3		−101.2	109.6	105.1
CBS-Q		−105.5	104.6	104.6

increasing basis sets. For example, the results from the MP2/6-311+G(2df,p) level of theory were better than that from the MP2/6-31+G(d) level of theory, and MP2 predictions were improved with the cc-pVTZ basis set as compared to cc-pVDZ.

The DFT methods include the effects of electron correlation at only a moderate increase in computing cost, as compared to the HF method. Therefore, DFT methods can provide the benefits of some more expensive ab initio methods at essentially HF cost. However, in this work the B3LYP results were poor with all of the basis sets. The differences between reactions 1 and 2 were very large even with large basis sets. For hydrogen peroxide in reaction 3, the calculated values from the B3LYP/6-31+G(d) level of theory had an error of nearly 54 kJ·mol^{-1}, as compared to the experimental value. Similar values were obtained using the large basis set, 6-311+G(2df,p). There was still a large error of about 17 kJ·mol^{-1} for the calculated molar enthalpy of formation.

The composite theories (G2, G2MP2, G3, G3B3, and CBS-Q) are expected to yield the best results because they have been developed to model accurately thermochemical quantities especially for small, light-atom, main group molecules. Previous results have shown that the means of absolute deviation associated with enthalpy of formation values obtained using G2 and G2MP2 theories are (5.0 and 6.7) kJ·mol^{-1}, respectively.[37] The G3 and G3B3 theories are a further improvement over G2 theory, and the accuracy of the theory (and derivatives thereof) has been tested extensively for enthalpies of formation.[38] The CBS-Q theory accounts for errors due to basis set truncation by an extrapolation, and the mean of absolute deviation associated with the method is 4.2 kJ·mol^{-1}.[37] From Table 2, all of these composite theories performed well (a difference around 4 kJ·mol^{-1} or less) and predicted accurate enthalpies of formation for hydrogen peroxide.

After the analysis of all of the data, the appropriate theory can be selected to obtain accurate values of enthalpy of formation. The values calculated from HF and B3LYP methods were left out because they did not demonstrate an improvement in the prediction with increasing basis set. Results from the MP2 method were also left out because of poor prediction results for hydrogen peroxide. Therefore, predicted values from the composite theories were used to calculate the averages.

The calculated average enthalpy of formation for hydrogen peroxide was −136.8 kJ·mol^{-1} with a standard deviation of 2.1 kJ·mol^{-1} (the experimental value is −136.3 kJ·mol^{-1}). On the basis of the six best predicted values of enthalpy of formation, from the reaction 1, an average value of 54.8 kJ·mol^{-1} with a standard deviation of 2.9 kJ·mol^{-1} was calculated. With the reaction 2, the average value was 55.7 kJ·mol^{-1} with a standard deviation of 2.9 kJ·mol^{-1}. Generally, more consistent results should be obtained with the reaction 2, which is a more balanced isodesmic reaction. Therefore, in this work we recommended the molar enthalpy of formation value for ammonia oxide to be (55.7 ± 2.9) kJ·mol^{-1}. The calculated average value of enthalpy of formation for hydrogen peroxide is only greater than the experimental value by 0.5 kJ·mol^{-1}, which suggests our calculated average value of enthalpy of formation for gaseous ammonia oxide is very reliable.

Gibbs Energy of Formation. Similarly to the method, as discussed in the last section, the molar Gibbs energy of formation, ΔG_{f}, can be obtained using the same isodesmic reactions 1 and 2 according to eqs 7 and 8. Equation 9 was used to calculate the molar Gibbs energy of formation for hydrogen peroxide, which was used to compare with the experimental value to check the computed values for ammonia oxide.

$$\Delta G_{\mathrm{f,NH_3O}} = \Delta G^{\mathrm{exp}}_{\mathrm{f,NH_3}} + \Delta G^{\mathrm{exp}}_{\mathrm{f,H_2O}} - \Delta G^{\mathrm{exp}}_{\mathrm{f,H_2}} - \Delta G^{\mathrm{cal}}_{\mathrm{Rxn1}} \tag{7}$$

$$\Delta G_{\mathrm{f,NH_3O}} = \Delta G^{\mathrm{exp}}_{\mathrm{f,NH_3}} + \Delta G^{\mathrm{exp}}_{\mathrm{f,H_2O_2}} - \Delta G^{\mathrm{exp}}_{\mathrm{f,H_2O}} - \Delta G^{\mathrm{cal}}_{\mathrm{Rxn2}} \tag{8}$$

$$\Delta G_{\mathrm{f,H_2O_2}} = 2\Delta G^{\mathrm{exp}}_{\mathrm{f,H_2O}} - \Delta G^{\mathrm{exp}}_{f,\mathrm{H_2}} - \Delta G^{\mathrm{cal}}_{\mathrm{Rxn3}} \tag{9}$$

where $\Delta G^{\mathrm{exp}}_{\mathrm{f}}$ is the experimental Gibbs energy of formation of the known compound and $\Delta G^{\mathrm{cal}}_{\mathrm{Rxn}}$ is the calculated Gibbs energy of reaction (Gibbs energy change) using theoretical calculations.

The summarized results of the molar Gibbs energy of formation are shown in Table 3. As we expected, the HF and B3LYP methods yielded poor predictions even with large basis sets. The HF/cc-pVDZ level of theory yielded a good prediction on Gibbs energy of formation for hydrogen peroxide, but the values obtained for ammonia oxide differed significantly from that obtained from the composite methods. The MP2 predictions were poor with the basis sets 6-31+G(d) and cc-pVDZ, but they were improved with the basis sets 6-311+G (2df,p) and cc-pVTZ, respectively. However, MP2 theory failed to predict a reasonable Gibbs energy of formation for hydrogen peroxide. The theoretical results differed from the experimental value by substantially more than 8.4 $\text{kJ}\cdot\text{mol}^{-1}$. Therefore, all of the values obtained from HF, B3LYP, and MP2 theories were left out. As expected, the composite theories performed well for both ammonia oxide and hydrogen peroxide, and hence the predicted values were used to calculate the averages. In all composite theories, excellent agreement was found between calculated values and the experimental data for hydrogen peroxide (see Table 1). The differences between the values obtained from reactions 1 and 2 were also small.

The calculated average Gibbs energy of formation for hydrogen peroxide was -103.4 $\text{kJ}\cdot\text{mol}^{-1}$ with a standard deviation of 3.8 $\text{kJ}\cdot\text{mol}^{-1}$ (the experimental value is -105.6 $\text{kJ}\cdot\text{mol}^{-1}$). From reaction 1, an average value of 106.3 $\text{kJ}\cdot\text{mol}^{-1}$ with a standard deviation of 2.9 $\text{kJ}\cdot\text{mol}^{-1}$ was calculated. With the reaction 2, the average value was 103.8 $\text{kJ}\cdot\text{mol}^{-1}$ with a standard deviation of 2.9 $\text{kJ}\cdot\text{mol}^{-1}$. We expected reliable results from reaction 3 because this reaction is more balanced. Hence, the recommended value of molar Gibbs energy of formation for ammonia oxide is (103.8 ± 2.9) $\text{kJ}\cdot\text{mol}^{-1}$. The calculated average value of Gibbs energy of formation for hydrogen peroxide is only greater than the experimental value by 2.2 $\text{kJ}\cdot\text{mol}^{-1}$, which suggests our calculated average value of molar Gibbs energy of formation for gaseous ammonia oxide has a pretty high accuracy.

Entropy and Heat Capacity. Entropy, S, is a thermodynamic parameter that is related to the uniformity of a system, and it can provide a measure of the amount of energy in a system that cannot be used to do work.[39] From statistical mechanics, the entropy is defined to be the Boltzmann constant times the natural logarithm of the number of microstates. Unlike the molar enthalpy of formation and molar Gibbs energy of formation, the value of molar entropy is an absolute. Heat capacity at constant volume, C_v, is a measurable thermal energy that characterizes the amount of heat which is required to change the system temperature.[39] Specific heat capacity is a function of the molecule structure. In particular, it depends on the number of degrees of freedom that are available to the particles in the molecule. For small molecules, nowadays quantum chemistry can provide highly accurate estimations of molar entropy and molar heat capacity via frequency calculations.[40] The attainable level of accuracy is impressive, often reaching into the sub-joule regime.

The summaries of calculated molar entropies (S) and molar heat capacities at constant volume (C_v) for gaseous ammonia oxide at 1 atm and 298.15 K are shown in Table 4. All of these levels of theory yielded good predictions for both S and C_v. Therefore, the computed values from all of the methods were used to calculate their averages. The calculated average molar entropy for ammonia oxide was 221.1 $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ with a standard deviation of 0.1 $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$. For molar heat capacity at constant volume, an average value of 28.9 $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ with a standard deviation of 0.3 $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ was obtained. The excellent agreement of the calculated hydrogen peroxide average value with the experimental value suggests that the calculated molar entropies and molar heat capacities at constant volume for ammonia oxide are very reliable.

Table 4. Summary of Calculated Molar Entropies and Molar Heat Capacities at Constant Volume for Ammonia Oxide at 1 atm and 298.15 K

		S	C_v
method	basis set	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
HF	6-31G(d,p)	221.2	29.0
	6-311+G(2df,p)	220.8	28.4
	cc-pVDZ	221.3	29.2
	cc-pVTZ	220.9	28.6
MP2	6-31G(d,p)	221.1	28.8
	6-311+G(2df,p)	221.0	28.7
	cc-pVDZ	221.1	29.0
	cc-pVTZ	221.1	28.8
B3LYP	6-31G(d,p)	221.1	29.0
	6-311+G(2df,p)	221.3	29.3
	cc-pVDZ	221.1	29.2
	cc-pVTZ	221.3	29.4
G2		221.2	28.9
G3		221.2	28.9
G3B3		221.1	28.8
CBS-Q		221.2	28.9

Table 5. Summary of the Recommended Values of Thermochemical Properties for Ammonia Oxide at 1 atm and 298.15 K

ΔH_f	ΔG_f	S	C_v
$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
55.7 ± 2.9	103.8 ± 2.9	221.1 ± 0.1	28.9 ± 0.3

Conclusions

Various computational methods have been employed to determine reliable thermochemical data, including the molar enthalpy of formation, molar Gibbs energy of formation, molar entropy, and molar heat capacity at constant volume, for gaseous ammonia oxide, which is an unstable substance and is difficult to measure its thermodynamic properties experimentally. We have demonstrated that isodesmic reactions are very useful to calculate accurate thermochemical data at different levels of theory. As expected, the composite theories, including G2, G2MP2, G3, G3B3, and CBS-Q, yielded the most accurate values, as compared to other ab initio and density functional methods (HF, MP2, B3LYP). On the basis of this work, we recommended a value of (55.7 ± 2.9) $\text{kJ}\cdot\text{mol}^{-1}$ for the molar enthalpy of formation, (103.8 ± 2.9) $\text{kJ}\cdot\text{mol}^{-1}$ for the molar Gibbs energy of formation, (221.1 ± 0.1) $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ for molar entropy, and (28.9 ± 0.3) $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ for the molar heat capacity at constant volume, for gaseous ammonia oxide at 1 atm and 298.15 K. All of the results are summarized in Table 5. The accuracy of the prediction is high due to excellent agreement of the calculated value for hydrogen peroxide with the experimental value. These thermochemical data are important for the design of safe and economical chemical processes. It should be noted that the thermochemical data reported here are for ammonia oxide in the gas phase, at 1 atm and 298.15 K.

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