Thermochimica Acta, 197 (1992) 181–189
Elsevier Science Publishers B.V., Amsterdam

On thermodynamics of the gas-phase isomeric heterodimers of nitrous oxide and hydrogen fluoride [α]

Zdeněk Slanina [1]
Max-Planck-Institut für Chemie (Otto-Hahn-Institut), Mainz (Germany)

(Received 28 May 1991)

Abstract

Recent experimental and theoretical results have revealed the existence of two isomeric heterodimers in the nitrous oxide–hydrogen fluoride system, namely linear $ON_2 \cdot HF$ and bent $N_2O \cdot HF$. A computational evaluation of the thermodynamics of these isomeric species has been carried out on the basis of available quantum-chemical data of ab initio type. It has been shown that at moderate and higher temperatures the relative stabilities of both species are of the same order of magnitude. This stability interplay leads to quite distinct isomerism contributions to overall values of thermodynamic quantities. Isomeric enhancement of the heat capacity term reaches its maximum at temperatures slightly above 100 K and is about 5 J K^{-1} mol^{-1}.

INTRODUCTION

Quite recently, sophisticated ab initio studies [2,3] considerably extended the scope of the theoretical knowledge [4–10] concerning the associating system of N_2O and HF. In accordance with observations [11–17], theory confirms the existence of two isomeric heterodimers, namely a linear structure $ON_2 \cdot HF$ with a hydrogen bond to the nitrogen atom, and a bent structure $N_2O \cdot HF$ with a hydrogen bond to the oxygen atom. This two-fold isomerism in the N_2O–HF system represents so far the most thoroughly investigated (both theoretically and experimentally) case of this structural phenomenon. However, this isomerism has also been indicated in observations of other species [18–28].

At present, the predominant theoretical description is that in terms of geometric parameters and the energetics of isolated local potential minima, see refs. 29–31. In addition, computational studies have been published

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[α] Part LII in the series Multi-Molecular Clusters and Their Isomerism; for Part LI, see ref. 1.

[1] The permanent and reprint request address: The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Dolejškova 3, CS-18223 Prague 8-Kobylisy, Czech and Slovak Federal Republic.

which involve temperature effects [32–41]. For this purpose, however, it is necessary to have certain pieces of information about vibrational motions which at present are predominantly supplied by quantum-chemical calculations at the level of harmonic vibrational frequencies. Approaches beyond this framework are, at present, quite exceptional [33]; the involvement of temperature effects in isomeric systems [42–50] has a special importance, because it enables the possible temperature interchanges in relative stabilities of the individual isomers to be revealed. The present paper deals with this aspect and its further thermodynamic consequences for the gas phase system N_2O–HF.

DESCRIPTION OF COMPUTATIONS

The information necessary for construction of partition functions will be taken from the computations [2,3]. In ref. 2 the computation used a basis set of triple-zeta plus double polarisation quality (TZ2P) combined with Møller–Plesset second-order (MP2) treatment of correlation effects. In terms of this computational scheme, structural, energy, and harmonic vibrational characteristics of both isomeric complexes were obtained. For the potential energy term as an option, the correction for the basis set superposition error (BSSE) was also considered, which led to two different evaluations of this term. The more recent study [3] was carried out in an extensive polarised basis set of the CGTO type [51,52] combined with many-body perturbation theory (MBPT) up to the fourth order (and with inclusion of the BSSE contribution). Three different approaches [3] to the potential energy term will be used for the purposes of the present study: the MBPT treatment up to the second order (MBPT2); the treatment up to the fourth order without triple excitations, i.e. only single, double and quadruple excitations, SDQ–MBPT4; and the full fourth order (MBPT4). However, because the results in the third treatment are only available [3] for the linear structure, the MBPT2 energy was applied for the other isomer (MBPT4–MBPT2). The energetics of the associations

$$N_2O(g) + HF(g) = ON_2 \cdot HF(g) \qquad (1)$$

$$N_2O(g) + HF(g) = N_2O \cdot HF(g) \qquad (2)$$

are given in Table 1. In addition to the ΔE_i term ($i = 1$, 2 or linear, bent) of potential energy, the changes $\Delta H_{0,i}^{\ominus}$ in the ground-state energy term, i.e. after correcting the ΔE_i term for zero-point vibrations, are also presented.

In our contexts, further starting terms are represented by the partition functions q_i of the isomers. These partition functions are constructed in the usual approximation of rigid rotor and harmonic oscillator, RRHO. This approximation was used in its standard version, although in connection with descriptions of molecular complexes, interesting progress has

TABLE 1

Potential energy change ΔE and ground-state energy change $\Delta H_0^{\ominus}$ for formation of the linear $ON_2 \cdot HF$ and the bent $N_2O \cdot HF$ complexes evaluated in various approximations to energy (kJ mol^{-1}) [2,3]

Approximation	$N_2O+HF=ON_2 \cdot HF$		$N_2O+HF=N_2O \cdot HF$	
	ΔE	$\Delta H_0^{\ominus}$	ΔE	$\Delta H_0^{\ominus}$
TZ2P/MP2	−15.34	−9.46	−11.09	−5.80
TZ2P/MP2+BSSE	−12.52	−6.65	−8.10	−2.81
MBPT2	−12.34	−6.46	−8.82	−3.54
SDQ–MBPT4	−9.71	−3.83	−10.08	−4.80
MBPT4–MBPT2	−12.76	−6.88	−8.82	−3.54

recently been made in the replacement of torsional motion by free internal rotation [53–60]. Reference 2 reports, for both isomers, all the necessary parameters for construction of the RRHO partition functions, namely in the MP2 approximation (but without the reoptimisation with BSSE). It must be mentioned that in the first, second and third approximations, ref. 3 only contains energy and structural information but practically no vibrational data. Therefore, for the three energy treatments described above, we used, the SDQ–MBPT4 geometries [3] and MP2 harmonic vibrational frequencies [2] for the construction of RRHO partition functions.

For a description of the thermodynamics of isomeric clusters, it is possible to adopt the formalism developed for general isomeric systems [61–71]. Let us consider a system of n isomers under the conditions of their thermodynamic equilibrium. Their mole fractions w_i in the above-defined molecular terms are

$$w_i = \frac{q_i \exp(-\Delta H_{0,i}^{\ominus}/RT)}{\sum_{j=1}^{n} q_j \exp(-\Delta H_{0,j}^{\ominus}/RT)} \tag{3}$$

From a methodical standpoint it is also possible to consider the simple Boltzmann factors

$$w_i' = \frac{\exp(-\Delta E_i/RT).}{\sum_{j=1}^{n} \exp(-\Delta E_j/RT)} \tag{4}$$

For the association processes (1) and (2) with participation of a particular isomer, it is possible to construct their corresponding standard partial terms $\Delta X_i^{\ominus}$: enthalpy changes ($X=H$), entropy changes ($X=S$) or changes of heat capacity at constant pressure ($X=C_p$). In addition to these partial terms, the overall terms ($\Delta X_T^{\ominus}$) can also be considered useful, the processes (1) and (2) both contributing to the latter terms according to the weight factors w_i. These overall terms will apply to the situations in which the individual isomers are not differentiated. The partial and overall terms are mutually related [61–71]

$$\Delta H_{\mathrm{T}}^{\ominus} = \sum_{i=1}^{n} w_i \, \Delta H_i^{\ominus} \tag{5}$$

$$\Delta S_{\mathrm{T}}^{\ominus} = \sum_{i=1}^{n} w_i \left(\Delta S_i^{\ominus} - R \ln w_i \right) \tag{6}$$

$$\Delta C_{p,\mathrm{T}}^{\ominus} = \Delta C_{p,w}^{\ominus} + \frac{1}{RT^2} \left[\sum_{i=1}^{n} w_i \left(\Delta H_i^{\ominus} \right)^2 - \left(\Delta H_{\mathrm{T}}^{\ominus} \right)^2 \right] \tag{7}$$

where $\Delta C_{p,w}^{\ominus}$ is the so-called isofractional term

$$\Delta C_{p,w}^{\ominus} = \sum_{i=1}^{n} w_i \, \Delta C_{p,i}^{\ominus} \tag{8}$$

It has been suggested that the overall term $\Delta C_{p,\mathrm{T}}^{\ominus}$ be called relaxation [70]. Moreover it is useful to delimit explicitly an intrinsic contribution of isomerism to the thermodynamic terms by using the so-called isomerism contributions to the values of thermodynamic functions $\delta X_1^{\mathrm{iso}}$. These isomerism contributions are related to the isomer which predominates at low temperatures (by convention this isomer is labelled with subscript 1) and they are introduced by the definition relation

$$\delta X_1^{\mathrm{iso}} = \Delta X_{\mathrm{T}}^{\ominus} - \Delta X_1^{\ominus} \tag{9}$$

RESULTS AND DISCUSSION

Table 2 gives two representative temperature courses for weight factors w_1 and w_1' for the linear structure $ON_2 \cdot HF$. For this purpose we selected

TABLE 2

Temperature dependence of the weight factors (the mole fractions) w_1 and w_1' of the linear $ON_2 \cdot HF$ complex in the gas phase equilibrium mixture with the bent $N_2O \cdot HF$ isomer evaluated within the SDQ–MBPT4 and MBPT4–MBPT2 approaches to energy

T (K)	SDQ–MBPT4		MBPT4–MBPT2	
	w_1 (%)	w_1' (%)	w_1 (%)	w_1' (%)
50	2.55	28.8	99.9	100.0
100	9.64	38.9	95.0	99.1
200	20.5	44.4	77.5	91.4
298.15	27.3	46.2	68.2	83.0
500	36.0	47.7	61.3	72.0
1000	46.7	48.9	59.6	61.6

the energy approximations SDQ–MBPT4 and MBPT4–MBPT2 which can be considered the most sophisticated of the five treatments considered (Table 1). Moreover, the temperature course of the remaining three approaches is qualitatively similar to that of the MBPT4–MBPT2 treatment. A substantial difference exists between this approximation and SDQ–MBPT4: these two approximations lead to mutually reversed stability orders of the isomers (in terms of $\Delta H_{0,i}^{\ominus}$ or ΔE). Because in the SDQ–MBPT4 approximation the linear structure is richer in energy than the bent isomer, the latter species must increasingly predominate with decreasing temperature. In the MBPT4–MBPT2 (and the remaining three) approach(es), the opposite situation is encountered. However, at medium and high temperatures the populations of both isomers become similar in all five approximations considered (tens of %). If the temperature evolution is continued beyond the upper temperature limit in Table 2, we find that both structures reach equimolarity at 1254 K in the case of the SDQ–MBPT4 treatment. The situation is different in the remaining four approximations to potential energy. The w_1 term decreases until it reaches a certain minimum and then it slowly increases without any interchange in relative stabilities of both isomers. The lowest value of the w_1 term (59.4%) is reached at about 848 K in the MBPT4–MBPT2 approximation. Finally, the simple Boltzmann factors w_i' are generally not good substitutes for the w_i terms.

Table 3 presents the temperature dependence of partial standard enthalpy changes, entropy changes and changes of heat capacity at constant pressure for reactions (1) and (2) as well as the corresponding overall terms of the total association

$$N_2O(g) + HF(g) = N_2O\text{–}HF(g) \qquad (10)$$

again for the two presumably most sophisticated approaches to the potential energy. The $\Delta S_i^{\ominus}$ and $\Delta C_{p,i}^{\ominus}$ terms must be the same for both these energy approximations, because identical sets of input data were used for construction of partition functions. It is self-evident that the partial enthalpy terms are different for these two energy approximations, the same being true of all the parent overall terms. All the quantities presented exhibit distinct temperature dependences, these courses involving minima for the enthalpy and entropy terms. For the heat capacity terms, the temperature course shows no extremes.

Table 4 provides an evaluation of the importance of the intrinsic isomeric contributions to the thermodynamics, namely in terms of the isomerism contributions to enthalpy, entropy and heat capacity, again within the limits of the SDQ–MBPT4 and MBPT4–MBPT2 approximations to potential energy. As, however, these two approximations provide substantially different pictures of stability at low temperatures (Table 2), the $\delta X_1^{\mathrm{iso}}$ terms are related to different reference isomers in these approximations. It

TABLE 3

Partial and overall standard [a] enthalpies $\Delta H_x^\ominus$, entropies $\Delta S_x^\ominus$ and heat capacities at constant pressure $\Delta C_{p,x}^\ominus$ of N_2O(g) and HF(g) associations evaluated within the SDQ–MBPT4 and MBPT4–MBPT2 approaches to energy

T (K)	$\Delta H_x^\ominus$ [b] (kJ mol^{-1})		$\Delta S_x^\ominus$ [b] (J K^{-1} mol^{-1})		$\Delta C_{p,x}^\ominus$ [b] (J K^{-1} mol^{-1})	
	SDQ–MBPT4	MBPT4–MBPT2	SDQ–MBPT4	MBPT4–MBPT2	SDQ–MBPT4	MBPT4–MBPT2
$N_2O(g) + HF(g) = ON_2 \cdot HF(g)$						
50	−4.59	−7.65	−77.8	−77.8	−10.2	−10.2
100	−4.96	−8.02	−83.1	−83.1	−4.83	−4.83
200	−4.99	−8.04	−83.6	−83.6	3.57	3.57
298.15	−4.41	−7.47	−81.3	−81.3	7.60	7.60
500	−2.53	−5.59	−76.6	−76.6	10.4	10.4
1000	3.14	0.09	−68.8	−68.8	11.9	11.9
$N_2O(g) + HF(g) = N_2O \cdot HF(g)$						
50	−5.68	−4.42	−69.1	−69.1	−14.8	−14.8
100	−6.27	−5.01	−77.6	−77.6	−9.18	−9.18
200	−6.71	−5.46	−81.0	−81.0	−0.54	−0.54
298.15	−6.54	−5.29	−80.3	−80.3	3.52	3.52
500	−5.47	−4.22	−77.7	−77.7	6.44	6.44
1000	−1.77	−0.51	−72.6	−72.6	7.93	7.93
$N_2O(g) + HF(g) = N_2O\text{–}HF(g)$						
50	−5.65	−7.64	−68.4	−77.7	−13.3	−9.61
100	−6.14	−7.87	−75.5	−81.2	−6.97	0.09
200	−6.36	−7.46	−77.3	−78.6	1.77	6.15
298.15	−5.96	−6.77	−75.7	−75.8	5.85	7.70
500	−4.41	−5.06	−71.8	−71.5	8.83	9.10
1000	0.53	−0.16	−65.1	−64.7	10.5	10.3

[a] The standard state is an ideal gas at 1 atm = 101325 Pa pressure.

[b] The parameter x denotes either 1 or 2 (i.e. the partial processes), or T (the overall process).

is evident that the isomerism contribution to the overall values of the thermodynamic functions is significant, at least in certain temperature intervals. In the case of the MBPT4–MBPT2 approximation both the enthalpy and entropy terms show a course with a maximum, which however is not distinct in the SDQ–MBPT4 approximation.

A relatively distinct course with a maximum was found with the $\delta C_{p,1}^{iso}$ term for some systems [49,66,70]. Therefore, Table 5 specifies the position of this maximum for all the five approximations to potential energy (as far as the maximum exists: it was not found in the SDQ–MBPT4 approach). When a maximum is present, there is considerable uniformity in its position. In all four approximations, it is found at temperatures slightly above 100 K, and its height is about 5 J K^{-1} mol^{-1}. Hence these maxima are relatively less distinct than those found, so far, to be the most pro-

TABLE 4

Isomerism contributions [a] to enthalpy $\delta H_1^{\mathrm{iso}}$, entropy $\delta S_1^{\mathrm{iso}}$ and heat capacity $\delta C_{p,1}^{\mathrm{iso}}$ for the isomeric system N_2O–HF(g) evaluated within the SDQ–MBPT4 and MBPT4–MBPT2 approaches to energy

T (K)	$\delta H_1^{\mathrm{iso}}$ (kJ mol^{-1})		$\delta S_1^{\mathrm{iso}}$ (J K^{-1} mol^{-1})		$\delta C_{p,1}^{\mathrm{iso}}$ (J K^{-1} mol^{-1})	
	SDQ–MBPT4	MBPT4–MBPT2	SDQ–MBPT4	MBPT4–MBPT2	SDQ–MBPT4	MBPT4–MBPT2
50	0.028	0.004	0.766	0.088	1.51	0.597
100	0.126	0.150	2.10	1.93	2.21	4.93
200	0.354	0.581	3.68	5.02	2.30	2.58
298.15	0.581	0.695	4.61	5.52	2.33	0.101
500	1.06	0.530	5.82	5.13	2.39	−1.33
1000	2.29	−0.241	7.53	4.07	2.56	−1.58

[a] Related to the isomer more stable at low temperatures, i.e. the bent $N_2O\cdot HF$ and the linear $ON_2\cdot HF$ structure in the SDQ–MBPT4 and MBPT4–MBPT2 approaches, respectively.

nounced in cluster isomeric systems [70]. Interestingly, the isofractional component is rather indistinct in these maxima (Table 5).

The whole study is presented in the RRHO approximation which is the only treatment which can be carried out within the scope of existing information. More sophisticated approximations to the partition functions would definitely bring quantitative changes; nevertheless, it is presumed [64] that qualitative features are already reflected by the RRHO treatment. At the same time it can be seen that the isomerism contributions to values of thermodynamics functions at low temperatures can markedly exceed the values of possible corrections [64] for the RRHO behaviour.

TABLE 5

Positions of the maxima in the isomerism contribution [a] to heat capacity $\delta C_{p,1}^{\mathrm{iso}}$ for the isomeric system N_2O–HF(g) evaluated within various energy approximations [b]

Approximation [b]	T (K)	$\delta C_{p,1}^{\mathrm{iso}}$ (J K^{-1} mol^{-1})	$\delta C_{p,w,1}^{\mathrm{iso}}$ [a] (J K^{-1} mol^{-1})
TZ2P/MP2	129	4.90	−0.33
TZ2P/MP2+BSSE	136	4.80	−0.32
MBPT2	102	5.57	−0.37
SDQ—MBPT4	No maximum		
MBPT4–MBPT2	118	5.28	−0.35

[a] Related to the isomer more stable at low temperatures, see Table 4. The relaxation term $\delta C_{p,1}^{\mathrm{iso}}$ is presented together with its isofractional component $\delta C_{p,w,1}^{\mathrm{iso}}$.

[b] See Table 1 for details.

ACKNOWLEDGEMENTS

The author is indebted to Drs Joanna Sadlej and Nicholas Handy for the valuable information exchange on refs. 2 and 3. This study was carried out during a stay at the Max-Planck-Institut für Chemie in Mainz supported by the Alexander von Humboldt-Stiftung. The support of and valuable discussions with Professor Karl Heinzinger and his kind hospitability are gratefully acknowledged.

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