Thermochimica Acta, 197 (1992) 169–180
Elsevier Science Publishers B.V., Amsterdam

A computational–thermodynamic study of the B_2H_4 and $B_2H_4^+$ isomerism

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(Received 24 June 1991)

Abstract

A computational evaluation of the relative stabilities of isomers of B_2H_4 (staggered D_{2d} and doubly bridged C_{2v} species) and of $B_2H_4^+$ (doubly bridged C_{2v}, triply bridged C_{3v} and staggered D_{2d} species) in an ideal gas phase has been carried out on the basis of recent quantum-chemical data. In both systems, relative stability interchange can take place, so that after passing a temperature threshold the global energy minimum becomes a less significant component of the isomeric mixture, being surpassed by a higher local energy minimum. The stability interchange has pronounced consequences in the heat capacity term, recalling phase transition behaviour.

INTRODUCTION

Borane chemistry has in recent years been the subject of vigorous theoretical interest; see e.g., refs. 1–6. Isomerism, discovered by computational means in some borane species, represents an interesting and distinct structural phenomenon. From the computational point of view, the isomerism means the presence of (at least) two local energy minima at potential hypersurface(s), as has been well exemplified by the B_2H_4 [7–19] and $B_2H_4^+$ [17–19] systems. Manifold occurrence of several relevant local energy minima on a potential hypersurface represents a relatively frequent event in contemporary computational studies. A generally preferred approach to the manifold occurrence consists in evaluation of a stability order according simply to the potential energy terms, (intuitive) preference of the structure with the lowest value of this term, or even straightforward abandonment of all the higher species. Nowadays, however, a more advanced treatment has become feasible [20–24], making use of isomeric partition functions in order to consider effects of temperature excitations

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0040-6031/92/$05.00

of rotational–vibrational motions upon the stability ordering at finite temperatures. In this article the treatment is applied to the evaluation of the relative stabilities of B_2H_4 and $B_2H_4^+$ isomers, based on recent quantum-chemical characterization of the potential hypersurface local energy minima [14,15,17].

LOCAL ENERGY MINIMA AND TEMPERATURE

The still predominant approach to the manifold occurrence of local minima has actually followed the state of the art of numerical quantum chemistry, for which, until recently, the characterization of stationary points of a hypersurface in terms of energy vs. structure represented a kind of upper limit. At present, however, the accepted standard of quantum-chemical description of a system is being shifted towards location of all relevant local energy minima and evaluation of harmonic frequencies for vibrational motions in the points. With the latter terms available the first correction is transfer from potential energy terms ΔE_i to the ground state energies $\Delta H^\circ_{0,i}$ through correction of the former terms by (harmonic) vibrational zero-point energies (from the thermochemical point of view the ground state energy represents the standard enthalpy change at absolute zero temperature). However, the extended standard of quantum chemical description (energy–structure–vibrational frequencies) offers practically all that is necessary for construction of partition functions q_i of the individual local energy minima in the usual approximation or rigid rotor and harmonic oscillator (RRHO) [22]. This approach to the local minima as isolated domains of configurational space actually requires the minima to be separated by insurmountable potential barriers.

Proportions (relative stabilities) between n individual local energy minima can be treated in terms of their equilibrium isomeric mixture mole fractions w_i. It holds [22,23] for the weighting factors in the above terms

$$w_i = \frac{q_i \exp[-\Delta H^\circ_{0,i}/(RT)]}{\sum_{j=1}^{n} q_j \exp[-\Delta H^\circ_{0,j}/(RT)]} \qquad (1)$$

Let us mention here that, although ideal gas phase behaviour is mostly assumed, in eqn. (1) applications to other media are also possible. It should also be noted that the $\Delta H^\circ_{0,i}$ terms can belong to various types of processes (isomerization, association), as in fact only relative ground-state energies of the individual local minima with respect to some common (however arbitrary) reference state are important for eqn. (1). Hence we can understand the $\Delta H^\circ_{0,i}$ terms in eqn. (1) as the ground-state energies related to one of the isomers taken as the reference structure (it is useful to choose, as the reference structure, the isomer which is the most stable in the low temperature region and to assign, formally, the index 1 to it). Then the $\Delta H^\circ_{0,i}$ terms denote the standard enthalpy changes accompanying the isomerization of the first isomer to the i-th one at absolute zero temperature. Clearly enough, the isomer 1 (which usually, but not necessarily, represents the global minimum at the potential energy hypersurface—the zero-point correction can in principle change isomeric ordering), in spite of being predominant at low temperatures, can become the minor component of the equilibrium isomeric mixture with increasing temperature. Such an event, of course, would represent a very interesting situation from the physico-chemical point of view, having substantial consequences for theory–experiment comparisons. Finally, there are arguments [20] in support of a good RRHO approximation applicability, as corrections for deviations from RRHO behaviour should extensively cancel between the numerator and denominator of eqn. (1).

There is still an intermediate, simplified possibility of reflecting temperature effects on relative stabilities of local minima, viz. by means of so called simple Boltzmann factors [22]

$$w_i' = \frac{\exp[-\Delta E_i/(RT)]}{\sum_{j=1}^{n} \exp[-\Delta E_j/(RT)]} \tag{2}$$

However, these Boltzmann factors do not reflect any kind of rotational–vibrational motion and they do not admit of the possibility of interchange in stability order with changing temperature (i.e., if $\Delta E_i > \Delta E_j$ then, always, $w_i' < w_j'$). Hence the simple Boltzmann factors cannot be generally applicable.

Two limiting situations can be considered: the isolated local energy minima and a single pseudospecies created by the equilibrium mixture of the isomeric structures. Then, for any structure-dependent quantity X (in our context it is, first of all, a standard thermodynamic function X°), we can differentiate two classes of values: the partial terms (X_i°) corresponding to the individual isomers, and the overall one (X_T°) corresponding to their equilibrium mixture. From both the methodological and the applications standpoints it appears useful to introduce [21–23] the so called isomerism contribution δX_1 to the values X_T° as follows

$$\delta X_1 = X_T^\circ - X_1^\circ \tag{3}$$

A particularly interesting factor is the contribution of isomerism to heat capacity at constant pressure ($X = C_p$), since the isomeric interplay can be manifested in the $\delta C_{p,1}$ term by a fairly distinct temperature maximum [23], which persists even in the overall (total) standard heat capacity term and is thus observable. It holds [23] for the $\delta C_{p,1}$ term that

$$\delta C_{p,1} = \delta C_{p,w,1} + \frac{1}{RT^2}\left[\sum_{i=1}^{n} w_i(\Delta H_i^\circ - \Delta H_1^\circ)^2 - (\delta H_1)^2\right] \tag{4}$$

where $\delta C_{p,w,1}$ denotes the so called isofractional [21,23] isomerism contribution to heat capacity

$$\delta C_{p,w,1} = \sum_{i=1}^{n} w_i(\Delta C^\circ_{p,i} - \Delta C^\circ_{p,1}) \tag{5}$$

while the isomerism contribution to enthalpy is given simply by [21]

$$\delta H_1 = \sum_{i=1}^{n} w_i(\Delta H^\circ_i - \Delta H^\circ_1) \tag{6}$$

The isofractional contribution (5) is a somewhat auxiliary quantity as it supposes temperature-independent w_i terms. However, the full $\delta C_{p,1}$ term (4) takes account of the (frequently crucial) effects of changes in composition upon a temperature change. The latter term is therefore called the relaxation [21,23] isomerism contribution to heat capacity.

THE B_2H_4 AND $B_2H_4^+$ SYSTEMS

The quantum-chemical extended description of the B_2H_4 system is given in refs. 15 and 17, each paper revealing two local energy minima (staggered D_{2d} and doubly bridged C_{2v} species). An earlier study [15], employing the 6-311G**(6d) basis set up to the CCSD + T(CCSD) level† (abbreviated in this paper as CC), gives the D_{2d} isomer as the global minimum, whereas a newer evaluation [17] prefers the C_{2v} structure (Table 1). In the newer study [17] the structural parameters were evaluated at the MP2/6-13G* level, considering all electrons for calculated correlation energies, and the energetics in the geometries were evaluated at the MP4/6-311G** level modified by a number of subsequent corrections (here coded by MP4). The harmonic vibrational frequencies were evaluated within an MP2 treatment and in terms of the HF/6-31G* approach in refs. 15 and 17, respectively. In both treatments, scaling factors for vibrational frequencies were suggested, viz. a factor of 0.96 or 0.893 in ref. 15 or 17, respectively, introduced in order to account for overestimation of the values of vibrational frequencies in a particular quantum-chemical calculation. In our connections each energy term was combined with related, both unscaled and scaled, vibrational frequencies (the approaches coded by CC/1.0, CC/0.96 and MP4/1.0, MP4/0.893). Finally, in a study [14] preceding the CC treatment [15] the energetics were evaluated at the MP2/6-31G** level (here coded by MP2), and the results almost coincide with the CC energetics (the C_{2v} isomer lies somewhat higher in energy in the former than in the latter approach; see survey in Table 1). The MP2 energetics [14] are in the

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† The coupled cluster (CC) method with single and double (CCSD) excitations and with an evaluation of triple excitations (CCSD + T(CCSD)).

TABLE 1

Survey of the relative energetics (kJ mol^{-1}) in the B_2H_4 [a] and $B_2H_4^+$ [b] systems

B_2H_4 Source	Isomer	ΔE_i [c]	$\Delta H^{\circ}_{0,i}$ [d]
MP2/6-31G** (ref. 14)	D_{2d}	0.0	0.0
	C_{2v}	6.360	9.296 [e]
			8.982 [e]
CCSD+T(CCSD)/6-311G**(6d) (ref. 15)	D_{2d}	0.0	0.0
	C_{2v}	5.439	8.986 [f]
			8.844 [f]
Corrected [17] MP4/6-311G**	C_{2v}	0.0	0.0
	D_{2d}	3.095	0.158 [e]
			0.473 [e]
$B_2H_4^+$ Source	Isomer	ΔE_i [c]	$\Delta H^{\circ}_{0,i}$ [d]
Corrected [17] MP4/6-311G**	C_{2v}	0.0	0.0
	C_{3v}	42.050	48.324 [e]
			47.653 [e]
	D_{2d}	87.762	78.569 [e]
			79.553 [e]

[a] Doubly bridged and staggered isomers of C_{2v} and D_{2d} symmetry, respectively.

[b] Doubly bridged, triply bridged and staggered isomers of C_{2v}, C_{3v} and D_{2d} symmetry, respectively.

[c] Potential energy difference with respect to the first structure.

[d] Ground-state energy difference with respect to the first structure (i.e., ΔE_i corrected for zero-point vibrations).

[e] Zero-point vibrational correction based on harmonic vibrational frequencies [17], either unscaled (the upper line) or scaled by 0.893 (the lower line).

[f] Zero-point vibrational correction based on harmonic vibrational frequencies [15], either unscaled (the upper line) or scaled by 0.96 (the lower line).

present paper combined with the unscaled and scaled vibrational frequencies [17] (coded by MP2/1.0 and MP2/0.893). These six approaches altogether create a rather broad interval of the isomeric ground-state energy separations. It should nevertheless be mentioned that by use of a much larger basis set the CC value may be changed [15] by as much as ±21 kJ mol^{-1}.

The extended quantum-chemical description for the cationic $B_2H_4^+$ system is available in ref. 17. With the MP4 treatment, three different local energy minima were found there (doubly bridged C_{2v}, triply bridged C_{3v} and staggered D_{2d}; see Table 1). In this three-membered system the C_{2v} isomer seems to be well separated from the remaining two. Harmonic vibrational frequencies are again employed in our connections, both unscaled (1.0) and scaled (0.893).

RESULTS AND DISCUSSION

Figure 1 presents the temperature dependences of the weight factors w_i' and w_i evaluated within the MP2, CC and MP4 approaches for the two-membered B_2H_4 system. As the results are quite similar for the unscaled and scaled frequencies, only the results from the scaled treatments are given. It can be seen that in the MP2 and CC energetics the structure D_{2d} is populated more significantly than C_{2v} within the whole temperature interval studied. A different picture is however created by the MP4 treatment. Although the C_{2v} isomer (which is the ground-state structure here) is more populated at the lowest temperatures, with increasing temperature the relative stabilities of both structures become closer, until the order of their relative stabilities is interchanged towards the end of the temperature interval studied. Concerning the simple Boltzmann factors, Fig. 1 demonstrates that they are rather insufficient as an approximation for simulation of w_i terms of the system.

Figure 2 deals with temperature dependences of the isomerism contributions to heat capacity in the B_2H_4 system for the three treatments. Whereas in the MP2 and CC approaches there is one temperature maxi-

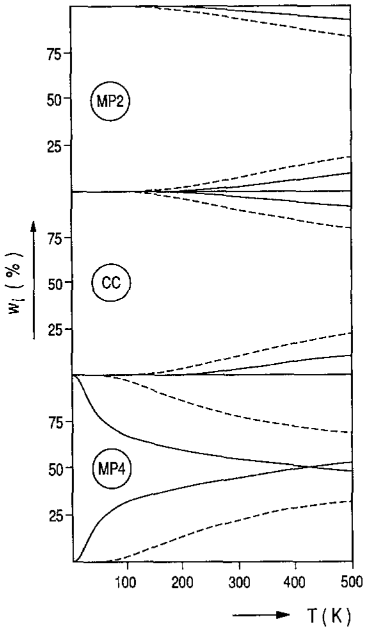

Fig. 1. Temperature dependences of the simple Boltzmann factors w_i' (broken curves) and the weights w_i in the B_2H_4 two-membered isomeric set in the MP2/0.893, CC/0.96, and MP4/0.893 approaches (see Table 2). The ordering at the highest presented temperature (from top to bottom) reads D_{2d}, D_{2d}, C_{2v}, C_{2v} in the MP2 and CC approaches, and C_{2v}, D_{2d}, C_{2v}, D_{2d} in the MP4 approach.

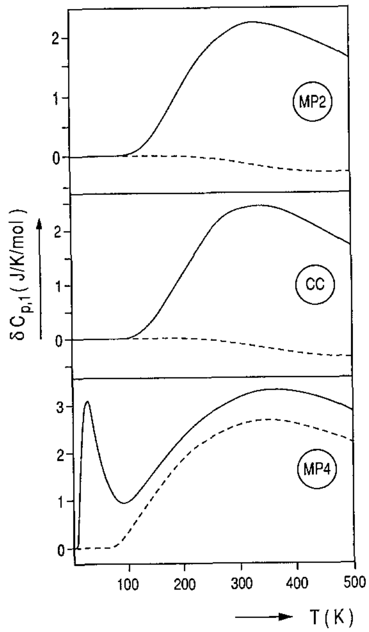

Fig. 2. Temperature dependences of the isomerism contribution (related to the species more stable at very low temperature; see Table 2) to heat capacity at constant pressure $\delta C_{p,1}$ (relaxation term) or $\delta C_{p,w,1}$ (isofractional term, broken lines) for the B_2H_4 two-membered isomeric system in the MP2/0.893, CC/0.96, and MP4/0.893 approaches (cf. Table 2).

mum on the dependence, the MP4 treatment leads to two maxima of about the same height. However, upon transfer from the isomerism contribution to the overall heat capacity at constant pressure C_p°, the extremum behaviour is conserved only in the case of the MP4 approach, and only for the low-temperature maximum (Fig. 3). It should be noticed that in the

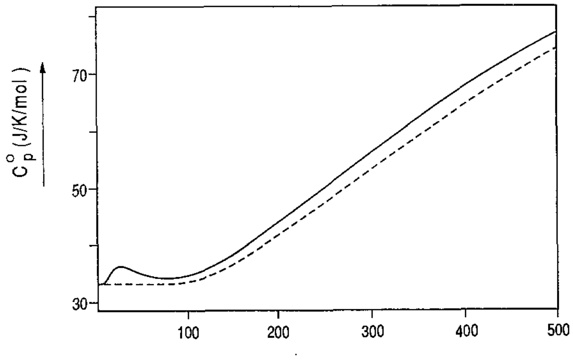

Fig. 3. Temperature dependence of the standard molar heat capacity at constant pressure for the pure C_{2v} isomer ($C_{p,1}^\circ$, the broken line) and for the B_2H_4 two-membered equilibrium isomeric mixture (C_p°) in the MP4/0.893 approach (Table 2).

TABLE 2

Characterization of some significant [a] points of the B_2H_4 isomeric interplay

Approach [b]	Type [a]	T (K)	w_1 [c] (%)	w_2 [c] (%)	$\delta C_{p,1}$ [d] ($\mathrm{J\ K^{-1}\ mol^{-1}}$)	C_p° ($\mathrm{J\ K^{-1}\ mol^{-1}}$)	$\dfrac{\delta C_{p,1}}{C_p^\circ}$ (%)
MP2/1.0	M: $\delta C_{p,1}$	342	96.3	3.7	2.3	62.1	3.7
	M: %	305	97.4	2.6	2.2	58.1	3.8
MP2/0.893	M: $\delta C_{p,1}$	330	96.4	3.6	2.2	64.8	3.4
	M: %	294	97.5	2.5	2.1	60.6	3.5
CC/1.0	M: $\delta C_{p,1}$	336	96.0	4.0	2.5	62.5	3.9
	M: %	301	97.2	2.8	2.4	58.6	4.1
CC/0.96	M: $\delta C_{p,1}$	330	96.1	3.9	2.4	63.3	3.8
	M: %	295	97.2	2.8	2.3	59.3	3.9
MP4/1.0	Cross	392	50.0	50.0	3.2	62.4	5.1
	M: $\delta C_{p,1}$	8	92.7	7.3	3.1	36.4	8.5
	M: $\delta C_{p,1}$	397	49.9	50.1	3.2	62.9	5.1
	M: C_p°	8	92.7	7.3	3.1	36.4	8.5
	M: %	8	92.7	7.3	3.1	36.4	8.5
	M: %	296	52.9	47.2	2.9	52.3	5.5
MP4/0.893	Cross	428	50.0	50.0	3.1	70.6	4.4
	M: $\delta C_{p,1}$	24	92.7	7.3	3.1	36.4	8.5
	M: $\delta C_{p,1}$	357	52.6	47.4	3.3	63.3	5.1
	M: C_p°	24	92.7	7.3	3.1	36.4	8.5
	M: %	24	92.7	7.3	3.1	36.4	8.5
	M: %	263	56.6	43.4	2.9	52.2	5.6

[a] I.e., point of two-isomer equimolarity (Cross), maximum in the isomerism contribution to heat capacity $\delta C_{p,1}$(M: $\delta C_{p,1}$), maximum in the standard overall heat capacity at constant pressure C_p°(M: C_p°), or maximum of the relative enhancement $\delta C_{p,1}/C_p^\circ$ of the C_p° term by isomeric interplay (M: %).

[b] The coding X/Y is used where X is an energy acronym and Y is a scaling factor. The acronyms MP2, CC and MP4 denote the approaches [14,15,17] MP2/6-31G**, CCSD+T(CCSD)/6-311G**(6d) and MP4/6-311G**, respectively (Table 1).

[c] The mole fraction of the species in the equilibrium isomeric mixture; 1 and 2 denote the staggered D_{2d} and doubly bridged C_{2v} (doubly bridged C_{2v} and staggered D_{2d} in the MP4 approach) species, respectively.

[d] Isomerism contribution to heat capacity related to the species more stable in very low temperature region, i.e. to the staggered D_{2d} (doubly bridged C_{2v} in the MP4 approach) isomer.

low-temperature limit the C_p° term approaches the classical value of $4R$ (instead of the rigorous zero). This is a result of the use of one-term translational and rotational partition functions, the one-term approximation however, not being critical for the low-temperature maximum description.

Table 2 gives a detailed specification of some distinct points of the B_2H_4 isomeric interplay. In addition to the maxima in the isomerism contribution to heat capacity $\delta C_{p,1}$, the maximum in the standard overall heat capacity

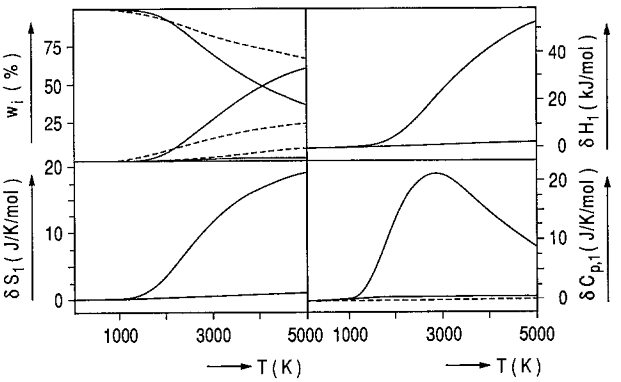

Fig. 4. Temperature dependence of the $B_2H_4^+$ isomeric interplay evaluated within the approach using the 0.893 scaling factor (Table 3). Upper left part: the simple Boltzmann factors w_i' (broken curves) and the weights w_i in the three-membered isomeric set; the ordering at the highest presented temperature (from top to bottom) reads C_{2v}, D_{2d}, C_{2v}, C_{3v}, D_{2d}, C_{3v}. The remaining three sub-pictures show the temperature dependence of the isomerism contributions δX_1 (related to the C_{2v} isomer; see Table 3): upper right part $X = H$ (enthalpy), lower left part $X = S$ (entropy), lower right part $X = C_p$ (heat capacity at constant pressure: $\delta C_{p,1}$ (relaxation term) or $\delta C_{p,w,1}$ (isofractional term, broken line)). In each related pair of the isomerism contributions the higher and lower (nearly constant) curve refer to the three- and two-membered (i.e., abandoning the D_{2d} isomer) isomeric set, respectively.

at constant pressure C_p° and the point of two-isomer equimolarity, maxima in the relative enhancement $\delta C_{p,1}/C_p^\circ$ of the C_p° term by isomeric interplay are also considered. Results for unscaled and scaled frequencies are presented side by side, showing that the scaling is not particularly significant for the considered quantities (with perhaps an exception for the MP4 treatment). The highest relative enhancement of the overall standard heat capacity by isomeric interplay is found in the MP4 approach in the low-temperature region (8.5%).

Figure 4 presents the temperature interplay in the $B_2H_4^+$ system (again for the scaled vibrational set). In order to see some interesting effects, a wider temperature interval is to be considered. A relative stability interchange can then be observed; however, it is an exchange between the ground-state structure C_{2v} and the species of highest potential energy, D_{2d} (the interchange between the C_{3v} and D_{2d} species takes places at considerably lower temperatures and cannot be seen in the figure, being specified in Table 3). The isomerism contributions to enthalpy, entropy and heat capacity can reach quite substantial values, and the last mentioned term again exhibits a temperature maximum. The maximum is, moreover, conserved in the overall heat capacity course (Fig. 5). It should be noted that the interplay between the C_{2v} and D_{2d} structures is mainly responsible for the effects. In a reduced two-membered isomeric set composed of the C_{2v} and C_{3v} species the isomerism effects are negligible.

TABLE 3

Characterization of some significant [a] points of the $B_2H_4^+$ isomeric interplay

Scaling	Type [a]	T (K)	w_1 [b] (%)	w_2 [b] (%)	w_3 [b] (%)	$\delta C_{p,1}$ [c] (J K^{-1} mol^{-1})	C_p° (J K^{-1} mol^{-1})	$\frac{\delta C_{p,1}}{C_p^\circ}$ (%)
1.0	Cross	1145	99.7	0.1	0.1	1.2	106	1.1
	Cross	4055	49.2	1.7	49.2	13.8	144	9.6
	M: $\delta C_{p,1}$	2774	75.7	1.4	22.8	21.1	148	14.3
	M: C_p°	2997	70.4	1.5	28.1	20.7	148	14.0
	M: %	2735	76.7	1.4	21.9	21.1	147	14.3
0.893	Cross	1150	99.7	0.1	0.1	1.2	110	1.1
	Cross	4056	49.2	1.7	49.2	13.8	144	9.6
	M: $\delta C_{p,1}$	2775	75.8	1.4	22.8	21.1	149	14.2
	M: C_p°	2957	71.3	1.5	27.2	20.8	149	14.0
	M: %	2743	76.5	1.4	22.1	21.1	149	14.2

[a] I.e., point of two-isomer equimolarity (Cross), maximum in the isomerism contribution to heat capacity $\delta C_{p,1}$ (M: $\delta C_{p,1}$), maximum in the standard overall heat capacity at constant pressure C_p° (M: C_p°), or maximum of the relative enhancement $\delta C_{p,1}/C_p^\circ$ of the C_p° term by isomeric interplay (M: %).

[b] The mole fraction of the species in the equilibrium isomeric mixture; 1, 2 and 3 denote the doubly bridged C_{2v}, triply bridged C_{3v} and staggered D_{2d} isomer, respectively.

[c] Isomerism contribution to heat capacity related to the species most stable in the very low temperature region, i.e. to the doubly bridged C_{2v} isomer.

Table 3 gives a specification of the significant points in the temperature behaviour of the three-membered $B_2H_4^+$ isomeric set. Again, differences between results from unscaled and scaled vibrational frequency sets are not too pronounced. The highest relative enhancement of the overall standard heat capacity by the isomeric interplay is over 14% in this system.

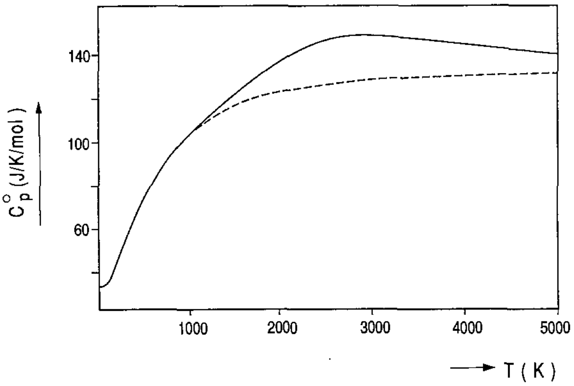

Fig. 5 Temperature dependence of the standard molar heat capacity at constant pressure for the pure C_{2v} isomer ($C_{p,1}^\circ$, the broken line) and for the $B_2H_4^+$ three-membered equilibrium isomeric mixture (C_p°) in the approach using the 0.893 scaling factor (Table 3).

The results obtained for both isomeric systems indicate the possibility of a relative stability interchange in some temperature regions. In particular, the conventional concept of a global energy minimum is questioned by the findings, as a local energy minimum can be more stable than the deepest minimum at some temperatures. Moreover, the stability interchanges can be connected with a temperature maximum in the heat capacity term, resembling to some extent effects known from phase transitions. The temperature maximum could serve for an experimental proof of an isomerism suggested by potential hypersurface search. In any case, the computational procedure for isomerism interplay treatment is available [24], and the results in this paper represent another argument for the application of the procedure as a standard complement to routine quantum-chemical or molecular–mechanical studies of hypersurfaces with manifold local energy minima.

ACKNOWLEDGEMENTS

This study was carried out during a research stay at the Max-Planck-Institut für Chemie (Otto-Hahn-Institut), supported by the Alexander von Humboldt-Stiftung. This support, as well as the valuable discussions with Professor Karl Heinzinger and the kind hospitality of him, of his group, and of the Max-Planck-Institut für Chemie are gratefully acknowledged. Last, but certainly not least, the information exchange with Prof. W.N. Lipscomb on the results [15] is also highly appreciated.

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