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Determination of dissociation energies and thermal functions of hydrogen-bond formation using high resolution FTIR spectroscopy

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Institute of Optics, University of Rochester, Rochester, New York 14627

In my paper a reduced equation of motion [Eq. (19a)] was derived. Equation (19a) contains two terms. The first term is the mean-field term and the second term is the kernel term which represents the fluctuations of the disordered system. In the paper I argued that the second term is zero due to the definition of the projection operator. This is not correct. Although the projection operator defined in the paper contains the entire dynamic operators of the disordered system, the projection operator contains an average over the disorder ensemble also. Since the Hamiltonian of the disordered system given by Eq. (1) contains the random variable \( r_m \), the factors \( PLQ \) and \( QLP \) are not zero. Therefore the kernel term is not zero. In the paper only the mean-field term was calculated explicitly. Therefore the result of the paper is based on the mean-field approximation.

In a recent paper by Deng, Grad, and Mukamel \(^1\) a set of reduced equations, which contains only the zero- and one-body operators, was derived. It has been shown that the population transport is obtained by calculating the kernel term to the second order in the molecule–molecule interactions. In my paper I have shown that by defining a complete set of the dynamic operators of the disordered system, the population transport can be obtained from the mean-field term.


Erratum: Molecular beam translational spectroscopy of physisorption bound states of molecules on metal surfaces. I. HD on Cu(111) and Au(111) single crystal surfaces [J. Chem. Phys. 85, 2249 (1986)]

U. Harten, J. P. Toennies, and Ch. Wöll
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Equation (3) should read

\[
f(x) = 1 - \left[ 1 + \alpha x + \frac{(\alpha x)^2}{2} + \frac{(\alpha x)^3}{6} \right] \exp \left( -\alpha x \right).
\]

None of the results reported are affected since the correct formula was used in the calculations. We thank J. Frenken for calling this to our attention.


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Some errata and misprints have been detected in this paper. The following corrections are presented to clarify the previous text.

Abstract:

The last sentence in the abstract should read:

Rovibrational band information available for HCN---HF also permits evaluation of thermal functions of dimer formation in kJ mol\(^{-1}\): \( \Delta U^{0}_{298.2} = -20.5(2) \), \( \Delta H^{0}_{298.2} = -23.0(2) \), \( \Delta G^{0}_{298.2} = 8.27(2) \); and \( \Delta S^{0}_{298.2} = -0.1050 \) kJ mol\(^{-1}\) K\(^{-1}\), respectively.

Equation (9):

\[
\Delta U^{0} = U^{0}_{HCN-HF} - U^{0}_{HCN} - U^{0}_{HF} - D_0
\]
where
\[ \Delta U^0 = (U^0 - U^0_0) = \frac{\sum \epsilon_i e^{-\epsilon_i/kT}}{\sum g_i e^{-\epsilon_i/kT}}. \]

**Equation (11):**
\[ \Delta H^0_T = \Delta U^0_T - RT. \]

**Equation (14):**
\[ K_p = \frac{Q_{HCN-HF} N_0 (HCN-HF)}{Q_{HCN} N_0 (HCN) Q_{HF} N_0 (HF)} \]
\[ \frac{1}{kT}, \]

where \( Q \) is the respective total partition function.

**Table I:**
Table I stated experimental temperatures are interchanged:
At 233 K should read At 243 K.
At 243 K should read At 233 K.

---

**TABLE III. Comparison of thermal functions of hydrogen-bond formation at various levels of approximation.**

<table>
<thead>
<tr>
<th></th>
<th>( \Delta U^0 )</th>
<th>( \Delta H^0 )</th>
<th>( \Delta G^0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anharmonic</td>
<td>20.5(2)</td>
<td>-23.0(2)</td>
<td>8.27(2)</td>
</tr>
<tr>
<td>Harmonic</td>
<td>-21.0</td>
<td>-23.4</td>
<td>8.72</td>
</tr>
<tr>
<td>Observed frequencies</td>
<td>-20.7</td>
<td>-23.2</td>
<td>8.15</td>
</tr>
</tbody>
</table>

\( \Delta U^0, \Delta H^0, \Delta G^0 \) in kJ mol\(^{-1}\). 
Comparable estimated errors apply to each column.

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**TABLE IV. Results for the five thermal functions using the anharmonic potential model.**

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>( \Delta U^0 )</th>
<th>( \Delta H^0 )</th>
<th>( \Delta G^0 )</th>
<th>( \Delta S^0_T )</th>
<th>( \Delta C^0_T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.2</td>
<td>-20.5(2)</td>
<td>-23.0(2)</td>
<td>8.27(2)</td>
<td>-0.1050(2)</td>
<td>-0.0077(3)</td>
</tr>
<tr>
<td>250.2</td>
<td>-20.7</td>
<td>-22.8</td>
<td>3.25</td>
<td>-0.1042</td>
<td>-0.0016</td>
</tr>
<tr>
<td>200.2</td>
<td>-21.1</td>
<td>-22.8</td>
<td>1.96</td>
<td>-0.1042</td>
<td>+0.0006</td>
</tr>
<tr>
<td>150.2</td>
<td>-21.5</td>
<td>-22.8</td>
<td>-7.16</td>
<td>-0.1040</td>
<td>-0.0026</td>
</tr>
<tr>
<td>100.2</td>
<td>-21.7</td>
<td>-22.5</td>
<td>-12.32</td>
<td>-0.1018</td>
<td>-0.0081</td>
</tr>
</tbody>
</table>

\( \Delta U^0, \Delta H^0, \Delta G^0, \Delta S^0_T, \Delta C^0_T \) in kJ mol\(^{-1}\). 

* Also to be corrected on p. 5679.

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We thank Professor S. H. Bauer and members of the Thermodynamic Research Center, Texas A&M University for comments and discussion.