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Erratum: Determination of Dissociation Energies and Thermal Functions of Hydrogen Bond Formation Using High Resolution FTIR Spectroscopy [J. Chem. Phys. 87, 5674 (1987)]

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Erratum: Determination of dissociation energies and thermal functions of hydrogen bond formation using high resolution FTIR spectroscopy [J. Chem. Phys. 87, 5674 (1987)]

B. A. Wofford, M. Eliades, S. G. Lieb, and J. W. Bevan

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Erratum: Density expansion in a disordered system and its application in nonlinear optics [J. Chem. Phys. 87, 2413 (1987)]

Z. Deng

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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 Mukamel¹ 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.

¹Z. Deng, J. Grad, and S. Mukamel, J. Chem. Phys. (to be published).

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)]

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Equation (3) should read

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

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.

Erratum: Determination of dissociation energies and thermal functions of hydrogen bond formation using high resolution FTIR spectroscopy [J. Chem. Phys. 87, 5674 (1987)]

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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} : $\Delta U_{298.2}^0 = -20.5(2)$, $\Delta H_{298.2}^0 = -23.0(2)$, $\Delta G_{298.2}^0 = 8.27(2)$; and $\Delta S_{298.2}^0 = -0.1050 \text{ kJ mol}^{-1} \text{ K}^{-1}$, respectively.

Equation (9):

$$\Delta U_T^0 = U_{\text{HCN---HF}}^0 - U_{\text{HCN}}^0 - U_{\text{HF}}^0 - D_0,$$

where

$$\Delta U_0^0 = (U_T^0 - U_0^0) = \frac{\sum_i g_i \epsilon_i e^{-\epsilon_i/kt}}{\sum_i g_i e^{-\epsilon_i/kt}}$$

Equation (11):

$$\Delta H_T^0 = \Delta U_T^0 - RT.$$

Equation (14):

$$K_p = \frac{Q_{\text{HCN--HF}} N_{00}(\text{HCN--HF})}{Q_{\text{HCN}} N_{00}(\text{HCN}) Q_{\text{HF}} N_{00}(\text{HF})} \frac{1}{kT},$$

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.^a

	$\Delta U_{298.16}^0$	$\Delta H_{298.16}^0$	$\Delta G_{298.16}^0$	$\Delta S_{298.16}^0$	$\Delta Cp_{298.16}^0$
Anharmonic approx.	-20.5(2) ^b	-23.0(2)	8.27(2)	-0.1050(2)	-0.0077(3)
Harmonic approx.	-21.0	-23.4	8.72	-0.1079	-0.0062
Observed frequencies	-20.7	-23.2	8.15	-0.1051	-0.0058

^a $\Delta U_{298.16}^0$, $\Delta H_{298.16}^0$, $\Delta G_{298.16}^0$ in kJ mol^{-1} , $\Delta Cp_{298.16}^0$, $\Delta S_{298.16}^0$ in $\text{kJ mol}^{-1} \text{K}^{-1}$.

^b Comparable estimated errors apply to each column.

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

Temperature (K)	ΔU_T^0 (kJ mol^{-1})	ΔH_T^0 (kJ mol^{-1})	ΔG_T^0 (kJ mol^{-1})	ΔS_T^0 ($\text{kJ mol}^{-1} \text{K}^{-1}$)	ΔCp_T^0 ($\text{kJ mol}^{-1} \text{K}^{-1}$)
298.2	-20.5(2)	-23.0(2)	8.27(2)	-0.1050(2) ^a	-0.0077(3)
250.2	-20.7	-22.8	3.25	-0.1042	-0.0016
200.2	-21.1	-22.8	1.96	-0.1042	+0.0006
150.2	-21.5	-22.8	-7.16	-0.1040	-0.0026
100.2	-21.7	-22.5	-12.32	-0.1018	-0.0081

^a Also to be corrected on p. 5679.

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