ADDITIONS AND CORRECTIONS

2002, Volume 106A

M. Ohara, K. Miyajima, A. Pramann, A. Nakajima,* K. Kaya: : Geometric and Electronic Structures of Terbium−Silicon Mixed Clusters (TbSi$_n$; 6 ≤ n ≤ 16)

Page 3703. Incorrect photoelectron (PE) spectra of TbSi$_n^-$ (n = 12−16) were shown in Figure 2. Since the mass difference between TbSi$_n^-$ and Tb$_3$OSi$_{n-12}^-$ is 3 amu, the PE spectra for TbSi$_n^-$ might be contaminated by those for Tb$_3$OSi$_{n-12}^-$ at n ≥ 12, especially when the deceleration processes made the mass separation worse. The corrected PE spectra for TbSi$_n^-$ (n = 12−16) appear below, when the laser vaporization of a Tb rod was controlled not to produce Tb clusters, together with the improvement of mass resolution.

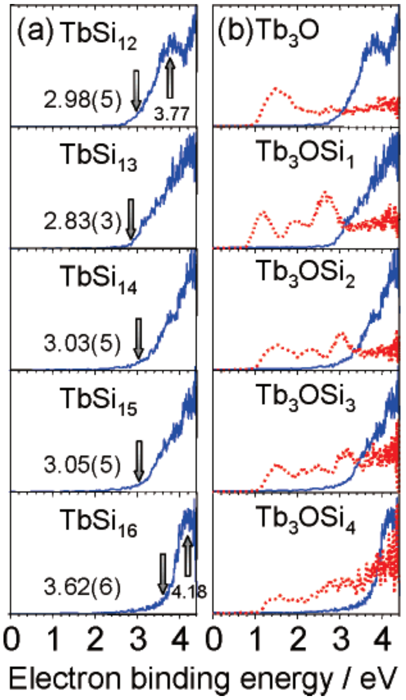

Figure 2. Photoelectron spectra of (a) TbSi$_n^-$ (n = 12−16) and (b) Tb$_3$OSi$_n^-$ (n = 0−4) at 266 nm (4.66 eV). In (b), the spectra of TbSi$_n^-$ were traced together, and the spectra reported previously can be reproduced by the sum of the two spectra.

TABLE 1: Electron Affinities of TbSi$_n$, Si$_n$, Tb$_3$OSi$_{n-12}$, and Clusters in eV

cluster size n	TbSi$_n$	Si$_n$	Tb$_3$OSi$_{n-12}$
6	1.95	1.8[a]	
7	2.08	1.7[a]	
8	2.23	2.3[a]	
9	2.20	2.4[a]	
10	3.60	2.2[a]	
11	3.55	2.5[a]	
12	2.98	2.6[a]	0.91
13	2.83	3.2[b]	0.70
14	3.03	3.2[b]	0.84
15	3.05	3.1[b]	0.98
16	3.62	3.2[b]	1.01

[a] Ref 2. [b] Ref 33.

Page 3704. The electron affinities were reported in Table 1. In this correction, the complete table is reported for TbSi$_n$, Si$_n$, and Tb$_3$OSi$_{n-12}$ (n = 6−16). The PE spectra for TbSi$_n$ feature local maxima of electron affinities of n = 10 and 16.

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Anne-Marie Boulanger, Emma E. Rennie, David M. P. Holland, David A. Shaw, and Paul M. Mayer* : Threshold-Photoelectron Spectroscopic Study of Methyl-Substituted Hydrazine Compounds

Page 8563. The heats of formation of methylhydrazine, 1,1-dimethylhydrazine, and tetramethylhydrazine are reported in Table 6. However, the heat of formation of the ionic methylhydrazine is incorrect and thus is the calculated ionization energy (IE$_a$) of neutral methylhydrazine listed in Table 5. The corrected values are reported in Tables 5 and 6 below. Figure 5 has also been corrected with the proper G3 IE$_a$ of methylhydrazine.

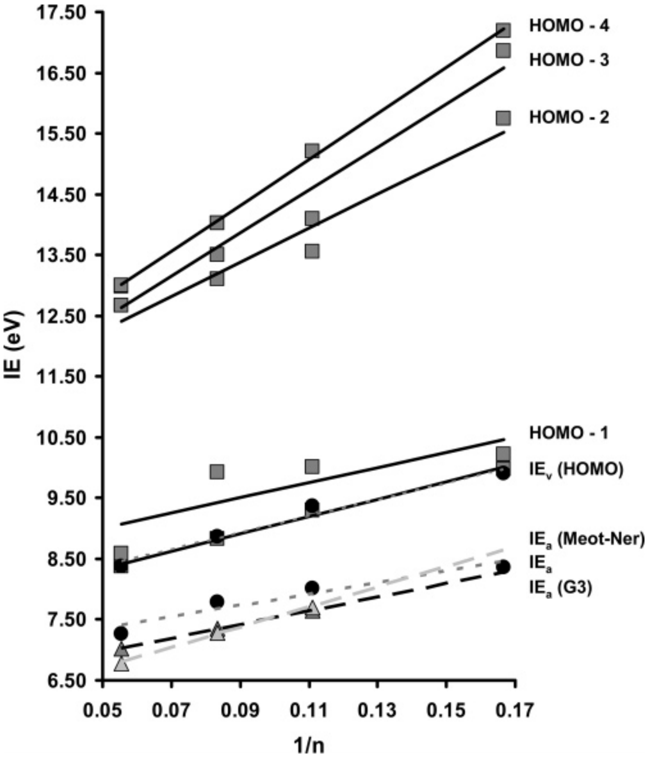

Figure 5. Plot of the experimental ionization energies as a function of the inverse of the size (1/n) of the molecule, including the ionization energies of hydrazine (IE$_v$ = 9.91 eV[10,14] and IE$_a$ = 8.36 eV[14]) as well as the calculated ROVGF energies of the first five highest occupied molecular orbitals (HOMO). The experimental data are shown in (●), the theoretical results for the HOMO are shown in (■), and the G3 and Meot-Ner[15] IEs are shown in (▲).

TABLE 5: Comparison of the Present Experimental Adiabatic and Vertical Ionization Energies with Previously Reported Values and Calculated G3 Adiabatic Ionization Energies

molecule	IE$_a$ (eV)	IE$_v$ (eV)	G3[a] (eV)
methylhydrazine	8.02 ± 0.16[a]	9.36 ± 0.02[a]	7.64
	7.7 ± 0.15[b]	9.32[i]	
	7.67 ± 0.02[c]	8.67[j]	
	8.05[d]	9.30[e]	
	8.40[e]	9.36[k]	
	8.63 ± 0.1[f]		
	7.67 ± 0.02[g]		
	8.00 ± 0.06[g]		
1,1-dimethylhydrazine	7.78 ± 0.16[a]	8.86 ± 0.01[a]	7.36
	7.29 ± 0.04[b]	8.88[l]	
	7.28 ± 0.04[c]	8.88[i]	
	7.87[d]	8.28[j]	
	8.05[e]	8.80[e]	
	8.12 ± 0.1[f]	8.85[k]	
	7.46 ± 0.02[g]		
	7.67 ± 0.05[g]		
tetramethylhydrazine	7.26 ± 0.16[a]	8.38 ± 0.01[a]	7.02
	6.78 ± 0.04[b]	8.43[m]	
	6.87[c]	8.27[i]	
	7.76 ± 0.05[f]	8.26[h]	
	6.87 ± 0.03[h]	7.93[j]	
		8.38[n]	
		8.27[o]	

[a] Present work. [b] Meot-Ner.[15] [c] Lias.[35] [d] Syage.[14] [e] Vovna.[3] [f] Dibeler.[33] [g] Akopyan.[38] [h] Nelsen.[13] [i] Nelsen.[5] [j] Bodor.[28] [k] Kimura.[10] [l] Nelsen.[6] [m] Nelsen.[12] [n] Rademacher.[2] [o] Nelsen.[16]

TABLE 6: Comparison of the Calculated 298 K Heats of Formation of the Neutral and Ion Compounds with Reported Values

	$\Delta_f H°$(neutral) (kJ mol^{-1})		$\Delta_f H°$(ion) (kJ mol^{-1})	
molecule	lit.	G3	lit.[d]	G3
methylhydrazine	94.6 ± 0.6,[a] 81,[b] 96[b]	107	835	844
1,1-dimethylhydrazine	83.9 ± 3.2,[a] 77[b]	94	786	804
tetramethylhydrazine	69.5[c]	95	732	772

[a] Pedley et al.[32] [b] Bohn.[36] [c] Dibeler et al.[33] [d] Lias.[35]

The ionization energies derived from the G3 heats of formation are in rough agreement with those listed by Lias et al.[35] For methylhydrazine, 1,1-dimethylhydrazine, and tetramethylhydrazine the calculated energies are 0.03, 0.08, and 0.15 eV lower than those given by Lias et al.

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Milind M. Deshmukh, Shridhar R. Gadre,* and Libero J. Bartolotti: : Estimation of Intramolecular Hydrogen Bond Energy via Molecular Tailoring Approach

Page 12519. While comparing our recent results with those in this Article, we found some inadvertent errors in reporting the electron density value in Table 1, column 4. Instead of reporting the electron density values at bond critical points (BCP) at MP2/6-311++G(2d,2p) level, in Table 1, column 4, by mistake we have reported the Hartree–Fock (HF), i.e., HF/6-311++G(2d,2p), results. However, this does not affect **either** the main results of the work **or** the hydrogen bond energy values reported using the scheme presented in the paper. The values in Table 1, column 4 (all values in a.u.) (0.02008, 0.02108, 0.02189, 0.02117, 0.02268, 0.03338, 0.02251, 0.02393, 0.02231, 0.02527, 0.02495, 0.02420, 0.01855, 0.00988, and 0.02426) should be replaced by new values (0.02178, 0.02287, 0.02339, 0.02298, 0.02421, 0.03581, 0.02558, 0.02404, 0.02418, 0.02704, 0.02665, 0.02585, 0.02001, 0.01004, and 0.02426), respectively. The corrected revised table is given as Supporting Information that accompanies this erratum on the Internet.

Also on page 12522 of the paper, right-hand side, line number 18, the electron density value (in a.u.) of 0.03338 should be replaced by 0.03581.

Similarly on page 12523 of the paper, left-hand side, line 1, the electron density values (in a.u.) of 0.009 and 0.033 should be replaced by 0.010 and 0.036, respectively.

Also, on p 12523, ref 2 should read “Pauling, L. *J. Am. Chem. Soc.* **1931**, *53*, 1367.”

Supporting Information Available: Corrected Table 1. This material is available free of charge via the Internet at http://pubs.acs.org.

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Leonid Belau, Kevin R. Wilson, Stephen R. Leone, and Musahid Ahmed*: : Vacuum Ultraviolet (VUV) Photoionization of Small Water Clusters

Page 10075. There is an error in calculating the dissociation energies (ΔE) that are reported in Table 1 and Figure 9 of the paper. This arose from using ΔE^+ values for $(H_2O)_n$ ($5 \leq n \leq 9$) from earlier published literature and not from Wang et al.,[1] as stated in the text of the paper. The appearance energy of H_3O^+ in Table A in the Supporting Information should read **11.74 ± 0.05 eV** and not 11.76 ± 0.05 eV. Using the correct ionization energy of **11.74 eV** reported in the text and the proton affinity from the NIST database[2] of **691 kJ/mol** (incorrectly written 690 kJ/mol in the paper) yields a dissociation energy of **19 ± 13 kJ/mol**. Corrections to the ΔE value for $(H_2O)_3$ arise solely from using **11.74 eV** as the ionization energy for H_3O^+. The error bars for the dissociation energies in the original paper did not include the errors in the measurements of the ionization energies (IE) from the experiments. These are included in the revised Table 1 and Figure 9 published here in this Correction. In the Discussion section of the paper, the dimer and trimer dissociation energies for single water loss should

TABLE 1: Experimental Values of Neutral Water Cluster Dissociation Energies for Single Water Molecule Loss: $(H_2O)_n \rightarrow (H_2O)_{n-1} + H_2O$

	dissociation energy (kJ/mol)	
cluster	this work	literature
$(H_2O)_2$	19 ± 13	15.3 ± 2.0[5]
$(H_2O)_3$	81 ± 18	
$(H_2O)_4$	65 ± 19	
$(H_2O)_5$	72 ± 16	
$(H_2O)_6$	50 ± 15	
$(H_2O)_7$	42 ± 15	
$(H_2O)_8$	40 ± 18	
$(H_2O)_9$	36 ± 18	

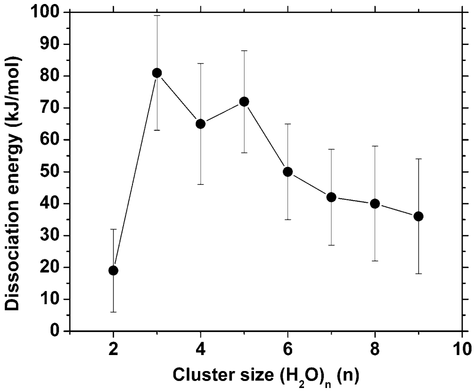

Figure 9. Neutral water cluster dissociation energies, for the process $(H_2O)_n \rightarrow (H_2O)_{n-1} + H_2O$.

read **19 ± 13** and **81 ± 18 kJ/mol**, respectively. (Numbers marked in bold are the correct values.)

A relaxation energy[3] has to be taken into account (assumed to be negligible in the paper) to bring the experimentally determined energies in this work in line with the theoretically calculated dissociation energies.[4,5]

Acknowledgment. We are grateful to Shawn Kathmann and Sotoris Xantheas (Pacific Northwest Laboratory) for pointing out the errors in the calculation of the dissociation energies.

References and Notes

(1) Wang, Y. S.; Tsai, C. H.; Lee, Y. T.; Chang, H. C.; Jiang, J. C.; Asvany, O.; Schlemmer, S.; Gerlich, D. *J. Phys. Chem. A* **2003**, *107*, 4217.

(2) http://webbook.nist.gov.

(3) Personal communication with S. Kathmann and S. Xantheas (Pacific Northwest Laboratory).

(4) Xantheas, S. S.; Burnham, C. J.; Harrison, R. J. *J. Chem. Phys.* **2002**, *116*, 1493.

(5) Xantheas, S. S. *Struc. Bond.* **2005**, *116*, 119.

10.1021/jp077381o