Erratum: Generalized moment expansion for observables of stochastic processes in dimensions *d*>1: Application to Mössbauer spectra of proteins [J. Chem. Phys. 84, 4015 (1986)]

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Erratum: Generalized moment expansion for observables of stochastic processes in dimensions $d>1$: Application to Mössbauer spectra of proteins [J. Chem. Phys. 84, 4015 (1986)]

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In our paper we tried to make a notational distinction between generalized moments μ_n, auxiliary functions $\mu_n(x)$ for the calculation of the generalized moments, and the (boldface written) discretized auxiliary functions $\boldsymbol{\mu}_n$. Due to a printing error this distinction got mixed up. For a better understanding of the paper we, therefore, would like to give the following guidelines for an interpretation of the boldface written quantities $\boldsymbol{\mu}_n(\mathbf{x})$ and $\boldsymbol{\mu}_n$ which occur in the published version of our paper:

(a) The quantities $\boldsymbol{\mu}_n(\mathbf{x})$ in Chap. III are auxiliary functions and should be written as $\mu_n(x)$.

(b) The quantities $\boldsymbol{\mu}_n$ in Eq. (2.27), Eq. (3.2), Eq. (3.28) left-hand side, and in the text on pages 4018 and 4021 are generalized moments and should be written as μ_n.

In addition, we would like to mention that the master-equation discretization we propose has been used before in a one-dimensional case in: N. Agmon and J. J. Hopfield, J. Chem. Phys. **78**, 6947 (1983).

Erratum: Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules [J. Chem. Phys. 82, 2418 (1985); 84, 4113 (E) (1986)]

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Ten of the smaller-basis-set calculations for geometry 2 were performed at an incorrect geometry. The calculations have been repeated for the correct geometry and the results are given in Tables I and II. We also show a corrected version of Fig. 4. There is no significant change in any of the conclusions or discussion.

We are grateful to Mark McGrath for bringing several of the errors to our attention.

TABLE I. Corrections to Tables III and VII.

Basis	$V(G_2)$	$V^{cc}(G_2)$	$V^{pc}(G_2)$
2	1.59	2.65	...
3	1.10	2.29	1.13
4	1.91	2.72	...
5	1.02	2.19	1.23
6	2.06	2.22	2.18
7	0.97	2.19	1.19
8	2.53	2.65	...
11	1.66	2.18	1.79
12	2.04	2.16	2.13
15	1.39	2.30	1.43

TABLE II. Corrections to Tables V and VI.

	$V(G_2)$		$V^{cc}(G_2)$	
	Mean	rms dev.	Mean	rms dev.
Small basis sets	1.45	0.06	2.21	0.59
Medium basis sets	1.87	0.57	2.28	0.14
$E_m > -100.04E_h$	1.56	0.69	2.22	0.52
$-100.04E_h > E_m > -100.06E_h$	1.99	0.31	2.27	0.05

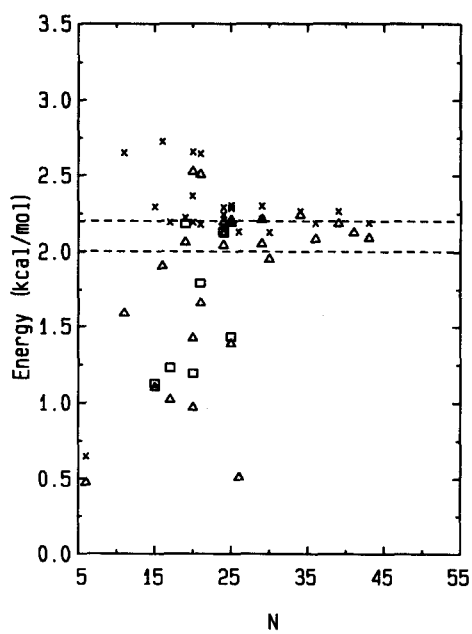

FIG. 4. Energy vs number of basis functions for geometry 2. Note that in Figs. 3 and 4, × marks V^{cc}, △ marks V, and □ marks V^{pc}.

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