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Citation: J. Chem. Phys. 100, 1780 (1994); doi: 10.1063/1.467292

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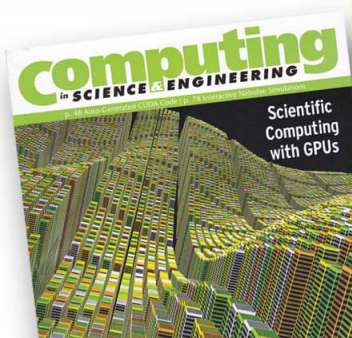
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Erratum: Fluxionality and low-lying transition structures of the water trimer [J. Chem. Phys. 99, 5228 (1993)]

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(Received 1 October 1993; accepted 6 October 1993)

In this work, the basis set superposition errors (BSSE) of the various conformers of $(\text{H}_2\text{O})_3$ were calculated using the full counterpoise (CP) procedure. Defining the three water monomers as X , Y , and Z , one has BSSE $(X-Y-Z) = E(X)_X + E(Y)_Y + E(Z)_Z - E(X)_{XYZ} - E(Y)_{XYZ} - E(Z)_{XYZ}$, where, e.g., $E(X)_X$ represents the energy of X calculated in the basis of X alone, and $E(X)_{XYZ}$ the energy of X calculated in the basis of X plus Y plus Z . The three BSSE contributions of the type $E(X)_X$ were erroneously calculated in the optimized monomer geometry, instead of the optimized geometry in the *trimer*. Hence, the different BSSE contributions and the BSSE corrected binding ener-

gies given in lines 3 to 6 of Table I are incorrect. The corrected Table I is thus presented here.

The CP corrected energies of the $\{uuu\}$, $\{upd\}$, and $\{ppp\}$ structures relative to the minimum-energy $\{uud\}$ structure given in Table II also change slightly. The corrected columns 7 and 8 of Table II are also presented here.

In all cases, the CP corrected and uncorrected energy values (column 7 of Table II) are now closer together, which strengthens the qualitative conclusions presented and discussed. Specifically, the $\{upd\}$ transition structure now lies energetically higher than the $\{uud\}$ structures at both the CP corrected and uncorrected levels.

TABLE I. Calculated binding energy contributions ΔE (kcal/mol) for the equilibrium structure and several transition structures of $(\text{H}_2\text{O})_3$, optimized at the Hartree-Fock (HF) and Møller-Plesset (MP2) levels.

Structure optimization level	$\{uud\}$		$C_3\{uuu\}$		$C_{3h}\{ppp\}$		$\{upd\}^a$
	HF	MP2	HF	MP2	HF	MP2	HF
$\Delta E(\text{HF})$	13.70	13.09	13.20	12.52	13.13	12.96	13.64
$\Delta E(\text{MP2})^b$	3.60	4.69	3.13	4.46	2.60	2.93	3.45
$\delta_{\text{HF}}^{\text{CP}^c}$	-1.22	-1.53	-1.07	-1.45	-0.91	-1.07	-1.16
$\delta_{\text{MP2}}^{\text{CP}^d}$	-2.18	-2.70	-1.86	-2.57	-1.43	-1.63	-2.06
$\delta^{\text{CP}} \equiv \delta_{\text{HF}}^{\text{CP}} + \delta_{\text{MP2}}^{\text{CP}}$	-3.39	-4.22	-2.93	-4.02	-2.33	-2.70	-3.22
$\Delta E(\text{HF}) + \Delta E(\text{MP2}) + \delta^{\text{CP}}$	13.91	13.56	13.41	12.96	13.40	13.19	13.87

^aHF optimized structure only.

^bMP2 contribution; frozen-core approximation employed.

^cCounterpoise correction at HF level.

^dCounterpoise correction at MP2 level.

TABLE II. Overview of $(\text{H}_2\text{O})_3$ calculated interaction energies $\Delta E(\text{cm}^{-1})$ for the stationary and "special" points. Structures are optimized at the HF and MP2 levels, as noted.

Structure	ΔE^{HF^a}	ΔE^{MP2^a}
"Chair" $\{uud\}$	0	0
"Crown" $\{uuu\}$	171(172)	209
"Planar" $\{ppp\}$	177(196)	128
$\{upd\}$	11(20)	
Saddle point		
$\{uup\}$	(140)	
Not stationary		
$\{upp\}$	(126)	
Not stationary		

^aCounterpoise corrected energies, relative to $\{uud\}$ structure; counterpoise uncorrected values in parentheses.