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ADDITION/CORRECTION

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Correction to "Influence of Hybridization and Cooperativity on the Properties of Au-Bonding Interaction: Comparison with Hydrogen Bonds" [*The Journal of Physical Chemistry A* **2011**, *115*, 2853–2858. DOI: 10.1021/jp110777g]. Qingzhong Li,* Hui Li, Ran Li, Bo Jing, Zhenbo Liu, Wenzuo Li, Feng Luan, Jianbo Cheng, Baoan Gong, and Jiazhong Sun

There are small errors in Table 3 of section 3.2 and Table 4 of section 3.3.

The interaction energies between the two molecular pairs in T1 should be calculated with formulas of $\Delta E_{\text{A-BC}} = E_{\text{ABC}} - E_{\text{A}} - E_{\text{BC}} - \Delta E_{\text{A-C}}$, where E_{ABC}, E_{A}, and E_{BC} are the energies of the optimized triad ABC, monomer A, and dyad BC, respectively, while $\Delta E_{\text{A-C}}$ is the interaction energy between A and C obtained as a difference between the energy of AC in the triad and the energy sum of the monomers with all of them frozen in the geometry of the triad.

Similarly, the cooperative energy should be calculated with $E_{\text{coop}} = \Delta E_{\text{total}} - \Delta E_{\text{AB}}(\text{D}) - \Delta E_{\text{BC}}(\text{D}) - \Delta E_{\text{A-C}}$, where ΔE_{total} is the total interaction energy in the triad, $\Delta E_{\text{AB}}(\text{D})$ is the interaction energy in the AB dyad, $\Delta E_{\text{BC}}(\text{D})$ is the interaction energy in the BC dyad, and $\Delta E_{\text{A-C}}$ is the interaction energy between A and C obtained as a difference between the energy of AC in the triad and the energy sum of the monomers with all of them frozen in the geometry of the triad.

The reason for correcting them is that the T1 trimer is cyclic and the interaction energy between A and C is large, as shown in Table 4; thus the interaction between A and C has a great effect on ΔE(O···Au), ΔE(O···HO), and E_{coop} in T1.

The corrected Table 3 and 4 are as follows with corrected data in bold type.

The corresponding discussions in section 3.2 and section 3.3 have been updated (corrections in bold).

At the MP2 level, the interaction energy of the OH···O hydrogen bond is calculated to be −19.67 kJ/mol in the water dimer. It is changed to be **−32.75** kJ/mol in T1. This value in the trimer is increased by about **66%** relative to the water dimer. The interaction energy of Au-bonding in D1 is −117.76 kJ/mol. This value is increased to **−131.11** kJ/mol in T1. The increased percentage is about **11%**. The CCSD method gives a similar increased percentage with the MP2 method for the Au-bonding but a smaller increased percentage than the MP2 method for the OH···O hydrogen bond. The increase of the interaction energy for both types of interactions in T1 indicates that there is interplay between the two interactions in the trimer. Furthermore, the effect of Au-bonding on the hydrogen bond is larger than that of the hydrogen bond on the Au-bonding. These conclusions are similar to those in hydrogen bonds.

The cooperative energy (E_{coop}) is the most effective method for evaluating the cooperativity of Au-bonding and the hydrogen bond. The E_{coop} is calculated to be the difference between the total interaction energy in the trimer and the sum of interaction energy in the respective dimers. The result is also given in Table 4. The E_{coop} value is negative in T1 and T2 but is positive in T3. The negative E_{coop} indicates a positive cooperativity in T1 and T2, while the positive E_{coop} shows a negative cooperativity in T3. The E_{coop} absolute value at the MP2 level is larger than that at the CCSD level. The E_{coop} is calculated to be **−10.08** kJ/mol in T1 at the CCSD level. It amounts to about **7%** of the total interaction energy in the trimer. The synergistic effect in T1 is

Table 4. Two-Body Interaction Energy ($E_{\text{two-body}}$, kJ/mol), Three-Body Interaction Energy ($E_{\text{three-body}}$, kJ/mol), Cooperative Energy (E_{coop}, kJ/mol), and Total Interaction Energy (E_{total}, kJ/mol) in the Trimers at the MP2 and CCSD Levels[a]

	T1		T2		T3	
	MP2	CCSD	MP2	CCSD	MP2	CCSD
$E_{\text{two-body}}$(A−B)	−117.68	−98.42	−118.77	−100.45	−118.81	−100.67
$E_{\text{two-body}}$(B−C)	−15.47	−13.70	−2.40	−2.42	−0.08	−0.09
$E_{\text{two-body}}$(A−C)	−15.48	−13.60	−13.55	−11.39	−8.80	−7.85
$E_{\text{three-body}}$	−20.67	−19.84	−3.71	−3.41	2.10	1.93
E_{coop}	**−12.78**	**−10.08**	−4.01	−2.70	3.02	2.05
E_{total}	−169.30	−145.55	−138.42	−117.67	−125.60	−106.68

[a] Note: Segments A, B, and C are seen in Figure 2.

Table 3. Total Interaction Energy (ΔE_{total}, kJ/mol), Interaction Energy (ΔE, kJ/mol) of Hydrogen Bond and Au-Bonding, and Its Change ($\Delta\Delta E$, kJ/mol) Relative to the Dimers in the Trimers at the MP2 and CCSD Levels[a]

	T1		T2		T3	
	MP2	CCSD	MP2	CCSD	MP2	CCSD
ΔE_{total}	−165.78	−143.92	−137.13	−118.17	−124.56	−107.42
ΔE(O···Au)	**−131.11** (−117.76)	**−112.00** (−101.55)	−121.32 (−117.76)	−103.80 (−101.55)	−114.31 (−117.76)	−99.12 (−101.55)
ΔE(O···HO)	**−32.75** (−19.67)	**−29.00** (−18.69)				
ΔE(π···HO)			−19.36 (−15.35)	−16.62 (−13.92)		
ΔE(O···HC)					−6.69 (−9.82)	−5.77 (−7.92)
$\Delta\Delta E$(O···Au)	**−13.35**	**−10.45**	−3.55	−2.25	3.45	2.43
$\Delta\Delta E$(O···HO)	**−13.08**	**−10.31**				
$\Delta\Delta E$(π···HO)			−4.01	−2.70		
$\Delta\Delta E$(O···HC)					3.13	2.15

[a] Note: Data in parentheses are the interaction energy in the dimers.

more muted than that in the cyclic hydrogen-bonded trimer of HCHO,[23] in which the synergistic effect is about 29%. The value of E_{coop} is small in T2 and T3 (−2.70 and 2.05 kJ/mol at the CCSD level, respectively).

However, we note that all conclusions and other parts of this article are not touched by this error.

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