THE JOURNAL OF PHYSICAL CHEMISTRY A

ADDITION/CORRECTION

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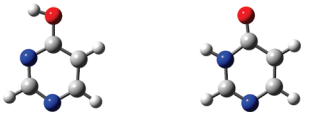
Correction to "Tautomerism in 4-Hydroxypyrimidine, *S*-Methyl-2-thiouracil, and 2-Thiouracil" [*The Journal of Physical Chemistry A* **2010**, *114*, 12725–12730. DOI: 10.1021/jp106883s]. Barbara M. Giuliano, Vitaliy Feyer,* Kevin C. Prince, Marcello Coreno, Luca Evangelisti, Sonia Melandri, and Walther Caminati

The Gibbs free energy (ΔG) reported in Tables 1−3, calculated using the B3LYP and MP2 basis sets, and the corresponding populations (P) are corrected in the tables here.

Table 1. Relative Energies and Populations (%) of 4HP and 4PO, at the B3LYP and MP2 Levels of Approximation, with 6-311++G(d,p) Basis Sets[a]

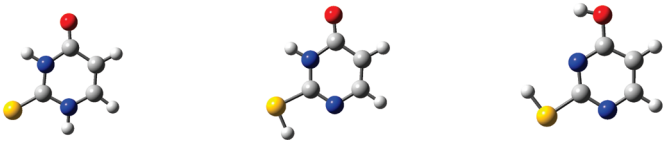
	4HP		4PO	
	B3LYP	MP2	B3LYP	MP2
ΔE/kJ mol^{-1}	8.4	0.0	0.0	4.2
ΔE_{ZPE}/kJ mol^{-1}	8.3	0.0	0.0	3.6
$\Delta G_{(348\ K)}$/kJ mol^{-1}	8.7	0.0	0.0	2.3
$P_{(348\ K)}$/%	4.7	69.1	95.3	30.9
$\Delta G_{(365\ K)}$ /kJ mol^{-1}	8.8	0.0	0.0	2.3
$P_{(365\ K)}$/%	5.3	68.3	94.7	31.7



[a] ΔE = electronic energy difference. ΔE_{ZPE} = zero-point corrected energy difference. ΔG = Gibbs free energy difference calculated at 348 and 365 K. P = population in % of the tautomers, estimated using the calculated ΔG value.

Table 2. Relative Energies and Populations (%) of the Most Stable Species of 2TU, at the B3LYP and MP2 Levels of Approximation, with 6-311++G(d,p) Basis Sets[a]

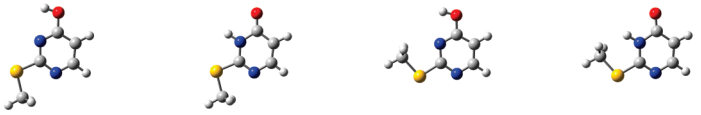
	2TU/diketo		2TU/keto		2TU/enol	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
ΔE/kJ mol^{-1}	0.0	0.0	48.8	36.4	52.3	28.7
ΔE_{ZPE}/kJ mol^{-1}	0.0	0.0	38.2	23.8	42.1	17.4
$\Delta G_{(339\ K)}$/kJ mol^{-1}	0.0	0.0	37.4	19.9	42.2	16.1
$P_{(339\ K)}$/%	100.0	99.4	0.0	0.1	0.0	0.5
$\Delta G_{(435\ K)}$ /kJ mol^{-1}	0.0	0.0	36.8	18.0	42.0	16.0
$P_{(435\ K)}$/%	100.0	98.1	0.0	0.7	0.0	1.2



[a] ΔE = electronic energy difference. ΔE_{ZPE} = zero-point corrected energy difference. ΔG = Gibbs free energy difference calculated at 339 and 435 K. P = population in % of the tautomers, estimated using the calculated ΔG value.

Table 3. Relative Energies and Populations (%) of the Most Stable Species of SM2T, at the B3LYP and MP2 Levels of Approximation, with 6-311++G(d,p) Basis Sets[a]

	SM2T/hydroxyl-1		SM2T/oxo-1		SM2T/hydroxyl-2		SM2T/oxo-2	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
ΔE/kJ mol^{-1}	6.6	0.0	0.0	5.2	9.2	2.7	12.5	18.7
ΔE_{ZPE}/kJ mol^{-1}	6.7	0.0	0.0	4.2	9.1	2.6	12.4	18.7
$\Delta G_{(343\ K)}$/kJ mol^{-1}	8.2	0.0	0.0	1.5	10.6	2.5	13.2	18.4
$P_{(343\ K)}$/%	4.9	48.9	92.2	29.9	2.1	21.1	0.8	0.1
$\Delta G_{(360\ K)}$/kJ mol^{-1}	8.3	0.0	0.0	1.3	10.7	2.5	13.3	18.4
$P_{(360\ K)}$/%	5.4	48.0	91.2	31.1	2.4	20.8	1.0	0.1



[a] ΔE = electronic energy difference. ΔE_{ZPE} = zero-point corrected energy difference. ΔG = Gibbs free energy difference calculated at 343 and 360 K. P = population in % of the tautomers, estimated using the calculated ΔG value.

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