THE JOURNAL OF PHYSICAL CHEMISTRY B

Addition/Correction

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Correction to "Redox Mechanism of Glycosidic-Bond Hydrolysis Catalyzed by 6-Phospho-α-Glucosidase (GlvA): A DFT Study"

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In our previously published article, an error was made in the tables within the article in which Table 2 was mistakenly also reproduced in place of part B of Table 1. The tables should of appeared as given herein.

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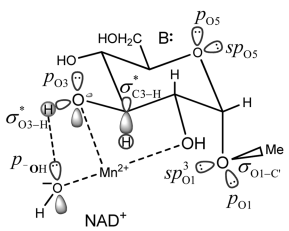
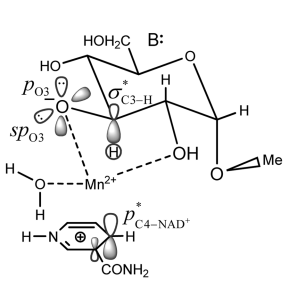
Table 1. B3LYP/6-31G(d) Second-Order Perturbation Estimates (in kJ mol^{-1}) of Hyperconjugative Interactions in Selected Equilibrium Structures of αGlc1Me



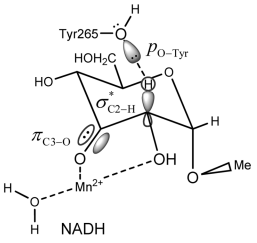
RC

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
	$p_{O3} \rightarrow \sigma^*_{C3-H}$	11.7
	$p_{-OH} \rightarrow \sigma^*_{O3-H}$	79.2
e-endo-An.	$sp_{O5} \rightarrow \sigma^*_{C1-C2}$	9.3
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	4.2
a-endo-An.	$p_{O5} \rightarrow \sigma^*_{C1-O1}$	60.9
	$\sigma_{C2-H} \rightarrow \sigma^*_{C1-O1}$	19.5
exo-An.	$p_{O1} \rightarrow \sigma^*_{C1-O5}$	36.2
	$sp^3_{O1} \rightarrow \sigma^*_{C1-H}$	17.8
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	7.4



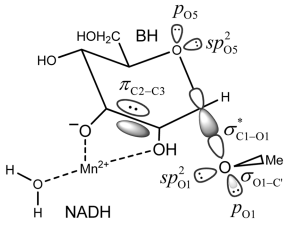
IC1

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
	$p_{O3} \rightarrow \sigma^*_{C3-H}$	33.9
	$\sigma_{C3-H} \rightarrow p^*_{C4-NAD^+}$	0.4
e-endo-An.	$sp_{O5} \rightarrow \sigma^*_{C1-C2}$	10.4
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	4.5
a-endo-An.	$p_{O5} \rightarrow \sigma^*_{C1-O1}$	67.6
	$\sigma_{C2-H} \rightarrow \sigma^*_{C1-O1}$	21.1
exo-An.	$sp^4_{O1} \rightarrow \sigma^*_{C1-O5}$	32.1
	$sp^3_{O1} \rightarrow \sigma^*_{C1-H}$	17.7
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	7.0



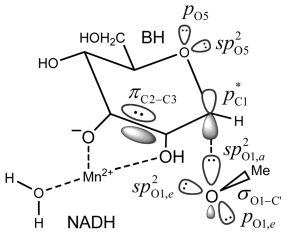
IC2

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
	$\pi_{C3-O} \rightarrow \sigma^*_{C2-H}$	5.6
	$p_{O-Tyr} \rightarrow \sigma^*_{C2-H}$	0.0
e-endo-An.	$sp^2_{O5} \rightarrow \sigma^*_{C1-C2}$	7.7
	$sp^2_{O5} \rightarrow \sigma^*_{C1-H}$	7.5
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	16.6
a-endo-An.	$p_{O5} \rightarrow \sigma^*_{C1-O1}$	53.2
	$\sigma_{C2-H} \rightarrow \sigma^*_{C1-O1}$	21.1
exo-An.	$p_{O1} \rightarrow \sigma^*_{C1-O5}$	44.5
	$sp^2_{O1} \rightarrow \sigma^*_{C1-H}$	15.2
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	8.0



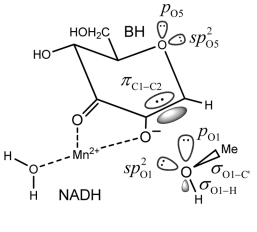
IC3

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
e-endo-An.	$sp^2_{O5} \rightarrow \sigma^*_{C1-C2}$	14.8
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	4.8
a-endo-An.	$p_{O5} \rightarrow \sigma^*_{C1-O1}$	56.3
	$\pi_{C2-C3} \rightarrow \sigma^*_{C1-O1}$	39.0
exo-An.	$p_{O1} \rightarrow \sigma^*_{C1-O5}$	47.0
	$sp^2_{O1} \rightarrow \sigma^*_{C1-H}$	14.6
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	6.2



TS4

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
	$sp^2_{O1,a} \rightarrow p^*_{C1}$	429.2
e-endo-An.	$sp^2_{O5} \rightarrow \sigma^*_{C1-C2}$	23.0
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	7.4
a-endo-An.	$p_{O5} \rightarrow p^*_{C1}$	286.4
	$\pi_{C2-C3} \rightarrow p^*_{C1}$	306.1
exo-An.	$p_{O1} \rightarrow \sigma^*_{C1-O5}$	4.1
	$sp^2_{O1,e} \rightarrow \sigma^*_{C1-O5}$	1.8
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	0.0



IC4···MeOH

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
	$p_{O1} \rightarrow \pi^*_{C1-C2}$	0.0
e-endo-An.	$sp^{1.6}_{O5} \rightarrow \sigma^*_{C1-C2}$	12.4
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	3.7
a-endo-An.	$p_{O5} \rightarrow \pi^*_{C1-C2}$	0.0
exo-An.	$\sigma_{O1-H} \rightarrow \sigma^*_{C1-O5}$	0.0
	$sp^2_{O1} \rightarrow \sigma^*_{C1-H}$	0.0
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	0.0

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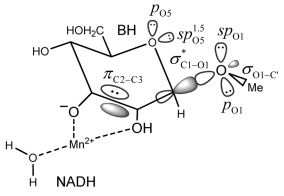
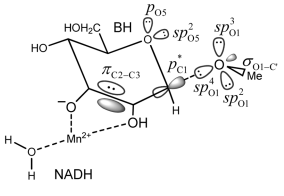
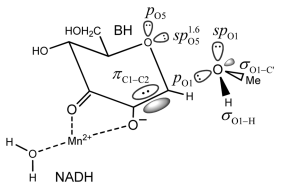
Table 2. B3LYP/6-31G(d) Second-Order Perturbation Estimates (in kJ mol^{-1}) of Hyperconjugative Interactions in Selected Equilibrium Structures of βGlc1Me



IC3



TS4



IC4···MeOH

Component	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$	$i \rightarrow j^*$	$\varepsilon_{i\rightarrow j^*}$
			$sp^4_{O1} \rightarrow p^*_{C1}$	778.0	$p_{O1} \rightarrow \pi^*_{C1-C2}$	0.0
e-endo-An.	$sp^{1.5}_{O5} \rightarrow \sigma^*_{C1-C2}$	10.3	$sp^2_{O5} \rightarrow \sigma^*_{C1-C2}$	27.9	$sp^{1.6}_{O5} \rightarrow \sigma^*_{C1-C2}$	27.6
	$p_{O5} \rightarrow \sigma^*_{C1-C2}$	10.6	$p_{O5} \rightarrow p^*_{C1}$	114.9		
	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	3.4	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	5.4	$\sigma_{C2-O} \rightarrow \sigma^*_{C1-O5}$	7.5
	$sp^{1.5}_{O5} \rightarrow \sigma^*_{C1-O1}$	11.5				
	$\pi_{C2-C3} \rightarrow \sigma^*_{C1-O1}$	16.4	$\pi_{C2-C3} \rightarrow p^*_{C1}$	200.6		
a-endo-An.	$p_{O5} \rightarrow \sigma^*_{C1-H}$	22.6	$p_{O5} \rightarrow \sigma^*_{C1-H}$	18.6	$p_{O5} \rightarrow \pi^*_{C1-C2}$	143.4
	$\pi_{C2-C3} \rightarrow \sigma^*_{C1-H}$	17.8	$\pi_{C2-C3} \rightarrow \sigma^*_{C1-H}$	0.0		
exo-An.	$p_{O1} \rightarrow \sigma^*_{C1-O5}$	59.8	$sp^3_{O1} \rightarrow p^*_{C1}$	44.8		
	$p_{O1} \rightarrow \sigma^*_{C1-H}$	14.3	$sp^2_{O1} \rightarrow p^*_{C1}$	44.1		
	$sp_{O1} \rightarrow \sigma^*_{C1-H}$	10.3				
	$\sigma_{O1-C'} \rightarrow \sigma^*_{C1-C2}$	0.0	$\sigma_{O1-C'} \rightarrow p^*_{C1}$	6.0		

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