

	ΔG_{+W}^o		ΔG_{+A}^o		ΔG_{+S}^o	
	QC	Experimental	QC	Experimental	QC	Experimental
S ₁ A ₁			-7.77 ^a (-7.29 ^b , -7.61 ^c , -6.60 ^d)	- 8.2 ^e	-7.77 ^a (-7.29 ^b , -7.61 ^c , -6.60 ^d)	-8.2 ^e
S ₁ A ₁ W ₁	-1.39 ^a		-6.88 ^a			
S ₁ A ₁ W ₂	-2.30 ^a		-6.18 ^a			
S ₁ A ₁ W ₃	-1.52 ^a		-5.81 ^a			
S ₁ A ₂			-4.75			
S ₁ A ₂ W ₁	-0.78		-4.15			
S ₂ A ₁			-13.84 ^a		-11.65 ^a	
S ₂ A ₁ W ₁	-2.31 ^a		-12.77		-12.59 ^a	
S ₂ A ₁ W ₂	-1.21 ^a		-11.00		-11.52 ^a	
S ₂ A ₁ W ₃	-2.04 ^a		-9.69		-12.04 ^a	
S ₂ A ₂			-8.75		-15.65	
S ₂ A ₂ W ₁	-1.96		-8.37		-16.83	
S ₂ A ₂ W ₂	-1.19		-8.35		-15.49	
S ₂ A ₂ W ₃	0.60		-5.71		-14.42	
S ₂ A ₃			-4.19			
S ₃ A ₁			-16.14		-7.08	
S ₃ A ₂			-13.84		-12.17	
S ₃ A ₃			-8.93		-16.92	
S ₃ A ₄			-7.42			
S ₄ A ₁			-15.74		-4.16	
S ₄ A ₂			-17.16		-7.48	
S ₄ A ₃			-13.79		-12.34	
S ₄ A ₄			-11.34		-16.26	
S ₄ A ₅			-7.63			