

	$\Delta G_{+W}^o$		$\Delta G_{+A}^o$		$\Delta G_{+S}^o$	
	QC	Experimental	QC	Experimental	QC	Experimental
H <sup>+</sup> W <sub>1</sub> S <sub>1</sub>					-28.59	-24.65 <sup>f</sup>
H <sup>+</sup> W <sub>2</sub> S <sub>1</sub>	-15.66				-15.33	-13.76 <sup>f</sup>
H <sup>+</sup> W <sub>3</sub> S <sub>1</sub>	-9.40				-10.12	-11.93 <sup>f</sup>
H <sup>+</sup> W <sub>4</sub> S <sub>1</sub>	-7.83				-9.18	-9.71 <sup>f</sup>
H <sup>+</sup> W <sub>5</sub> S <sub>1</sub>	-6.77	-5.79 <sup>a</sup>			-9.52	-9.82 <sup>f</sup>
H <sup>+</sup> W <sub>6</sub> S <sub>1</sub>	-5.32	-4.24 <sup>a</sup>			-9.70	-9.94 <sup>f</sup>
H <sup>+</sup> W <sub>7</sub> S <sub>1</sub>	-3.18	-3.28 <sup>a</sup>			-9.64	-9.96 <sup>f</sup>
H <sup>+</sup> W <sub>8</sub> S <sub>1</sub>	-2.80	-2.67 <sup>a</sup>			-9.84	-10.10 <sup>f</sup>
H <sup>+</sup> W <sub>9</sub> S <sub>1</sub>	-2.30	-2.12 <sup>a</sup>			-10.24	-10.86 <sup>f</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>1</sub>	-13.47	-13.01 <sup>b</sup> , -11.43 <sup>c</sup>	-52.08			
H <sup>+</sup> A <sub>1</sub> W <sub>2</sub>	-9.85	-7.14 <sup>b</sup> , -8.17 <sup>c</sup>	-33.02			
H <sup>+</sup> A <sub>1</sub> W <sub>3</sub>	-6.60	-5.92 <sup>b</sup> , -5.88 <sup>c</sup>	-25.01			
H <sup>+</sup> A <sub>1</sub> W <sub>4</sub>	-3.50	-3.94 <sup>b</sup> , -4.06 <sup>c</sup>	-19.73			
H <sup>+</sup> A <sub>1</sub> W <sub>5</sub>	-2.50	-2.55 <sup>b</sup> , -3.02 <sup>c</sup>	-15.80			
H <sup>+</sup> A <sub>1</sub> W <sub>6</sub>	-2.26	-2.54 <sup>b</sup>	-12.93			
H <sup>+</sup> A <sub>1</sub> W <sub>7</sub>	-1.15	-1.84 <sup>b</sup>	-10.84			
H <sup>+</sup> A <sub>1</sub> W <sub>8</sub>	-1.02		-9.26			
H <sup>+</sup> A <sub>1</sub> W <sub>9</sub>	0.25		-8.32			
H <sup>+</sup> A <sub>2</sub>			-22.97	-18.25 <sup>c</sup>		
H <sup>+</sup> A <sub>2</sub> W <sub>1</sub>	-7.04	-6.85 <sup>c</sup>	-16.53	-11.54 <sup>c</sup> , -12.75 <sup>d</sup>		
H <sup>+</sup> A <sub>2</sub> W <sub>2</sub>	-4.29	-5.25 <sup>c</sup>	-10.97	-9.13 <sup>c</sup> , -9.50 <sup>d</sup>		
H <sup>+</sup> A <sub>2</sub> W <sub>3</sub>	-3.41	-3.70 <sup>c</sup>	-7.78	-6.83 <sup>c</sup> , -7.02 <sup>d</sup>		
H <sup>+</sup> A <sub>2</sub> W <sub>4</sub>	-3.08		-7.36			
H <sup>+</sup> A <sub>2</sub> W <sub>5</sub>	-1.97		-6.82			
H <sup>+</sup> A <sub>2</sub> W <sub>6</sub>	-0.42		-4.99			
H <sup>+</sup> A <sub>1</sub> W <sub>1</sub> S <sub>1</sub>	-8.99		-33.14		-9.65	-8.3 <sup>d</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>2</sub> S <sub>1</sub>	-8.11		-25.59		-7.90	-7.1 <sup>d</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>3</sub> S <sub>1</sub>	-6.09		-22.28		-7.40	-6.7 <sup>d</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>4</sub> S <sub>1</sub>	-4.25		-18.71		-8.15	-6.9 <sup>d</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>5</sub> S <sub>1</sub>	-1.92		-13.85		-7.56	-7.5 <sup>d</sup>
H <sup>+</sup> A <sub>1</sub> W <sub>6</sub> S <sub>1</sub>	-2.04		-10.57		-7.34	-8.0 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>0</sub> S <sub>1</sub>			-22.09	-22.14 <sup>e</sup>	-13.35	-16.8 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>1</sub> S <sub>1</sub>	-5.72		-18.92		-12.03	-15.8 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>2</sub> S <sub>1</sub>	-4.97		-15.78		-12.71	-15.9 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>3</sub> S <sub>1</sub>	-4.58		-14.27		-13.89	-16.3 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>4</sub> S <sub>1</sub>	-4.26		-14.27		-15.06	-17.3 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>5</sub> S <sub>1</sub>	-2.01		-14.37		-15.11	-18.8 <sup>d</sup>
H <sup>+</sup> A <sub>2</sub> W <sub>6</sub> S <sub>1</sub>	-1.29		-13.63		-15.98	-19.9 <sup>d</sup>