

Supporting Information for:**Computational Electrochemistry:****The Aqueous Ru³⁺|Ru²⁺ Reduction Potential**

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TABLE S1: Partial Atomic Charge (Löwdin Population Analysis) on Ru and Water Molecules in Aqua Complexes ($[\text{Ru}(\text{H}_2\text{O})_n]^{q+}$; $n = 6, 18$; $q = 2, 3$) Determined with Various DFT Methods Combined with LANL2DZ/6-31+G(d,p).

$[\text{Ru}(\text{H}_2\text{O})_6]^{2+}$					$[\text{Ru}(\text{H}_2\text{O})_6]^{3+}$			
GGA	Ru	O _I	H _I	6H ₂ O	Ru	O _I	H _I	6H ₂ O
BLYP	0.40	-0.40	0.34	1.60	0.91	-0.37	0.36	2.09
BP86	0.42	-0.41	0.34	1.58	0.88	-0.37	0.36	2.13
BPBE	0.42	-0.41	0.34	1.58	0.88	-0.37	0.36	2.12
BPW91	0.43	-0.41	0.34	1.58	0.89	-0.37	0.36	2.11
G96LYP	0.46	-0.42	0.34	1.54	0.90	-0.37	0.36	2.09
HCTH	0.47	-0.40	0.33	1.53	0.92	-0.36	0.35	2.08
mPWLYP	0.46	-0.42	0.34	1.54	0.91	-0.37	0.36	2.09
mPWPBE	0.42	-0.41	0.34	1.58	0.88	-0.37	0.36	2.12
mPWPW	0.43	-0.41	0.34	1.58	0.88	-0.37	0.36	2.12
OLYP	0.48	-0.40	0.33	1.52	0.93	-0.36	0.35	2.07
PBE	0.42	-0.41	0.34	1.58	0.88	-0.37	0.36	2.12
H								
B3LYP	0.55	-0.43	0.33	1.44	1.03	-0.39	0.36	1.97
B3P86	0.52	-0.42	0.33	1.48	1.01	-0.38	0.36	1.99
B3PW91	0.53	-0.42	0.33	1.48	1.01	-0.38	0.36	1.99
B97-1	0.56	-0.42	0.33	1.43	1.05	-0.39	0.36	1.95
B97-2	0.55	-0.42	0.33	1.45	1.03	-0.38	0.35	1.97
B98	0.57	-0.42	0.33	1.44	1.06	-0.39	0.36	1.94
BH&HLYP	0.68	-0.43	0.33	1.32	1.19	-0.40	0.35	1.81
mPW1PW	0.54	-0.42	0.33	1.46	1.05	-0.39	0.36	1.95
O3LYP	0.53	-0.41	0.33	1.47	1.00	-0.37	0.35	2.00
PBEh	0.54	-0.42	0.33	1.46	1.03	-0.39	0.36	1.97
MGGA								
BB95	0.42	-0.41	0.34	1.58	0.86	-0.37	0.36	2.14
mPWB95	0.42	-0.41	0.34	1.59	0.86	-0.37	0.36	2.14
mPWKCIS	0.43	-0.41	0.34	1.57	0.88	-0.37	0.36	2.12
PBEKCIS	0.43	-0.41	0.34	1.57	0.88	-0.37	0.36	2.13
TPSSKCIS	0.47	-0.42	0.34	1.53	0.93	-0.38	0.36	2.07
TPSS	0.46	-0.42	0.34	1.54	0.93	-0.38	0.36	2.07
VSXC	0.59	-0.43	0.33	1.41	1.00	-0.38	0.35	2.00
HM								
B1B95	0.55	-0.42	0.33	1.45	1.04	-0.39	0.36	1.97
BB1K	0.61	-0.43	0.33	1.39	1.12	-0.39	0.35	1.88
MPW1B95	0.56	-0.43	0.33	1.44	1.05	-0.39	0.36	1.95
MPW1KCIS	0.50	-0.42	0.33	1.50	0.97	-0.38	0.36	2.02
MPWKCIS1K	0.62	-0.43	0.33	1.39	1.13	-0.39	0.35	1.88
PBE1KCIS	0.54	-0.42	0.33	1.47	1.02	-0.38	0.36	1.98
MPWB1K	0.61	-0.43	0.33	1.38	1.13	-0.40	0.35	1.87
TPSS1KCIS	0.52	-0.42	0.33	1.48	1.01	-0.38	0.36	1.99
TPSSh	0.51	-0.42	0.34	1.50	0.99	-0.38	0.36	2.01

$[\text{Ru}(\text{H}_2\text{O})_{18}]^{2+}$		$[\text{Ru}(\text{H}_2\text{O})_{18}]^{3+}$												
GGA	Ru	O _I	H _I	6H ₂ O	O _{II}	H _{II}	12H ₂ O	Ru	O _I	H _I	6H ₂ O	O _{II}	H _{II}	12H ₂ O
BLYP	0.32	-0.46	0.32	1.04	-0.58	0.32	0.64	0.72	-0.45	0.33	1.28	-0.56	0.32	1.00
BP86	0.26	-0.45	0.31	1.07	-0.58	0.32	0.66	0.68	-0.45	0.33	1.23	-0.56	0.32	1.09
BPBE	0.27	-0.45	0.31	1.05	-0.58	0.32	0.67	0.69	-0.45	0.33	1.26	-0.55	0.32	1.06
BPW91	0.28	-0.45	0.31	1.05	-0.58	0.32	0.67	0.69	-0.45	0.33	1.26	-0.55	0.32	1.05
G96LYP	0.31	-0.46	0.32	1.05	-0.58	0.32	0.64	0.71	-0.45	0.33	1.27	-0.56	0.32	1.01
HCTH	0.33	-0.43	0.31	1.16	-0.57	0.31	0.51	0.73	-0.43	0.33	1.36	-0.55	0.31	0.90
mPWLYP	0.31	-0.46	0.32	1.03	-0.58	0.32	0.66	0.71	-0.45	0.33	1.28	-0.56	0.32	1.01
mPWPBE	0.27	-0.46	0.31	1.04	-0.58	0.32	0.69	0.69	-0.45	0.33	1.25	-0.56	0.32	1.06
mPWPW	0.27	-0.46	0.31	1.04	-0.58	0.32	0.68	0.69	-0.45	0.33	1.25	-0.56	0.32	1.06
OLYP	0.34	-0.43	0.31	1.18	-0.58	0.31	0.49	0.75	-0.43	0.33	1.37	-0.55	0.31	0.88
PBE	0.27	-0.46	0.31	1.03	-0.58	0.32	0.70	0.68	-0.45	0.33	1.25	-0.56	0.32	1.07
H														
B3LYP	0.41	-0.46	0.32	1.00	-0.58	0.31	0.59	0.84	-0.46	0.33	1.23	-0.56	0.32	0.92
B3P86	0.37	-0.46	0.31	0.97	-0.57	0.31	0.66	0.81	-0.46	0.33	1.18	-0.55	0.32	1.01
B3PW91	0.38	-0.46	0.31	1.01	-0.58	0.31	0.61	0.82	-0.46	0.33	1.22	-0.55	0.32	0.97
B97-1	0.42	-0.46	0.31	1.00	-0.58	0.31	0.58	0.86	-0.45	0.33	1.23	-0.56	0.32	0.92
B97-2	0.40	-0.45	0.31	1.04	-0.57	0.31	0.56	0.84	-0.45	0.33	1.25	-0.55	0.31	0.92
B98	0.42	-0.46	0.31	1.00	-0.58	0.31	0.58	0.86	-0.46	0.33	1.22	-0.56	0.32	0.92
BH&HLYP	0.53	-0.47	0.31	0.95	-0.58	0.31	0.52	1.00	-0.46	0.33	1.17	-0.56	0.31	0.83
mPW1PW	0.40	-0.46	0.31	1.00	-0.57	0.31	0.60	0.83	-0.46	0.33	1.18	-0.55	0.32	1.00
O3LYP	0.39	-0.44	0.31	1.12	-0.57	0.31	0.50	0.82	-0.44	0.33	1.30	-0.55	0.31	0.88
PBEh	0.39	-0.46	0.31	0.99	-0.57	0.31	0.62	0.82	-0.46	0.33	1.17	-0.55	0.32	1.00
MGA														
BB95	0.27	-0.46	0.32	1.08	-0.58	0.32	0.65	0.67	-0.45	0.33	1.31	-0.56	0.32	1.02
mPWB95	0.27	-0.46	0.32	1.06	-0.58	0.32	0.67	0.65	-0.45	0.33	1.28	-0.56	0.32	1.06
mPWKCIS	0.28	-0.45	0.32	1.06	-0.58	0.32	0.66	0.68	-0.45	0.33	1.29	-0.56	0.32	1.03
PBEKCIS	0.28	-0.46	0.32	1.05	-0.58	0.32	0.68	0.68	-0.45	0.33	1.28	-0.56	0.32	1.03
TPSSKCIS	0.32	-0.46	0.32	1.03	-0.58	0.32	0.66	0.73	-0.45	0.33	1.26	-0.56	0.32	1.01
TPSS	0.31	-0.46	0.31	1.02	-0.58	0.32	0.67	0.74	-0.45	0.33	1.24	-0.56	0.32	1.03
V5XC	0.48	-0.47	0.33	1.12	-0.58	0.31	0.37	0.85	-0.44	0.34	1.51	-0.57	0.31	0.64
HM														
B1B95	0.41	-0.46	0.31	1.01	-0.58	0.31	0.58	0.85	-0.45	0.33	1.25	-0.56	0.32	0.90
BB1K	0.47	-0.46	0.31	0.98	-0.57	0.31	0.55	0.93	-0.46	0.33	1.21	-0.56	0.31	0.86

MPW1B95	0.42	-0.46	0.31	1.00	-0.58	0.31	0.58	0.87	-0.46	0.33	1.23	-0.56	0.32	0.90
MPW1KCIS	0.36	-0.46	0.31	1.04	-0.58	0.31	0.62	0.78	-0.45	0.33	1.25	-0.56	0.32	0.97
MPWKCSIK	0.47	-0.46	0.31	0.99	-0.57	0.31	0.54	0.93	-0.46	0.33	1.20	-0.55	0.31	0.87
PBEIKCIS	0.39	-0.46	0.31	1.01	-0.58	0.31	0.59	0.82	-0.45	0.33	1.24	-0.56	0.32	0.94
MPWBIK	0.48	-0.46	0.31	0.97	-0.57	0.31	0.56	0.94	-0.46	0.33	1.20	-0.56	0.31	0.86
TPSS1KCIS	0.38	-0.46	0.31	1.01	-0.58	0.31	0.61	0.81	-0.45	0.33	1.23	-0.56	0.32	0.96
TPSSh	0.36	-0.46	0.31	1.01	-0.58	0.32	0.63	0.80	-0.46	0.33	1.22	-0.56	0.32	0.98

TABLE S2: Solvation Free Energy for Optimized Gas-Phase Aqua Complexes and for Partially Optimized Aqua Complex with Ru-O Distances Constrained to Their Experimental Liquid-Phase Values.

All Calculations Were Done with MWB28 and All Values Are In eV.

[Ru(H₂O)₆]²⁺							
	Unconstrained			Constrained			
GGA	ΔG_{EP}	G_{CDS}	ΔG_S	ΔG_{EP}	G_{CDS}	ΔG_S	$\Delta \Delta G_S$
BLYP	-8.63	-0.22	-8.85	-8.67	-0.19	-8.86	0.02
mPWPW	-8.67	-0.22	-8.89	-8.69	-0.20	-8.89	0.00
G96LYP	-8.64	-0.22	-8.86	-8.68	-0.19	-8.87	0.01
OLYP	-8.65	-0.23	-8.88	-8.69	-0.20	-8.89	0.00
H							
mPW1PW	-8.65	-0.21	-8.85	-8.66	-0.20	-8.86	0.00
PBEh	-8.65	-0.21	-8.86	-8.66	-0.20	-8.86	0.00
MGGA							
TPSSKCIS	-8.66	-0.21	-8.87	-8.68	-0.20	-8.88	0.00
HM							
MPWB1K	-8.62	-0.20	-8.82	-8.64	-0.19	-8.84	0.01
MPWKCIS1K	-8.61	-0.21	-8.82	-8.64	-0.19	-8.84	0.02
<i>Average</i>	-8.64	-0.21	-8.86	-8.67	-0.20	-8.86	0.01
<i>Std Dev</i>	0.02	0.00	0.02	0.02	0.00	0.02	0.01
[Ru(H₂O)₆]³⁺							
	Unconstrained			Constrained			
GGA	ΔG_{EP}	G_{CDS}	ΔG_S	ΔG_{EP}	G_{CDS}	ΔG_S	$\Delta \Delta G_S$
BLYP	-19.23	-0.18	-19.41	-19.44	-0.15	-19.59	0.18
mPWPW	-19.33	-0.18	-19.50	-19.46	-0.15	-19.61	0.11
G96LYP	-19.26	-0.18	-19.44	-19.45	-0.15	-19.60	0.16
OLYP	-19.32	-0.19	-19.51	-19.49	-0.16	-19.65	0.14
H							
mPW1PW	-19.40	-0.17	-19.57	-19.51	-0.15	-19.67	0.10
PBEh	-19.41	-0.17	-19.58	-19.51	-0.15	-19.66	0.09
MGGA							
TPSSKCIS	-19.32	-0.18	-19.50	-19.46	-0.15	-19.61	0.11
HM							
MPWB1K	-19.47	-0.16	-19.64	-19.55	-0.15	-19.70	0.07
MPWKCIS1K	-19.44	-0.17	-19.61	-19.55	-0.15	-19.70	0.10
<i>Average</i>	-19.35	-0.17	-19.53	-19.49	-0.15	-19.64	0.12
<i>Std Dev</i>	0.08	0.01	0.07	0.04	0.00	0.04	0.03

[Ru(H₂O)₁₈]²⁺							
	Unconstrained			Constrained			
GGA	ΔG_{EP}	G_{CDS}	ΔG_S	ΔG_{EP}	G_{CDS}	ΔG_S	$\Delta \Delta G_S$
BLYP	-6.24	-0.79	-7.03	-6.23	-0.74	-6.97	-0.06
mPWPW	-6.28	-0.77	-7.05	-6.24	-0.76	-7.00	-0.05
G96LYP	-6.23	-0.79	-7.03	-6.23	-0.75	-6.98	-0.05
OLYP	-6.11	-0.94	-7.04	-6.19	-0.75	-6.94	-0.10
H							
mPW1PW	-6.19	-0.77	-6.95	-6.16	-0.76	-6.92	-0.03
PBEh	-6.20	-0.76	-6.96	-6.16	-0.76	-6.93	-0.03
MGGA							
TPSSKCIS	-6.25	-0.77	-7.02	-6.22	-0.75	-6.97	-0.05
HM							
MPWB1K	-6.12	-0.77	-6.89	-6.12	-0.76	-6.88	0.00
MPWKCIS1K	-6.12	-0.78	-6.90	-6.12	-0.76	-6.88	-0.02
<i>Average</i>	-6.19	-0.79	-6.98	-6.18	-0.76	-6.94	-0.04
<i>Std Dev</i>	0.06	0.05	0.06	0.04	0.00	0.04	0.03

[Ru(H₂O)₁₈]³⁺							
	Unconstrained			Constrained			
GGA	ΔG_{EP}	G_{CDS}	ΔG_S	ΔG_{EP}	G_{CDS}	ΔG_S	$\Delta \Delta G_S$
BLYP	-13.30	-0.73	-14.03	-13.30	-0.72	-14.01	-0.02
mPWPW	-13.40	-0.71	-14.11	-13.32	-0.73	-14.05	-0.06
G96LYP	-13.31	-0.74	-14.05	-13.31	-0.72	-14.03	-0.01
OLYP	-12.84	-1.05	-13.89	-13.30	-0.72	-14.02	0.13
H							
mPW1PW	-13.40	-0.71	-14.12	-13.36	-0.73	-14.09	-0.03
PBEh	-13.42	-0.71	-14.13	-13.36	-0.73	-14.09	-0.04
MGGA							
TPSSKCIS	-13.37	-0.72	-14.09	-13.32	-0.72	-14.05	-0.04
HM							
MPWB1K	-13.38	-0.71	-14.09	-13.38	-0.73	-14.11	0.02
MPWKCIS1K	-13.37	-0.73	-14.10	-13.38	-0.73	-14.11	-0.01
<i>Average</i>	-13.31	-0.76	-14.07	-13.34	-0.73	-14.06	-0.02
<i>Std Dev</i>	0.18	0.11	0.07	0.03	0.01	0.04	0.03

TABLE S3: Individual Aqueous Solvation Free Energies Calculated with SM6 Employing Various DFT Methods and Basis Sets at Gas-Phase

Geometries When the First or First and Second Hydration Shells Are Included Explicitly. All Values Are in eV.

GGA	$[\text{Ru}(\text{H}_2\text{O})_6]^{2+}$				$[\text{Ru}(\text{H}_2\text{O})_6]^{3+}$				TZQ	
	LANL2DZ	DZQ	MWB28	TZQS	TZQ	LANL2DZ	DZQ	MWB28		TZQS
BLYP	-8.81	-8.80	-8.85	-8.84	-8.84	-19.50	-19.38	-19.41	-19.43	-19.42
BP86	-8.86	-8.85	-8.89	-8.89	-8.89	-19.59	-19.47	-19.50	-19.52	-19.52
BPBE	-8.87	-8.85	-8.90	-8.89	-8.89	-19.60	-19.47	-19.50	-19.53	-19.52
BPW91	-8.86	-8.85	-8.89	-8.89	-8.89	-19.59	-19.47	-19.50	-19.52	-19.52
G96LYP	-8.83	-8.82	-8.86	-8.85	-8.85	-19.52	-19.41	-19.44	-19.45	-19.45
HCTH	-8.87	-8.84	-8.89	-8.88	-8.88	-19.65	-19.50	-19.54	-19.56	-19.56
mPWLYP	-8.81	-8.80	-8.85	-8.84	-8.84	-19.50	-19.39	-19.42	-19.43	-19.43
mPWPBE	-8.87	-8.85	-8.89	-8.89	-8.89	-19.60	-19.48	-19.51	-19.53	-19.53
mPWPW91	-8.86	-8.85	-8.89	-8.88	-8.88	-19.59	-19.47	-19.50	-19.53	-19.52
OLYP	-8.86	-8.84	-8.88	-8.88	-8.88	-19.61	-19.47	-19.51	-19.53	-19.53
PBEPBE	-8.86	-8.85	-8.89	-8.89	-8.89	-19.60	-19.48	-19.51	-19.53	-19.53
<i>Average</i>	-8.85	-8.84	-8.88	-8.87	-8.87	-19.58	-19.45	-19.49	-19.50	-19.50
<i>Std Dev</i>	0.02	0.02	0.02	0.02	0.02	0.05	0.04	0.04	0.05	0.04
H										
B3LYP	-8.80	-8.78	-8.82	-8.81	-8.81	-19.63	-19.46	-19.48	-19.50	-19.50
B3P86	-8.85	-8.82	-8.87	-8.86	-8.86	-19.72	-19.54	-19.57	-19.62	-19.62
B3PW91	-8.84	-8.82	-8.86	-8.85	-8.85	-19.70	-19.52	-19.55	-19.60	-19.60
B97-1	-8.81	-8.79	-8.84	-8.82	-8.82	-19.62	-19.48	-19.50	-19.52	-19.52
B97-2	-8.84	-8.81	-8.85	-8.85	-8.85	-19.72	-19.57	-19.59	-19.62	-19.62
B98	-8.81	-8.79	-8.84	-8.82	-8.82	-19.62	-19.49	-19.51	-19.53	-19.53
BH&HLYP	-8.75	-8.72	-8.77	-8.76	-8.76	-19.74	-19.59	-19.60	-19.63	-19.63
mPW1PW91	-8.83	-8.81	-8.85	-8.85	-8.85	-19.69	-19.55	-19.57	-19.60	-19.59
O3LYP	-8.84	-8.81	-8.86	-8.85	-8.85	-19.66	-19.52	-19.55	-19.58	-19.58
PBE1PBE	-8.84	-8.82	-8.86	-8.85	-8.85	-19.73	-19.55	-19.58	-19.63	-19.60
<i>Average</i>	-8.82	-8.80	-8.84	-8.83	-8.83	-19.68	-19.53	-19.55	-19.58	-19.58
<i>Std Dev</i>	0.03	0.03	0.03	0.03	0.03	0.05	0.04	0.04	0.05	0.05
MGA										
BB95	-8.85	-8.84	-8.88	-8.87	-8.87	-19.56	-19.45	-19.48	-19.50	-19.50
mPWB95	-8.84	-8.83	-8.87	-8.87	-8.87	-19.57	-19.45	-19.49	-19.51	-19.51
mPWKCIS	-8.85	-8.84	-8.88	-8.87	-8.87	-19.56	-19.44	-19.47	-19.49	-19.49

PBEKCIS	-8.85	-8.83	-8.88	-8.87	-8.87	-19.56	-19.44	-19.47	-19.49	-19.49
TPSSKCIS	-8.85	-8.83	-8.87	-8.87	-8.87	-19.60	-19.47	-19.50	-19.52	-19.52
TPSS	-8.86	-8.84	-8.88	-8.88	-8.88	-19.62	-19.49	-19.52	-19.55	-19.55
VSXC	-8.76	-8.73	-8.76	-8.76	-8.76	-19.65	-19.51	-19.54	-19.55	-19.55
<i>Average</i>	-8.84	-8.82	-8.86	-8.86	-8.86	-19.59	-19.46	-19.50	-19.52	-19.51
<i>Std Dev</i>	0.04	0.04	0.04	0.04	0.04	0.03	0.03	0.03	0.03	0.03
HM										
BIB95	-8.82	-8.80	-8.84	-8.83	-8.83	-19.72	-19.54	-19.57	-19.59	-19.59
BBIK	-8.81	-8.78	-8.83	-8.82	-8.81	-19.76	-19.61	-19.62	-19.65	-19.65
MPWIB95	-8.82	-8.80	-8.84	-8.83	-8.83	-19.74	-19.56	-19.58	-19.61	-19.61
MPWIKCIS	-8.83	-8.81	-8.86	-8.85	-8.85	-19.65	-19.51	-19.53	-19.56	-19.56
MPWKCIS1K	-8.80	-8.77	-8.82	-8.81	-8.81	-19.75	-19.59	-19.61	-19.64	-19.64
PBEIKCIS	-8.83	-8.80	-8.85	-8.84	-8.84	-19.68	-19.54	-19.56	-19.59	-19.59
MPWB1K	-8.81	-8.78	-8.82	-8.81	-8.81	-19.77	-19.62	-19.64	-19.67	-19.67
TPSS1KCIS	-8.84	-8.81	-8.86	-8.85	-8.85	-19.67	-19.50	-19.53	-19.57	-19.56
TPSSh	-8.85	-8.83	-8.87	-8.87	-8.87	-19.67	-19.51	-19.54	-19.57	-19.57
<i>Average</i>	-8.82	-8.80	-8.84	-8.83	-8.83	-19.71	-19.55	-19.58	-19.61	-19.60
<i>Std Dev</i>	0.02	0.02	0.02	0.02	0.02	0.05	0.04	0.04	0.04	0.04

	$[\text{Ru}(\text{H}_2\text{O})_{18}]^{2+}$					$[\text{Ru}(\text{H}_2\text{O})_{18}]^{3+}$				
GGA	LANL2DZ	DZQ	MWB28	TZQS	TZQ	LANL2DZ	DZQ	MWB28	TZQS	TZQ
BLYP	-6.94	-6.94	-7.03	-7.02	-7.02	-14.09	-14.04	-14.03	-14.01	-14.01
BP86	-6.99	-6.98	-7.07	-7.06	-7.06	-14.19	-14.15	-14.14	-14.12	-14.12
BPBE	-6.97	-6.96	-7.04	-7.04	-7.04	-14.16	-14.12	-14.10	-14.08	-14.08
BPW91	-6.97	-6.96	-7.04	-7.04	-7.03	-14.16	-14.11	-14.10	-14.08	-14.08
G96LYP	-6.95	-6.94	-7.03	-7.02	-7.02	-14.11	-14.06	-14.05	-14.03	-14.03
HCTH	-6.97	-6.96	-7.01	-7.03	-7.03	-14.03	-13.98	-13.95	-13.93	-13.93
mPWLYP	-6.94	-6.93	-7.03	-7.02	-7.02	-14.10	-14.05	-14.04	-14.03	-14.03
mPWPBE	-6.97	-6.96	-7.05	-7.04	-7.04	-14.17	-14.13	-14.12	-14.10	-14.10
mPWPW	-6.97	-6.96	-7.05	-7.04	-7.04	-14.17	-14.12	-14.11	-14.09	-14.09
OLYP	-7.00	-6.99	-7.04	-7.08	-7.08	-13.95	-13.93	-13.89	-13.90	-13.91
PBEPBE	-6.97	-6.96	-7.06	-7.05	-7.05	-14.18	-14.13	-14.12	-14.10	-14.11
Average	-6.97	-6.96	-7.04	-7.04	-7.04	-14.12	-14.07	-14.06	-14.04	-14.04
Std Dev	0.02	0.02	0.02	0.02	0.02	0.08	0.07	0.08	0.07	0.07
H										
B3LYP	-6.88	-6.87	-6.95	-6.94	-6.94	-14.14	-14.09	-14.05	-14.05	-14.04
B3P86	-6.92	-6.91	-6.99	-6.97	-6.97	-14.24	-14.18	-14.16	-14.14	-14.14
B3PW91	-6.90	-6.89	-6.96	-6.96	-6.96	-14.19	-14.14	-14.11	-14.09	-14.09
B97-1	-6.89	-6.88	-6.95	-6.94	-6.94	-14.15	-14.10	-14.06	-14.05	-14.05
B97-2	-6.90	-6.88	-6.94	-6.94	-6.94	-14.15	-14.10	-14.06	-14.04	-14.04
B98	-6.88	-6.87	-6.94	-6.94	-6.94	-14.15	-14.10	-14.06	-14.05	-14.05
BH&HLYP	-6.83	-6.81	-6.87	-6.86	-6.86	-14.21	-14.15	-14.09	-14.08	-14.08
mPWIPW	-6.89	-6.88	-6.95	-6.94	-6.94	-14.19	-14.15	-14.12	-14.10	-14.10
O3LYP	-6.94	-6.93	-6.98	-7.00	-7.00	-13.96	-13.92	-13.89	-13.90	-13.90
PBEh	-6.90	-6.89	-6.96	-6.95	-6.95	-14.20	-14.16	-14.13	-14.11	-14.11
Average	-6.89	-6.88	-6.95	-6.94	-6.94	-14.16	-14.11	-14.07	-14.06	-14.06
Std Dev	0.03	0.03	0.03	0.03	0.04	0.08	0.07	0.07	0.06	0.06
MGGA										
BB95	-6.96	-6.95	-7.03	-7.03	-7.03	-14.11	-14.06	-14.05	-14.02	-14.02
mPWB95	-6.95	-6.94	-7.03	-7.03	-7.03	-14.11	-14.07	-14.07	-14.04	-14.04
mPWKCIS	-6.96	-6.95	-7.04	-7.03	-7.03	-14.13	-14.08	-14.07	-14.05	-14.05
PBEKCIS	-6.96	-6.95	-7.05	-7.04	-7.04	-14.13	-14.08	-14.07	-14.06	-14.06
TPSSKCIS	-6.95	-6.94	-7.02	-7.02	-7.01	-14.15	-14.10	-14.09	-14.07	-14.07
TPSS	-6.95	-6.94	-7.02	-7.02	-7.02	-14.18	-14.13	-14.11	-14.09	-14.09

VSXC	-6.44	-6.36	-6.31	-6.35	-6.35	-13.89	-13.80	-13.69	-13.69	-13.69
<i>Average</i>	-6.88	-6.86	-6.93	-6.93	-6.93	-14.10	-14.05	-14.02	-14.00	-14.00
<i>Std Dev</i>	0.19	0.22	0.27	0.26	0.26	0.10	0.11	0.15	0.14	0.14
HM										
BIB95	-6.87	-6.86	-6.93	-6.91	-6.91	-14.15	-14.10	-14.06	-14.06	-14.03
BB1K	-6.85	-6.83	-6.89	-6.91	-6.91	-14.19	-14.13	-14.08	-14.08	-14.05
MPW1B95	-6.86	-6.85	-6.92	-6.92	-6.93	-14.16	-14.11	-14.07	-14.07	-14.04
MPW1KCIS	-6.91	-6.90	-6.95	-6.97	-6.97	-14.14	-14.09	-14.07	-14.07	-14.05
MPWKCIS1K	-6.86	-6.84	-6.90	-6.89	-6.89	-14.20	-14.14	-14.10	-14.10	-14.07
PBE1KCIS	-6.89	-6.88	-6.96	-6.95	-6.95	-14.16	-14.11	-14.08	-14.08	-14.06
MPWBIK	-6.84	-6.83	-6.89	-6.88	-6.90	-14.20	-14.14	-14.09	-14.09	-14.05
TPSS1KCIS	-6.91	-6.89	-6.97	-6.97	-6.97	-14.17	-14.11	-14.08	-14.08	-14.06
TPSSh	-6.92	-6.91	-6.98	-6.98	-6.98	-14.19	-14.14	-14.11	-14.11	-14.09
<i>Average</i>	-6.88	-6.87	-6.93	-6.93	-6.93	-14.17	-14.12	-14.08	-14.08	-14.06
<i>Std Dev</i>	0.03	0.03	0.04	0.04	0.03	0.02	0.02	0.02	0.02	0.02

TABLE S4: Components (ΔG_{EP} and G_{CDS}) of Aqueous Solvation Free Energies Calculated with SM6 For Various Functionals and Basis Sets at Gas-Phase Geometries When the First or First and Second Hydration Shells are Included Explicitly. All Values are in eV.

[Ru(H₂O)₆]²⁺	LANL2DZ		DZQ		MWB28		TZQS		TZQ	
	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}
GGA										
BLYP	-8.59	-0.22	-8.58	-0.22	-8.63	-0.22	-8.62	-0.22	-8.61	-0.22
BP86	-8.65	-0.22	-8.63	-0.22	-8.68	-0.21	-8.67	-0.22	-8.67	-0.22
BPBE	-8.65	-0.22	-8.63	-0.22	-8.68	-0.21	-8.67	-0.22	-8.67	-0.22
BPW91	-8.64	-0.22	-8.63	-0.22	-8.67	-0.22	-8.67	-0.22	-8.67	-0.22
G96LYP	-8.61	-0.23	-8.59	-0.23	-8.64	-0.22	-8.63	-0.23	-8.63	-0.22
HCTH	-8.63	-0.23	-8.61	-0.23	-8.66	-0.22	-8.65	-0.23	-8.65	-0.22
mPWLYP	-8.59	-0.22	-8.58	-0.22	-8.63	-0.22	-8.61	-0.22	-8.61	-0.22
mPWPBE	-8.65	-0.22	-8.63	-0.22	-8.68	-0.21	-8.67	-0.22	-8.67	-0.22
mPWPW	-8.64	-0.22	-8.63	-0.22	-8.67	-0.22	-8.67	-0.22	-8.67	-0.22
OLYP	-8.62	-0.23	-8.60	-0.23	-8.65	-0.23	-8.65	-0.23	-8.65	-0.23
PBEPBE	-8.65	-0.22	-8.63	-0.22	-8.68	-0.21	-8.67	-0.22	-8.67	-0.22
H										
B3LYP	-8.58	-0.22	-8.56	-0.22	-8.61	-0.21	-8.59	-0.22	-8.59	-0.22
B3P86	-8.64	-0.21	-8.61	-0.21	-8.66	-0.21	-8.65	-0.21	-8.65	-0.21
B3PW91	-8.63	-0.21	-8.60	-0.21	-8.65	-0.21	-8.64	-0.21	-8.64	-0.21
B97-1	-8.60	-0.21	-8.57	-0.22	-8.62	-0.21	-8.61	-0.22	-8.61	-0.22
B97-2	-8.62	-0.22	-8.59	-0.22	-8.64	-0.21	-8.63	-0.22	-8.63	-0.22
B98	-8.60	-0.21	-8.57	-0.22	-8.62	-0.21	-8.61	-0.21	-8.61	-0.21
BH&HLYP	-8.54	-0.21	-8.51	-0.21	-8.57	-0.21	-8.55	-0.21	-8.55	-0.21
mPW1PW	-8.62	-0.21	-8.60	-0.21	-8.65	-0.21	-8.64	-0.21	-8.64	-0.21
O3LYP	-8.62	-0.22	-8.59	-0.23	-8.64	-0.22	-8.63	-0.22	-8.63	-0.22
PBEh	-8.63	-0.21	-8.60	-0.21	-8.65	-0.21	-8.64	-0.21	-8.64	-0.21
MGGA										
BB95	-8.63	-0.22	-8.62	-0.22	-8.66	-0.21	-8.65	-0.22	-8.65	-0.22
mPWB95	-8.63	-0.21	-8.62	-0.22	-8.66	-0.21	-8.65	-0.22	-8.65	-0.22
mPWKCIS	-8.63	-0.22	-8.61	-0.23	-8.66	-0.22	-8.65	-0.22	-8.65	-0.22
PBEKCIS	-8.63	-0.22	-8.61	-0.22	-8.66	-0.22	-8.65	-0.22	-8.65	-0.22
TPSSKCIS	-8.63	-0.22	-8.61	-0.22	-8.66	-0.21	-8.65	-0.22	-8.65	-0.22
TPSS	-8.65	-0.21	-8.63	-0.21	-8.67	-0.21	-8.67	-0.21	-8.67	-0.21
VSXC	-8.56	-0.19	-8.53	-0.20	-8.57	-0.19	-8.56	-0.20	-8.56	-0.20
HM										
B1B95	-8.62	-0.21	-8.59	-0.21	-8.63	-0.21	-8.62	-0.21	-8.62	-0.21
BB1K	-8.60	-0.21	-8.57	-0.21	-8.62	-0.20	-8.61	-0.21	-8.61	-0.21
MPW1B95	-8.61	-0.21	-8.59	-0.21	-8.63	-0.21	-8.62	-0.21	-8.62	-0.21
MPW1KCIS	-8.62	-0.22	-8.59	-0.22	-8.64	-0.22	-8.63	-0.22	-8.63	-0.22
MPWKCIS1K	-8.59	-0.21	-8.56	-0.21	-8.61	-0.21	-8.60	-0.21	-8.60	-0.21
PBE1KCIS	-8.61	-0.21	-8.58	-0.22	-8.63	-0.21	-8.62	-0.21	-8.62	-0.21
MPWB1K	-8.60	-0.20	-8.57	-0.21	-8.62	-0.20	-8.61	-0.20	-8.61	-0.20
TPSS1KCIS	-8.62	-0.21	-8.60	-0.22	-8.65	-0.21	-8.64	-0.21	-8.64	-0.21
TPSSh	-8.64	-0.21	-8.62	-0.21	-8.66	-0.21	-8.66	-0.21	-8.66	-0.21

[Ru(H₂O)₆]³⁺	LANL2DZ		DZQ		MWB28		TZQS		TZQ	
GGA	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}
BLYP	-19.31	-0.19	-19.19	-0.19	-19.23	-0.18	-19.24	-0.19	-19.24	-0.19
BP86	-19.41	-0.18	-19.28	-0.18	-19.32	-0.18	-19.34	-0.18	-19.34	-0.18
BPBE	-19.42	-0.18	-19.29	-0.18	-19.33	-0.18	-19.35	-0.18	-19.34	-0.18
BPW91	-19.41	-0.18	-19.28	-0.18	-19.32	-0.18	-19.34	-0.18	-19.34	-0.18
G96LYP	-19.34	-0.19	-19.22	-0.19	-19.26	-0.18	-19.27	-0.19	-19.27	-0.18
HCTH	-19.46	-0.19	-19.31	-0.19	-19.35	-0.18	-19.37	-0.19	-19.37	-0.19
mPWLYP	-19.32	-0.19	-19.20	-0.19	-19.24	-0.18	-19.25	-0.19	-19.25	-0.18
mPWPBE	-19.42	-0.18	-19.30	-0.18	-19.33	-0.18	-19.35	-0.18	-19.35	-0.18
mPWPW	-19.41	-0.18	-19.29	-0.18	-19.33	-0.18	-19.35	-0.18	-19.35	-0.18
OLYP	-19.42	-0.19	-19.28	-0.19	-19.32	-0.19	-19.34	-0.19	-19.34	-0.19
PBEPBE	-19.42	-0.18	-19.29	-0.18	-19.33	-0.18	-19.35	-0.18	-19.35	-0.18
H										
B3LYP	-19.46	-0.18	-19.28	-0.18	-19.31	-0.17	-19.33	-0.17	-19.33	-0.17
B3P86	-19.55	-0.17	-19.37	-0.17	-19.40	-0.17	-19.45	-0.17	-19.45	-0.17
B3PW91	-19.52	-0.17	-19.35	-0.17	-19.38	-0.17	-19.43	-0.17	-19.43	-0.17
B97-1	-19.45	-0.17	-19.30	-0.18	-19.33	-0.17	-19.35	-0.17	-19.35	-0.17
B97-2	-19.54	-0.18	-19.39	-0.18	-19.42	-0.18	-19.45	-0.18	-19.45	-0.18
B98	-19.45	-0.17	-19.31	-0.18	-19.33	-0.17	-19.36	-0.17	-19.36	-0.17
BH&HLYP	-19.57	-0.17	-19.41	-0.18	-19.43	-0.17	-19.46	-0.17	-19.46	-0.17
mPW1PW	-19.52	-0.17	-19.38	-0.17	-19.40	-0.17	-19.43	-0.17	-19.43	-0.17
O3LYP	-19.48	-0.18	-19.34	-0.19	-19.37	-0.18	-19.40	-0.18	-19.40	-0.18
PBEh	-19.56	-0.17	-19.38	-0.17	-19.41	-0.17	-19.46	-0.17	-19.44	-0.17
MGGA										
BB95	-19.38	-0.18	-19.26	-0.19	-19.30	-0.18	-19.32	-0.18	-19.32	-0.18
mPWB95	-19.39	-0.18	-19.27	-0.18	-19.31	-0.18	-19.33	-0.18	-19.33	-0.18
mPWKCIS	-19.38	-0.19	-19.25	-0.19	-19.29	-0.18	-19.31	-0.18	-19.31	-0.18
PBEKCIS	-19.38	-0.19	-19.25	-0.19	-19.29	-0.18	-19.30	-0.18	-19.30	-0.18
TPSSKCIS	-19.42	-0.18	-19.29	-0.18	-19.32	-0.18	-19.34	-0.18	-19.34	-0.18
TPSS	-19.45	-0.18	-19.31	-0.18	-19.35	-0.17	-19.37	-0.18	-19.37	-0.18
VSXC	-19.46	-0.18	-19.33	-0.18	-19.36	-0.18	-19.37	-0.18	-19.37	-0.18
HM										
B1B95	-19.55	-0.17	-19.37	-0.17	-19.40	-0.17	-19.42	-0.17	-19.42	-0.17
BB1K	-19.59	-0.16	-19.44	-0.17	-19.46	-0.16	-19.49	-0.16	-19.49	-0.16
MPW1B95	-19.57	-0.17	-19.39	-0.17	-19.42	-0.16	-19.44	-0.17	-19.44	-0.17
MPW1KCIS	-19.47	-0.18	-19.33	-0.18	-19.36	-0.18	-19.38	-0.18	-19.38	-0.18
MPWKCIS1K	-19.58	-0.17	-19.42	-0.17	-19.44	-0.17	-19.47	-0.17	-19.47	-0.17
PBE1KCIS	-19.51	-0.18	-19.36	-0.18	-19.38	-0.18	-19.41	-0.18	-19.41	-0.18
MPWB1K	-19.61	-0.16	-19.45	-0.17	-19.47	-0.16	-19.50	-0.16	-19.50	-0.16
TPSS1KCIS	-19.49	-0.18	-19.32	-0.18	-19.36	-0.17	-19.39	-0.17	-19.39	-0.17
TPSSh	-19.50	-0.17	-19.34	-0.17	-19.37	-0.17	-19.40	-0.17	-19.40	-0.17

[Ru(H₂O)₁₈]²⁺	LANL2DZ		DZQ		MWB28		TZQS		TZQ	
GGA	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}
BLYP	-6.15	-0.79	-6.15	-0.79	-6.24	-0.79	-6.21	-0.81	-6.21	-0.81
BP86	-6.22	-0.76	-6.22	-0.76	-6.31	-0.76	-6.28	-0.78	-6.28	-0.77
BPBE	-6.19	-0.78	-6.18	-0.78	-6.27	-0.78	-6.24	-0.80	-6.24	-0.80
BPW91	-6.19	-0.78	-6.18	-0.78	-6.26	-0.78	-6.24	-0.80	-6.24	-0.80
G96LYP	-6.15	-0.80	-6.15	-0.79	-6.23	-0.79	-6.20	-0.82	-6.20	-0.82
HCTH	-6.07	-0.90	-6.06	-0.90	-6.12	-0.89	-6.10	-0.93	-6.10	-0.93
mPWLYP	-6.16	-0.78	-6.16	-0.78	-6.25	-0.77	-6.22	-0.80	-6.22	-0.80
mPWPBE	-6.20	-0.77	-6.19	-0.77	-6.28	-0.76	-6.26	-0.78	-6.26	-0.78
mPWPW	-6.20	-0.77	-6.19	-0.77	-6.28	-0.77	-6.25	-0.79	-6.25	-0.78
OLYP	-6.06	-0.94	-6.05	-0.94	-6.11	-0.94	-6.09	-0.99	-6.09	-0.99
PBEPBE	-6.21	-0.77	-6.20	-0.76	-6.30	-0.76	-6.27	-0.78	-6.27	-0.78
H										
B3LYP	-6.10	-0.78	-6.10	-0.77	-6.17	-0.77	-6.15	-0.79	-6.15	-0.79
B3P86	-6.16	-0.75	-6.15	-0.75	-6.23	-0.75	-6.21	-0.77	-6.21	-0.77
B3PW91	-6.13	-0.77	-6.12	-0.77	-6.19	-0.77	-6.17	-0.79	-6.17	-0.79
B97-1	-6.10	-0.78	-6.10	-0.78	-6.17	-0.78	-6.14	-0.80	-6.14	-0.80
B97-2	-6.09	-0.80	-6.08	-0.80	-6.14	-0.80	-6.12	-0.82	-6.12	-0.82
B98	-6.10	-0.78	-6.09	-0.78	-6.16	-0.78	-6.14	-0.80	-6.14	-0.80
BH&HLYP	-6.05	-0.77	-6.04	-0.77	-6.09	-0.77	-6.08	-0.78	-6.07	-0.78
mPW1PW	-6.13	-0.77	-6.12	-0.76	-6.19	-0.77	-6.16	-0.78	-6.16	-0.78
O3LYP	-6.05	-0.88	-6.05	-0.88	-6.10	-0.88	-6.08	-0.92	-6.08	-0.92
PBEh	-6.13	-0.76	-6.12	-0.76	-6.20	-0.76	-6.17	-0.78	-6.17	-0.78
MGGA										
BB95	-6.17	-0.79	-6.16	-0.79	-6.25	-0.79	-6.22	-0.81	-6.22	-0.81
mPWB95	-6.17	-0.78	-6.17	-0.77	-6.26	-0.77	-6.23	-0.80	-6.23	-0.80
mPWKCIS	-6.17	-0.79	-6.16	-0.79	-6.25	-0.78	-6.23	-0.81	-6.22	-0.81
PBEKCIS	-6.18	-0.78	-6.17	-0.78	-6.27	-0.78	-6.24	-0.80	-6.24	-0.80
TPSSKCIS	-6.18	-0.77	-6.17	-0.77	-6.25	-0.77	-6.23	-0.79	-6.22	-0.79
TPSS	-6.19	-0.76	-6.18	-0.76	-6.26	-0.76	-6.24	-0.78	-6.24	-0.78
VSXC	-5.90	-0.55	-5.82	-0.55	-5.77	-0.55	-5.77	-0.57	-5.78	-0.57
HM										
B1B95	-6.09	-0.78	-6.08	-0.78	-6.15	-0.78	-6.11	-0.80	-6.11	-0.80
BB1K	-6.07	-0.78	-6.06	-0.78	-6.12	-0.78	-6.12	-0.79	-6.12	-0.79
MPW1B95	-6.09	-0.77	-6.08	-0.77	-6.14	-0.77	-6.13	-0.79	-6.14	-0.79
MPW1KCIS	-6.12	-0.78	-6.12	-0.78	-6.17	-0.78	-6.17	-0.80	-6.17	-0.80
MPWKCIS1K	-6.08	-0.78	-6.06	-0.78	-6.12	-0.78	-6.10	-0.79	-6.10	-0.79
PBE1KCIS	-6.11	-0.78	-6.10	-0.78	-6.18	-0.78	-6.16	-0.80	-6.15	-0.80
MPWB1K	-6.07	-0.77	-6.06	-0.77	-6.12	-0.77	-6.10	-0.78	-6.12	-0.78
TPSS1KCIS	-6.14	-0.77	-6.12	-0.77	-6.20	-0.77	-6.18	-0.79	-6.18	-0.79
TPSSh	-6.16	-0.76	-6.14	-0.76	-6.22	-0.76	-6.20	-0.78	-6.20	-0.78

[Ru(H₂O)₁₈]³⁺	LANL2DZ		DZQ		MWB28		TZQS		TZQ	
GGA	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}	ΔG_{EP}	G_{CDS}
BLYP	-13.35	-0.74	-13.30	-0.74	-13.30	-0.73	-13.26	-0.75	-13.26	-0.75
BP86	-13.49	-0.71	-13.44	-0.71	-13.44	-0.71	-13.40	-0.72	-13.40	-0.72
BPBE	-13.44	-0.73	-13.39	-0.73	-13.38	-0.73	-13.33	-0.75	-13.33	-0.75
BPW91	-13.43	-0.73	-13.38	-0.73	-13.37	-0.73	-13.33	-0.75	-13.33	-0.75
G96LYP	-13.36	-0.74	-13.31	-0.74	-13.31	-0.74	-13.26	-0.77	-13.26	-0.77
HCTH	-13.16	-0.86	-13.12	-0.87	-13.09	-0.86	-13.02	-0.91	-13.02	-0.92
mPWLYP	-13.37	-0.72	-13.33	-0.72	-13.32	-0.72	-13.29	-0.74	-13.29	-0.74
mPWPBE	-13.46	-0.72	-13.41	-0.72	-13.41	-0.71	-13.36	-0.73	-13.37	-0.73
mPWPW	-13.45	-0.72	-13.41	-0.72	-13.40	-0.71	-13.36	-0.73	-13.36	-0.73
OLYP	-12.90	-1.05	-12.85	-1.08	-12.84	-1.05	-12.80	-1.10	-12.80	-1.11
PBEPBE	-13.46	-0.71	-13.42	-0.71	-13.41	-0.71	-13.38	-0.73	-13.38	-0.72
H										
B3LYP	-13.42	-0.72	-13.36	-0.72	-13.33	-0.72			-13.30	-0.74
B3P86	-13.54	-0.70	-13.48	-0.70	-13.46	-0.70			-13.43	-0.71
B3PW91	-13.47	-0.72	-13.41	-0.72	-13.39	-0.72			-13.35	-0.74
B97-1	-13.43	-0.73	-13.37	-0.73	-13.34	-0.73			-13.30	-0.74
B97-2	-13.41	-0.74	-13.35	-0.75	-13.32	-0.75			-13.26	-0.77
B98	-13.43	-0.73	-13.37	-0.73	-13.34	-0.73			-13.30	-0.75
BH&HLYP	-13.49	-0.72	-13.43	-0.72	-13.37	-0.72			-13.35	-0.73
mPW1PW	-13.48	-0.71	-13.43	-0.72	-13.40	-0.71			-13.37	-0.73
O3LYP	-12.95	-1.01	-12.89	-1.03	-12.88	-1.01			-12.84	-1.07
PBEh	-13.49	-0.71	-13.45	-0.71	-13.42	-0.71			-13.38	-0.72
MGGA										
BB95	-13.38	-0.73	-13.33	-0.73	-13.33	-0.73	-13.27	-0.75	-13.27	-0.75
mPWB95	-13.40	-0.72	-13.35	-0.72	-13.35	-0.72	-13.31	-0.73	-13.31	-0.74
mPWKCIS	-13.39	-0.73	-13.35	-0.73	-13.34	-0.73	-13.30	-0.75	-13.30	-0.75
PBEKCIS	-13.40	-0.73	-13.35	-0.73	-13.35	-0.73	-13.31	-0.74	-13.31	-0.74
TPSSKCIS	-13.43	-0.72	-13.38	-0.72	-13.37	-0.72	-13.33	-0.74	-13.33	-0.74
TPSS	-13.47	-0.71	-13.41	-0.71	-13.40	-0.71	-13.37	-0.73	-13.37	-0.73
VSXC	-13.45	-0.44	-13.36	-0.44	-13.25	-0.44	-13.24	-0.45	-13.24	-0.45
HM										
B1B95	-13.42	-0.72	-13.37	-0.73	-13.33	-0.72			-13.29	-0.74
BB1K	-13.47	-0.72	-13.41	-0.72	-13.36	-0.72			-13.32	-0.73
MPW1B95	-13.45	-0.71	-13.40	-0.72	-13.36	-0.72			-13.31	-0.73
MPW1KCIS	-13.41	-0.73	-13.36	-0.73	-13.36	-0.73			-13.29	-0.75
MPWKCIS1K	-13.48	-0.72	-13.42	-0.73	-13.37	-0.73			-13.33	-0.74
PBE1KCIS	-13.44	-0.72	-13.39	-0.73	-13.35	-0.72			-13.32	-0.74
MPWB1K	-13.49	-0.71	-13.43	-0.71	-13.38	-0.71			-13.32	-0.73
TPSS1KCIS	-13.45	-0.72	-13.39	-0.72	-13.36	-0.72			-13.33	-0.74
TPSSh	-13.48	-0.71	-13.42	-0.71	-13.40	-0.71			-13.36	-0.73