Supporting Information

Theoretical Analysis of the Unusual Temperature Dependence of the Kinetic Isotope Effect in Quinol Oxidation

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Table S1. Structures of the truncated gas phase models

a) UQH_2 optimized structure of the truncated gas phase model calculated at the B3LYP/6-31G** level. The total energy is -1277.51381485 Hartrees.

group	atom	x	y	z	group	atom	x	y	z
PBIM	C	-3.112	-1.213	0.317	UQH2	C	3.665	-0.404	0.040
PBIM	C	-4.265	-0.605	-0.254	UQH2	C	1.335	-0.849	0.688
PBIM	C	-5.444	-1.353	-0.402	UQH2	C	3.725	-1.597	-0.690
PBIM	C	-5.441	-2.677	0.021	UQH2	C	1.454	-2.054	-0.055
PBIM	C	-4.288	-3.265	0.587	UQH2	C	2.612	-2.441	-0.737
PBIM	C	-3.108	-2.546	0.745	UQH2	H	0.578	-2.699	-0.088
PBIM	C	-2.728	0.880	-0.221	UQH2	O	0.248	-0.500	1.329
PBIM	H	-6.328	-0.896	-0.838	UQH2	O	4.897	-1.940	-1.345
PBIM	H	-6.343	-3.277	-0.084	UQH2	H	5.516	-1.231	-1.105
PBIM	H	-4.326	-4.304	0.907	UQH2	O	4.844	0.348	0.068
PBIM	H	-2.220	-2.990	1.184	UQH2	O	2.499	1.195	1.385
PBIM	N	-2.146	-0.243	0.325	UQH2	C	4.746	1.628	-0.557
PBIM	N	-3.996	0.704	-0.581	UQH2	H	4.050	2.272	-0.012
PBIM	C	-1.982	2.146	-0.371	UQH2	H	5.750	2.064	-0.534
PBIM	C	-1.944	4.302	-1.156	UQH2	H	4.415	1.538	-1.600
PBIM	C	-0.002	3.473	-0.038	UQH2	C	2.299	1.076	2.795
PBIM	C	-0.643	4.521	-0.698	UQH2	H	2.262	2.095	3.192
PBIM	H	-2.481	5.097	-1.675	UQH2	H	1.360	0.555	2.999
PBIM	H	1.012	3.571	0.340	UQH2	H	3.138	0.540	3.263
PBIM	H	-0.157	5.479	-0.859	UQH2	C	2.684	-3.731	-1.517
PBIM	C	-0.675	2.269	0.137	UQH2	H	2.891	-3.550	-2.580
PBIM	H	-0.196	1.442	0.657	UQH2	H	3.490	-4.379	-1.152
PBIM	N	-2.609	3.155	-1.009	UQH2	H	1.742	-4.282	-1.444
UQH2	C	2.503	-0.025	0.718	UQH2	H	-1.140	-0.381	0.689

b) PQH_2 optimized structure of the truncated gas phase model calculated at the B3LP/6-31G** level. The total energy is -1127.10462272 Hartrees.

group	atom	x	y	z	group	atom	x	y	z
PBIM	C	-1.885	1.791	-0.452	PQH2	C	3.019	-0.816	-1.030
PBIM	C	-3.253	1.907	-0.073	PQH2	C	4.250	-0.510	-0.422
PBIM	C	-3.867	3.170	-0.050	PQH2	C	1.796	-0.313	-0.481
PBIM	C	-3.104	4.278	-0.403	PQH2	C	4.287	0.313	0.714
PBIM	C	-1.747	4.148	-0.774	PQH2	C	1.896	0.498	0.679
PBIM	C	-1.116	2.908	-0.805	PQH2	C	3.113	0.823	1.277
PBIM	C	-2.740	-0.163	0.032	PQH2	H	0.976	0.884	1.113
PBIM	H	-4.910	3.265	0.238	PQH2	O	0.643	-0.601	-1.043
PBIM	H	-3.556	5.267	-0.392	PQH2	O	5.491	0.642	1.346
PBIM	H	-1.183	5.038	-1.040	PQH2	H	6.206	0.462	0.725
PBIM	H	-0.072	2.804	-1.084	PQH2	C	3.182	1.697	2.506

PBIM	N	-1.581	0.457	-0.376	PQH2	H	3.591	1.155	3.368
PBIM	N	-3.764	0.666	0.225	PQH2	H	3.840	2.561	2.347
PBIM	C	-2.812	-1.624	0.230	PQH2	H	2.188	2.066	2.776
PBIM	C	-4.081	-3.442	0.836	PQH2	H	-0.583	0.018	-0.630
PBIM	C	-1.812	-3.813	0.194	PQH2	C	5.560	-1.046	-0.965
PBIM	C	-3.031	-4.337	0.627	PQH2	H	6.171	-0.264	-1.445
PBIM	H	-5.051	-3.809	1.175	PQH2	H	6.174	-1.492	-0.171
PBIM	H	-0.960	-4.463	0.015	PQH2	H	5.399	-1.819	-1.718
PBIM	H	-3.167	-5.401	0.799	PQH2	C	2.925	-1.674	-2.271
PBIM	C	-1.691	-2.443	-0.010	PQH2	H	1.880	-1.694	-2.588
PBIM	H	-0.750	-2.012	-0.352	PQH2	H	3.533	-1.288	-3.100
PBIM	N	-3.993	-2.125	0.649	PQH2	H	3.245	-2.712	-2.096

Table S2. Structures of the truncated solvated models

a) UQH_2 optimized structure of the truncated solvated model calculated at the B3LYP/6-31G** level with PCM for acetonitrile. The total energy is -1277.57971768 Hartrees.

group	atom	x	y	z	group	atom	x	y	z
PBIM	C	2.417	-1.708	-0.231	UQH2	C	-3.869	-0.121	0.136
PBIM	C	3.763	-1.591	0.238	UQH2	C	-1.501	-0.123	-0.402
PBIM	C	4.517	-2.746	0.519	UQH2	C	-3.573	-0.040	1.504
PBIM	C	3.917	-3.986	0.330	UQH2	C	-1.229	-0.049	0.973
PBIM	C	2.584	-4.096	-0.132	UQH2	C	-2.243	-0.012	1.937
PBIM	C	1.822	-2.968	-0.416	UQH2	H	-0.191	-0.022	1.288
PBIM	C	2.973	0.363	-0.076	UQH2	O	-0.536	-0.151	-1.353
PBIM	H	5.542	-2.665	0.874	UQH2	O	-4.594	-0.007	2.423
PBIM	H	4.480	-4.892	0.540	UQH2	H	-5.414	-0.089	1.907
PBIM	H	2.151	-5.084	-0.267	UQH2	O	-5.214	-0.209	-0.190
PBIM	H	0.798	-3.052	-0.772	UQH2	O	-3.188	-0.221	-2.158
PBIM	N	1.927	-0.443	-0.428	UQH2	C	-5.734	0.887	-0.960
PBIM	N	4.096	-0.263	0.330	UQH2	H	-5.264	0.922	-1.945
PBIM	C	2.863	1.834	-0.156	UQH2	H	-6.806	0.708	-1.063
PBIM	C	3.813	3.900	0.224	UQH2	H	-5.573	1.840	-0.441
PBIM	C	1.642	3.827	-0.765	UQH2	C	-2.874	-1.461	-2.800
PBIM	C	2.715	4.586	-0.294	UQH2	H	-3.210	-1.366	-3.836
PBIM	H	4.671	4.456	0.602	UQH2	H	-1.798	-1.650	-2.777
PBIM	H	0.762	4.310	-1.181	UQH2	H	-3.407	-2.294	-2.324
PBIM	H	2.704	5.671	-0.326	UQH2	C	-1.934	0.069	3.412
PBIM	C	1.713	2.440	-0.698	UQH2	H	-2.375	0.964	3.866
PBIM	H	0.898	1.826	-1.060	UQH2	H	-2.346	-0.789	3.955
PBIM	N	3.902	2.568	0.299	UQH2	H	-0.855	0.096	3.584
UQH2	C	-2.847	-0.169	-0.820	UQH2	H	0.403	-0.242	-0.944

b) PQH_2 optimized structure of the truncated solvated model calculated at the B3LP/6-31G** level with PCM for acetonitrile. The total energy is -1127.19165281 Hartrees.

group	atom	x	y	z	group	atom	x	y	z
PBIM	C	2.103	-1.693	-0.428	PQH2	C	-3.158	0.121	-1.223
PBIM	C	3.409	-1.626	0.152	PQH2	C	-4.259	0.023	-0.348
PBIM	C	4.155	-2.802	0.359	PQH2	C	-1.856	-0.070	-0.715
PBIM	C	3.587	-4.016	-0.014	PQH2	C	-4.049	-0.298	1.004
PBIM	C	2.293	-4.077	-0.586	PQH2	C	-1.672	-0.359	0.646
PBIM	C	1.539	-2.927	-0.797	PQH2	C	-2.756	-0.484	1.516
PBIM	C	2.619	0.349	-0.003	PQH2	H	-0.661	-0.500	1.017
PBIM	H	5.151	-2.757	0.799	PQH2	O	-0.804	0.039	-1.569
PBIM	H	4.145	-4.939	0.135	PQH2	O	-5.116	-0.372	1.898
PBIM	H	1.883	-5.047	-0.864	PQH2	H	-5.679	-1.142	1.672
PBIM	H	0.546	-2.980	-1.238	PQH2	C	-2.553	-0.814	2.974
PBIM	N	1.615	-0.415	-0.523	PQH2	H	-2.866	0.014	3.622
PBIM	N	3.717	-0.314	0.416	PQH2	H	-3.150	-1.682	3.274
PBIM	C	2.504	1.821	0.075	PQH2	H	-1.502	-1.028	3.184
PBIM	C	3.414	3.828	0.760	PQH2	H	0.088	-0.138	-1.107
PBIM	C	1.324	3.875	-0.396	PQH2	C	-5.664	0.263	-0.852
PBIM	C	2.355	4.572	0.239	PQH2	H	-6.065	-0.612	-1.381
PBIM	H	4.240	4.335	1.264	PQH2	H	-6.337	0.481	-0.020
PBIM	H	0.475	4.408	-0.822	PQH2	H	-5.701	1.101	-1.554
PBIM	H	2.342	5.655	0.328	PQH2	C	-3.357	0.435	-2.688
PBIM	C	1.396	2.489	-0.480	PQH2	H	-2.417	0.324	-3.231
PBIM	H	0.612	1.923	-0.970	PQH2	H	-4.101	-0.226	-3.147
PBIM	N	3.502	2.494	0.690	PQH2	H	-3.710	1.464	-2.842

Table S3. Structures of the full system gas phase models

a) UQH_2 optimized structure of the full system gas phase model calculated at the B3LYP/LANL2DZ level. The total energy is -2361.70495900 Hartrees.

group	atom	x	y	z	group	atom	x	Y	z
PBIM	C	-1.451	1.431	1.214	BPY	C	5.027	3.683	1.465
PBIM	C	-0.021	1.614	1.252	BPY	H	5.387	2.509	3.266
PBIM	C	0.548	2.687	1.976	BPY	C	3.650	2.550	-0.188
PBIM	C	-0.323	3.554	2.644	BPY	C	4.390	3.677	0.216
PBIM	C	-1.739	3.373	2.604	BPY	H	5.597	4.548	1.787
PBIM	C	-2.317	2.316	1.895	BPY	C	2.948	2.443	-1.480
PBIM	C	-0.535	-0.159	0.046	BPY	H	4.469	4.541	-0.434
PBIM	H	1.622	2.837	2.023	BPY	C	2.890	3.477	-2.433
PBIM	H	0.083	4.389	3.211	BPY	C	2.183	3.283	-3.629
PBIM	H	-2.375	4.073	3.139	BPY	H	3.378	4.425	-2.243
PBIM	H	-3.392	2.171	1.865	BPY	C	1.631	1.055	-2.863
PBIM	N	-1.744	0.305	0.446	BPY	C	1.542	2.048	-3.846

PBIM	N	0.540	0.583	0.499	BPY	H	2.125	4.076	-4.368
PBIM	C	-0.258	-1.331	-0.769	BPY	H	1.141	0.098	-2.989
PBIM	C	1.457	-2.622	-1.758	BPY	H	0.975	1.858	-4.751
PBIM	C	-0.849	-3.300	-2.050	BPY	N	2.624	-1.440	1.476
PBIM	C	0.524	-3.518	-2.295	BPY	N	4.164	-1.131	-0.651
PBIM	H	2.519	-2.755	-1.924	BPY	N	2.320	1.236	-1.702
PBIM	H	-1.594	-3.980	-2.453	BPY	N	3.537	1.447	0.631
PBIM	H	0.867	-4.361	-2.886	UQH2	H	-5.958	-4.334	-0.387
PBIM	C	-1.246	-2.199	-1.279	UQH2	C	-5.836	-3.318	-0.771
PBIM	H	-2.293	-2.002	-1.066	UQH2	O	-6.371	-2.436	0.272
PBIM	N	1.085	-1.545	-1.012	UQH2	H	-4.778	-3.097	-0.943
RU	Ru	2.401	-0.126	-0.127	UQH2	H	-6.407	-3.199	-1.702
BPY	H	3.179	-4.109	4.258	UQH2	C	-6.371	-1.062	-0.025
BPY	C	3.025	-3.363	3.485	UQH2	C	-5.180	-0.323	-0.220
BPY	C	1.931	-2.479	3.546	UQH2	C	-7.606	-0.384	-0.069
BPY	C	3.916	-3.268	2.405	UQH2	C	-5.255	1.060	-0.489
BPY	C	1.761	-1.534	2.526	UQH2	O	-3.959	-0.994	-0.165
BPY	H	1.216	-2.519	4.361	UQH2	C	-7.660	1.002	-0.331
BPY	C	3.701	-2.298	1.408	UQH2	O	-8.859	-1.012	0.065
BPY	H	4.762	-3.943	2.342	UQH2	C	-6.485	1.746	-0.545
BPY	H	0.933	-0.837	2.525	UQH2	H	-4.334	1.610	-0.670
BPY	C	4.575	-2.108	0.233	UQH2	O	-8.901	1.646	-0.390
BPY	C	5.755	-2.842	0.001	UQH2	C	-9.106	-1.778	1.301
BPY	C	4.921	-0.880	-1.757	UQH2	C	-6.570	3.230	-0.833
BPY	C	6.526	-2.582	-1.141	UQH2	H	-9.608	0.969	-0.284
BPY	H	6.070	-3.606	0.702	UQH2	H	-10.124	-2.162	1.205
BPY	C	6.100	-1.580	-2.036	UQH2	H	-8.386	-2.596	1.383
BPY	H	4.556	-0.105	-2.420	UQH2	H	-9.032	-1.118	2.176
BPY	H	7.436	-3.142	-1.329	UQH2	H	-7.174	3.423	-1.728
BPY	H	6.667	-1.345	-2.931	UQH2	H	-7.061	3.764	-0.009
BPY	C	4.162	1.455	1.841	UQH2	H	-5.573	3.660	-0.984
BPY	C	4.912	2.548	2.292	UQH2	H	-3.168	-0.398	0.105
BPY	H	4.040	0.570	2.452					

b) PQH_2 optimized structure of the full system gas phase model calculated at the B3LYP/LANL2DZ level. The total energy is -2211.31950965 Hartrees.

group	**atom**	**x**	**y**	**z**	**group**	**atom**	**x**	**Y**	**z**
PBIM	C	-1.628	1.211	1.804	BPY	H	4.052	0.724	2.080
PBIM	C	-0.223	1.475	1.613	BPY	C	4.636	3.881	0.926
PBIM	C	0.390	2.591	2.226	BPY	H	5.391	2.758	2.635
PBIM	C	-0.414	3.423	3.014	BPY	C	3.061	2.639	-0.449
PBIM	C	-1.806	3.163	3.200	BPY	C	3.786	3.817	-0.187
PBIM	C	-2.426	2.062	2.602	BPY	H	5.196	4.786	1.138

PBIM	C	-0.819	-0.347	0.521	BPY	C	2.143	2.469	-1.590
PBIM	H	1.447	2.803	2.099	BPY	H	3.688	4.676	-0.841
PBIM	H	0.028	4.289	3.500	BPY	C	1.839	3.485	-2.515
PBIM	H	-2.389	3.838	3.821	BPY	C	0.937	3.230	-3.559
PBIM	H	-3.483	1.857	2.743	BPY	H	2.287	4.467	-2.418
PBIM	N	-1.975	0.057	1.104	BPY	C	0.689	0.979	-2.705
PBIM	N	0.269	0.462	0.789	BPY	C	0.353	1.952	-3.654
PBIM	C	-0.607	-1.510	-0.326	BPY	H	0.689	4.008	-4.274
PBIM	C	0.996	-2.696	-1.595	BPY	H	0.252	-0.010	-2.736
PBIM	C	-1.272	-3.533	-1.481	BPY	H	-0.359	1.713	-4.437
PBIM	C	0.050	-3.661	-1.960	BPY	N	2.646	-1.391	1.368
PBIM	H	2.020	-2.757	-1.944	BPY	N	3.738	-0.999	-1.007
PBIM	H	-2.028	-4.266	-1.747	BPY	N	1.568	1.220	-1.692
PBIM	H	0.343	-4.487	-2.599	BPY	N	3.173	1.541	0.377
PBIM	C	-1.606	-2.450	-0.656	PQH2	C	-6.567	-1.521	0.253
PBIM	H	-2.615	-2.317	-0.270	PQH2	C	-5.388	-0.740	0.304
PBIM	N	0.686	-1.636	-0.798	PQH2	C	-7.760	-0.913	-0.218
Ru	Ru	2.035	-0.117	-0.164	PQH2	C	-5.395	0.613	-0.096
BPY	H	3.903	-3.969	4.002	PQH2	O	-4.210	-1.351	0.748
BPY	C	3.554	-3.248	3.270	PQH2	C	-7.741	0.446	-0.607
BPY	C	2.428	-2.444	3.533	PQH2	C	-6.572	1.230	-0.554
BPY	C	4.219	-3.106	2.042	PQH2	H	-4.473	1.189	-0.053
BPY	C	2.002	-1.530	2.561	PQH2	O	-8.898	1.104	-1.083
BPY	H	1.883	-2.524	4.467	PQH2	C	-6.602	2.682	-0.981
BPY	C	3.751	-2.169	1.101	PQH2	H	-9.687	0.529	-1.055
BPY	H	5.086	-3.720	1.824	PQH2	H	-6.928	2.781	-2.024
BPY	H	1.140	-0.893	2.711	PQH2	H	-7.320	3.255	-0.380
BPY	C	4.375	-1.934	-0.216	PQH2	H	-5.613	3.143	-0.876
BPY	C	5.539	-2.588	-0.665	PQH2	H	-3.441	-0.708	0.936
BPY	C	4.255	-0.711	-2.235	PQH2	C	-9.070	-1.682	-0.312
BPY	C	6.064	-2.289	-1.931	PQH2	H	-9.848	-1.244	0.333
BPY	H	6.033	-3.319	-0.036	PQH2	H	-9.459	-1.698	-1.342
BPY	C	5.408	-1.331	-2.730	PQH2	H	-8.953	-2.722	-0.002
BPY	H	3.717	0.027	-2.818	PQH2	C	-6.524	-2.970	0.705
BPY	H	6.960	-2.788	-2.287	PQH2	H	-7.249	-3.166	1.507
BPY	H	5.779	-1.069	-3.715	PQH2	H	-6.752	-3.663	-0.118
BPY	C	4.004	1.607	1.455	PQH2	H	-5.528	-3.207	1.085
BPY	C	4.747	2.753	1.762					

Table S4. Structures of the superimposed full system models

a) UQH_2 structure of the superimposed full system model used for calculating solvent reorganization energy and proton potential energy curves.

group	atom	x	y	z	group	atom	x	y	z

PBIM	C	0.000	0.000	0.000	BPY	C	6.961	1.097	-0.562
PBIM	C	1.430	0.000	0.000	BPY	H	6.923	1.291	1.621
PBIM	C	2.137	1.217	0.000	BPY	C	5.428	-0.593	-1.424
PBIM	C	1.409	2.402	-0.002	BPY	C	6.410	0.408	-1.641
PBIM	C	-0.006	2.396	-0.003	BPY	H	7.713	1.864	-0.724
PBIM	C	-0.724	1.205	-0.003	BPY	C	4.754	-1.328	-2.481
PBIM	C	0.744	-2.017	0.007	BPY	H	6.729	0.639	-2.652
PBIM	H	3.225	1.225	0.001	BPY	C	4.982	-1.135	-3.867
PBIM	H	1.933	3.355	-0.002	BPY	C	4.225	-1.837	-4.807
PBIM	H	-0.539	3.344	-0.004	BPY	H	5.740	-0.433	-4.198
PBIM	H	-1.811	1.200	-0.003	BPY	C	3.045	-2.899	-2.977
PBIM	N	-0.423	-1.304	0.006	BPY	C	3.225	-2.734	-4.353
PBIM	N	1.882	-1.295	0.004	BPY	H	4.395	-1.690	-5.870
PBIM	C	0.735	-3.494	0.025	BPY	H	2.296	-3.578	-2.588
PBIM	C	1.922	-5.468	-0.050	BPY	H	2.601	-3.287	-5.048
PBIM	C	-0.450	-5.593	0.169	BPY	N	3.757	-2.604	2.089
PBIM	C	0.775	-6.253	0.067	BPY	N	5.236	-3.769	0.220
PBIM	H	2.900	-5.945	-0.132	BPY	N	3.793	-2.238	-2.049
PBIM	H	-1.376	-6.155	0.264	BPY	N	5.011	-0.896	-0.130
PBIM	H	0.844	-7.337	0.079	UQH2	C	-5.022	-1.939	-1.202
PBIM	C	-0.476	-4.204	0.149	UQH2	C	-5.666	-2.022	-2.442
PBIM	H	-1.412	-3.665	0.231	UQH2	C	-3.614	-1.871	-1.153
PBIM	N	1.922	-4.131	-0.072	UQH2	C	-4.933	-2.026	-3.636
RU	Ru	3.646	-2.441	0.013	UQH2	C	-2.901	-1.869	-2.363
BPY	H	4.326	-2.990	5.932	UQH2	C	-3.537	-1.941	-3.608
BPY	C	4.166	-2.890	4.862	UQH2	H	-1.819	-1.807	-2.318
BPY	C	3.063	-2.144	4.365	UQH2	O	-3.020	-1.811	0.063
BPY	C	5.039	-3.498	3.962	UQH2	O	-5.590	-2.097	-4.841
BPY	C	2.902	-2.031	2.982	UQH2	H	-6.538	-2.095	-4.623
BPY	H	2.356	-1.662	5.031	UQH2	O	-7.047	-2.047	-2.576
BPY	C	4.829	-3.367	2.560	UQH2	O	-5.785	-1.967	-0.050
BPY	H	5.880	-4.077	4.328	UQH2	C	-7.698	-3.208	-2.037
BPY	H	2.086	-1.460	2.553	UQH2	H	-7.576	-3.248	-0.952
BPY	C	5.634	-4.005	1.543	UQH2	H	-8.756	-3.111	-2.291
BPY	C	6.742	-4.859	1.806	UQH2	H	-7.299	-4.125	-2.488
BPY	C	5.919	-4.376	-0.793	UQH2	C	-5.802	-0.734	0.677
BPY	C	7.429	-5.467	0.759	UQH2	H	-6.450	-0.895	1.542
BPY	H	7.050	-5.039	2.831	UQH2	H	-4.796	-0.467	1.013
BPY	C	7.006	-5.224	-0.580	UQH2	H	-6.216	0.076	0.064
BPY	H	5.570	-4.156	-1.796	UQH2	C	-2.757	-1.939	-4.899
BPY	H	8.275	-6.118	0.961	UQH2	H	-2.949	-2.844	-5.486
BPY	H	7.517	-5.672	-1.426	UQH2	H	-3.037	-1.091	-5.535
BPY	C	5.555	-0.212	0.916	UQH2	H	-1.682	-1.880	-4.706

BPY	C	6.521	0.782	0.751	UQH2	H	-2.009	-1.636	-0.012
BPY	H	5.192	-0.484	1.900					

b) PQH_2 structure of the superimposed full system model used for calculating solvent reorganization energy and proton potential energy curves.

group	atom	x	y	z	group	atom	x	y	z
PBIM	C	0.000	0.000	0.000	BPY	H	5.245	-0.503	1.810
PBIM	C	1.430	0.000	0.000	BPY	C	6.947	1.092	-0.689
PBIM	C	2.141	1.215	0.000	BPY	H	6.973	1.269	1.495
PBIM	C	1.414	2.402	-0.001	BPY	C	5.385	-0.586	-1.520
PBIM	C	-0.002	2.397	-0.003	BPY	C	6.363	0.414	-1.758
PBIM	C	-0.722	1.207	-0.005	BPY	H	7.696	1.859	-0.867
PBIM	C	0.738	-2.018	0.010	BPY	C	4.678	-1.310	-2.562
PBIM	H	3.230	1.222	0.002	BPY	H	6.652	0.654	-2.775
PBIM	H	1.940	3.355	-0.001	BPY	C	4.865	-1.107	-3.953
PBIM	H	-0.535	3.346	-0.005	BPY	C	4.076	-1.797	-4.875
PBIM	H	-1.811	1.209	-0.005	BPY	H	5.617	-0.407	-4.300
PBIM	N	-0.425	-1.305	0.011	BPY	C	2.944	-2.865	-3.019
PBIM	N	1.879	-1.298	0.006	BPY	C	3.083	-2.690	-4.398
PBIM	C	0.734	-3.496	0.031	BPY	H	4.214	-1.642	-5.941
PBIM	C	1.936	-5.465	-0.040	BPY	H	2.201	-3.542	-2.613
PBIM	C	-0.438	-5.603	0.182	BPY	H	2.434	-3.232	-5.079
PBIM	C	0.793	-6.255	0.081	BPY	N	3.823	-2.627	2.023
PBIM	H	2.918	-5.935	-0.122	BPY	N	5.233	-3.780	0.094
PBIM	H	-1.361	-6.172	0.280	BPY	N	3.726	-2.219	-2.109
PBIM	H	0.868	-7.339	0.096	BPY	N	5.005	-0.900	-0.217
PBIM	C	-0.472	-4.213	0.157	PQH2	C	-5.041	-2.175	-1.210
PBIM	H	-1.412	-3.680	0.237	PQH2	C	-5.695	-2.225	-2.458
PBIM	N	1.926	-4.126	-0.066	PQH2	C	-3.655	-1.914	-1.170
RU	Ru	3.642	-2.444	-0.046	PQH2	C	-4.971	-1.979	-3.637
BPY	H	4.508	-3.066	5.841	PQH2	C	-2.949	-1.704	-2.364
BPY	C	4.317	-2.950	4.778	PQH2	C	-3.592	-1.724	-3.603
BPY	C	3.211	-2.179	4.325	PQH2	H	-1.882	-1.507	-2.311
BPY	C	5.151	-3.560	3.843	PQH2	O	-3.036	-1.880	0.040
BPY	C	3.007	-2.049	2.949	PQH2	O	-5.586	-2.052	-4.885
BPY	H	2.534	-1.693	5.019	PQH2	H	-6.227	-1.317	-4.977
BPY	C	4.899	-3.409	2.451	PQH2	C	-2.830	-1.478	-4.882
BPY	H	5.994	-4.156	4.177	PQH2	H	-2.814	-2.369	-5.521
BPY	H	2.189	-1.460	2.551	PQH2	H	-3.294	-0.683	-5.476
BPY	C	5.667	-4.040	1.401	PQH2	H	-1.795	-1.194	-4.673
BPY	C	6.774	-4.909	1.619	PQH2	H	-2.043	-1.663	-0.041
BPY	C	5.880	-4.377	-0.947	PQH2	C	-7.171	-2.544	-2.538
BPY	C	7.424	-5.506	0.543	PQH2	H	-7.792	-1.670	-2.298

BPY	H	7.108	-5.107	2.632	PQH2	H	-7.438	-2.870	-3.545
BPY	C	6.966	-5.238	-0.779	PQH2	H	-7.451	-3.333	-1.834
BPY	H	5.504	-4.139	-1.936	PQH2	C	-5.801	-2.406	0.075
BPY	H	8.269	-6.168	0.711	PQH2	H	-5.169	-2.183	0.935
BPY	H	7.447	-5.677	-1.647	PQH2	H	-6.698	-1.778	0.134
BPY	C	5.581	-0.225	0.819	PQH2	H	-6.138	-3.446	0.170
BPY	C	6.545	0.768	0.633					

Table S5. Partial charges used for the solvent reorganization energy calculations
a) UQH_2 superimposed full system model

group	atom	charge				group	atom	charge			
		diabatic state						diabatic state			
		1a	1b	2a	2b			1a	1b	2a	2b
PBIM	C	0.294	0.246	0.294	0.246	BPY	C	0.133	0.133	0.133	0.133
PBIM	C	0.398	0.401	0.398	0.401	BPY	H	0.083	0.083	0.083	0.083
PBIM	C	-0.305	-0.271	-0.305	-0.271	BPY	C	0.335	0.335	0.335	0.335
PBIM	C	-0.147	-0.104	-0.147	-0.104	BPY	C	-0.405	-0.405	-0.405	-0.405
PBIM	C	-0.168	-0.100	-0.168	-0.100	BPY	H	0.007	0.007	0.007	0.007
PBIM	C	-0.259	-0.267	-0.259	-0.267	BPY	C	0.335	0.335	0.335	0.335
PBIM	C	0.415	0.373	0.415	0.373	BPY	H	0.094	0.094	0.094	0.094
PBIM	H	0.114	0.152	0.114	0.152	BPY	C	-0.405	-0.405	-0.405	-0.405
PBIM	H	0.066	0.100	0.066	0.100	BPY	C	0.133	0.133	0.133	0.133
PBIM	H	0.067	0.099	0.067	0.099	BPY	H	0.094	0.094	0.094	0.094
PBIM	H	0.103	0.141	0.103	0.141	BPY	C	0.409	0.409	0.409	0.409
PBIM	N	-0.706	-0.619	-0.706	-0.619	BPY	C	-0.460	-0.460	-0.460	-0.460
PBIM	N	-0.730	-0.590	-0.730	-0.590	BPY	H	0.007	0.007	0.007	0.007
PBIM	C	0.469	0.469	0.469	0.469	BPY	H	-0.057	-0.057	-0.057	-0.057
PBIM	C	0.353	0.398	0.353	0.398	BPY	H	0.083	0.083	0.083	0.083
PBIM	C	0.104	0.180	0.104	0.180	BPY	N	-0.573	-0.573	-0.573	-0.573
PBIM	C	-0.375	-0.354	-0.375	-0.354	BPY	N	-0.573	-0.573	-0.573	-0.573
PBIM	H	-0.016	0.011	-0.016	0.011	BPY	N	-0.637	-0.637	-0.637	-0.637
PBIM	H	0.039	0.059	0.039	0.059	BPY	N	-0.637	-0.637	-0.637	-0.637
PBIM	H	0.096	0.130	0.096	0.130	UQH2	C	0.005	-0.050	0.080	0.025
PBIM	C	-0.307	-0.388	-0.307	-0.388	UQH2	C	0.062	0.095	-0.017	0.016
PBIM	H	0.092	0.113	0.092	0.113	UQH2	C	0.283	0.400	0.364	0.481
PBIM	N	-0.597	-0.572	-0.597	-0.572	UQH2	C	0.156	0.048	0.332	0.224
RU	Ru	3.000	3.000	2.000	2.000	UQH2	C	-0.348	-0.456	-0.313	-0.421
BPY	H	0.048	0.048	0.048	0.048	UQH2	C	0.009	0.015	0.051	0.057
BPY	C	0.199	0.199	0.199	0.199	UQH2	H	0.191	0.132	0.242	0.183
BPY	C	-0.359	-0.359	-0.359	-0.359	UQH2	O	-0.514	-0.667	-0.333	-0.485
BPY	C	-0.410	-0.410	-0.410	-0.410	UQH2	O	-0.477	-0.519	-0.432	-0.473
BPY	C	0.413	0.413	0.413	0.413	UQH2	H	0.364	0.342	0.421	0.399
BPY	H	0.127	0.127	0.127	0.127	UQH2	O	-0.307	-0.367	-0.277	-0.336
BPY	C	0.417	0.417	0.417	0.417	UQH2	O	-0.314	-0.260	-0.176	-0.122

BPY	H	0.139	0.139	0.139	0.139	UQH2	C	0.186	0.253	0.043	0.110
BPY	H	0.000	0.000	0.000	0.000	UQH2	H	0.006	-0.028	0.061	0.027
BPY	C	0.417	0.417	0.417	0.417	UQH2	H	0.022	-0.027	0.101	0.052
BPY	C	-0.410	-0.410	-0.410	-0.410	UQH2	H	0.013	-0.034	0.068	0.021
BPY	C	0.413	0.413	0.413	0.413	UQH2	C	0.188	0.150	-0.059	-0.096
BPY	C	0.199	0.199	0.199	0.199	UQH2	H	0.024	-0.026	0.117	0.067
BPY	H	0.139	0.139	0.139	0.139	UQH2	H	0.008	-0.029	0.140	0.103
BPY	C	-0.359	-0.359	-0.359	-0.359	UQH2	H	0.007	0.029	0.081	0.103
BPY	H	0.000	0.000	0.000	0.000	UQH2	C	-0.005	0.054	-0.082	-0.023
BPY	H	0.048	0.048	0.048	0.048	UQH2	H	0.026	-0.017	0.075	0.031
BPY	H	0.127	0.127	0.127	0.127	UQH2	H	0.030	-0.013	0.073	0.029
BPY	C	0.409	0.409	0.409	0.409	UQH2	H	0.009	-0.025	0.061	0.027
BPY	C	-0.460	-0.460	-0.460	-0.460	UQH2	H	0.376	0.392	0.376	0.392
BPY	H	-0.057	-0.057	-0.057	-0.057						

b) PQH_2 superimposed full system model

group	**atom**	**charge**				**group**	**atom**	**charge**			
		diabatic state						**diabatic state**			
		1a	**1b**	**2a**	**2b**			**1a**	**1b**	**2a**	**2b**
PBIM	C	0.294	0.246	0.294	0.246	BPY	H	-0.057	-0.057	-0.057	-0.057
PBIM	C	0.398	0.401	0.398	0.401	BPY	C	0.133	0.133	0.133	0.133
PBIM	C	-0.305	-0.271	-0.305	-0.271	BPY	H	0.083	0.083	0.083	0.083
PBIM	C	-0.147	-0.104	-0.147	-0.104	BPY	C	0.335	0.335	0.335	0.335
PBIM	C	-0.168	-0.100	-0.168	-0.100	BPY	C	-0.405	-0.405	-0.405	-0.405
PBIM	C	-0.259	-0.267	-0.259	-0.267	BPY	H	0.007	0.007	0.007	0.007
PBIM	C	0.415	0.373	0.415	0.373	BPY	C	0.335	0.335	0.335	0.335
PBIM	H	0.114	0.152	0.114	0.152	BPY	H	0.094	0.094	0.094	0.094
PBIM	H	0.066	0.100	0.066	0.100	BPY	C	-0.405	-0.405	-0.405	-0.405
PBIM	H	0.067	0.099	0.067	0.099	BPY	C	0.133	0.133	0.133	0.133
PBIM	H	0.103	0.141	0.103	0.141	BPY	H	0.094	0.094	0.094	0.094
PBIM	N	-0.706	-0.619	-0.706	-0.619	BPY	C	0.409	0.409	0.409	0.409
PBIM	N	-0.730	-0.590	-0.730	-0.590	BPY	C	-0.460	-0.460	-0.460	-0.460
PBIM	C	0.469	0.469	0.469	0.469	BPY	H	0.007	0.007	0.007	0.007
PBIM	C	0.353	0.398	0.353	0.398	BPY	H	-0.057	-0.057	-0.057	-0.057
PBIM	C	0.104	0.180	0.104	0.180	BPY	H	0.083	0.083	0.083	0.083
PBIM	C	-0.375	-0.354	-0.375	-0.354	BPY	N	-0.573	-0.573	-0.573	-0.573
PBIM	H	-0.016	0.011	-0.016	0.011	BPY	N	-0.573	-0.573	-0.573	-0.573
PBIM	H	0.039	0.059	0.039	0.059	BPY	N	-0.637	-0.637	-0.637	-0.637
PBIM	H	0.096	0.130	0.096	0.130	BPY	N	-0.637	-0.637	-0.637	-0.637
PBIM	C	-0.307	-0.388	-0.307	-0.388	PQH2	C	-0.082	-0.205	0.004	-0.120
PBIM	H	0.092	0.113	0.092	0.113	PQH2	C	-0.122	-0.116	-0.123	-0.118
PBIM	N	-0.597	-0.572	-0.597	-0.572	PQH2	C	0.260	0.454	0.299	0.492
RU	Ru	3.000	3.000	2.000	2.000	PQH2	C	0.141	0.039	0.287	0.185
BPY	H	0.048	0.048	0.048	0.048	PQH2	C	-0.403	-0.476	-0.303	-0.376
BPY	C	0.199	0.199	0.199	0.199	PQH2	C	0.106	0.105	0.101	0.100

BPY	C	-0.359	-0.359	-0.359	-0.359	PQH2	H	0.162	0.121	0.204	0.163
BPY	C	-0.410	-0.410	-0.410	-0.410	PQH2	O	-0.520	-0.684	-0.303	-0.466
BPY	C	0.413	0.413	0.413	0.413	PQH2	O	-0.514	-0.554	-0.432	-0.472
BPY	H	0.127	0.127	0.127	0.127	PQH2	H	0.394	0.368	0.423	0.397
BPY	C	0.417	0.417	0.417	0.417	PQH2	C	-0.082	-0.047	-0.118	-0.083
BPY	H	0.139	0.139	0.139	0.139	PQH2	H	0.043	0.005	0.081	0.043
BPY	H	0.000	0.000	0.000	0.000	PQH2	H	0.043	0.005	0.081	0.043
BPY	C	0.417	0.417	0.417	0.417	PQH2	H	0.025	-0.004	0.071	0.041
BPY	C	-0.410	-0.410	-0.410	-0.410	PQH2	H	0.390	0.392	0.390	0.392
BPY	C	0.413	0.413	0.413	0.413	PQH2	C	0.069	0.097	0.065	0.093
BPY	C	0.199	0.199	0.199	0.199	PQH2	H	-0.007	-0.044	0.025	-0.011
BPY	H	0.139	0.139	0.139	0.139	PQH2	H	-0.007	-0.044	0.025	-0.011
BPY	C	-0.359	-0.359	-0.359	-0.359	PQH2	H	0.019	-0.005	0.045	0.021
BPY	H	0.000	0.000	0.000	0.000	PQH2	C	0.078	0.116	-0.015	0.023
BPY	H	0.048	0.048	0.048	0.048	PQH2	H	0.011	-0.021	0.055	0.022
BPY	H	0.127	0.127	0.127	0.127	PQH2	H	-0.002	-0.054	0.069	0.017
BPY	C	0.409	0.409	0.409	0.409	PQH2	H	-0.002	-0.054	0.070	0.018
BPY	C	-0.460	-0.460	-0.460	-0.460						

Abbreviations: PBIM, 2-(2-pyridyl)-benzimidazolate; RU, ruthenium ion; BPY, 2,2′-dipyridyl; UQH2, 2,3-dimethoxy-5-methyl-1,4-benzoquinol; PQH2, 2,3,5-trimethyl-1,4-benzoquinol;

Table S6. Molecular mechanical parameters for gas phase proton potential energy curves.

Parameters	UQH_2	PQH_2
D_{OH}	78.5	78.5
D_{NH}	81.0	81.0
R^0_{OH} (1*a*)	0.97	0.96
R^0_{NH} (1*b*)	1.01	1.01
R^0_{OH} (2*a*)	0.98	0.97
R^0_{NH} (2*b*)	1.01	1.01
ω_{OH} (1*a*)	3607	3685
ω_{NH} (1*b*)	3545	3545
ω_{OH} (2*a*)	3513	3622
ω_{NH} (2*b*)	3545	3545
β_{OH} (1*a*)	2.58	2.64
β_{NH} (1*b*)	2.49	2.49
β_{OH} (2*a*)	2.51	2.59
β_{NH} (2*b*)	2.49	2.49
D'_{NH} (1*a*)	2335.5	1266.31
D'_{OH} (1*b*)	4227.32	2883.26
D'_{NH} (2*a*)	1596.06	764.065

D'_{OH} (2*b*)	605.573	442.146
β'_{NH} (1*a*)	2.5	2.5
β'_{OH} (1*b*)	2.5	2.5
β'_{NH} (2*a*)	2.5	2.5
β'_{OH} (2*b*)	2.5	2.5
ΔE_{1b}	64.262	73.0227
ΔE_{2a}	-4.680338	-7.126177
ΔE_{2b}	-40.058138	-34.283077
V^{PT} (1*a*/1*b*)	167.5	119.804
V^{PT} (2*a*/2*b*)	99.8	82.4474

Parameters defined in Ishikita, H.; Soudackov,, A. V.; and Hammes-Schiffer, S. *J. Am. Chem. Soc.* **2007**, *129*, 11146-11152.
D, D', ΔE, V^{PT} in units of kcal/mol, R^0 in units of Å, ω in units of cm^{-1}, β and β' in units of $Å^{-1}$.
R^0 and ω for OH and NH obtained from DFT calculations (B3LYP/6-31G**) of UQH_2, PQH_2, and pbimH.
ω is used for calculating β and is corrected with 0.9619 scaling factor (Andersson, M.P.; Uvdal, P. *J. Phys. Chem. A*. **2005**, 109, 2937-2941).
D_{OH} =78.5 kcal/mol (de Heer, M.I.; Korth, H.G.; Mulder, P. *J. Org. Chem*. **1999**, 64, 6969-6975).
D_{NH} = 81.0 kcal/mol (Clyne, M.A.A.; Thrush, B.A. *Proc. Chem. Soc*. **1962**, 227).
β' = 2.5 $Å^{-1}$ (Warshel, A. *Computer Modeling of Chemical Reaction in Enzymes and Solutions*, John Wiley & Sons, Inc, New York, 1991).

Table S7. Analysis of the contributions of pairs of reactant/product vibronic states μ/ν for UQH_2 and PQH_2 systems at 320 K with parameters given in Table 2. The free energies $\Delta G^0_{\mu\nu}$ and $\Delta G^{\ddagger}_{\mu\nu}$ are given in units of kcal/mol.

Quinol	Isotope	μ	ν	% Cont.	P_μ	$\Delta G^0_{\mu\nu}$	$\Delta G^{\ddagger}_{\mu\nu}$	$e^{-\Delta G^{\ddagger}_{\mu\nu}/k_B T}$	$S^2_{\mu\nu}$
UQH_2	H	0	0	9.36	0.9999797	-3.67	1.79	6.0×10^{-2}	8.2×10^{-4}
		0	1	89.9	0.9999797	2.40	2.89	1.1×10^{-2}	4.5×10^{-2}
		1	2	0.73	0.0000203	-0.74	0.017	9.7×10^{-1}	1.9×10^{-1}
	D	0	0	0.27	0.999722	-3.67	1.79	6.0×10^{-2}	1.1×10^{-5}
		0	1	82.1	0.999722	1.01	1.01	2.0×10^{-1}	9.9×10^{-4}
		1	2	16.3	0.000278	-0.53	0.056	9.2×10^{-1}	1.6×10^{-1}
		1	3	1.24	0.000278	1.73	1.87	5.3×10^{-2}	2.1×10^{-2}
PQH_2	H	0	0	31	0.999993	-3.34	1.09	1.8×10^{-1}	1.2×10^{-4}
		0	1	66.7	0.999993	3.00	3.78	2.5×10^{-3}	1.9×10^{-2}
		1	2	2.33	0.000007	-1.15	1.2×10^{-4}	1.00	2.4×10^{-1}
		1	3	0.03	0.000007	1.64	1.70	6.9×10^{-2}	4.0×10^{-2}
	D	0	0	0.55	0.999854	-3.34	1.09	1.8×10^{-1}	6.7×10^{-7}
		0	1	52.3	0.999854	1.53	1.56	8.6×10^{-2}	1.3×10^{-4}
		1	2	34.6	0.000146	-0.22	0.18	7.5×10^{-1}	7.1×10^{-2}
		1	3	12.4	0.000146	1.54	1.58	8.4×10^{-2}	2.3×10^{-1}

Estimation of the driving forces (provided by Jon Cape, personal communication):

Useful Formulas:

$HA \rightarrow H^+ + A^-$ $\quad \Delta G^o = 1.368\ pK_a$ kcal/mol at 298.15 K

$M^+ + e^- \rightarrow M$ $\quad \Delta G^o = -23.061\ E$ kcal/mol E is the potential in Volts

$E = E^o - 0.05916\ pH$ $\quad E^o$ is standard potential in Volts at pH=0

QOH --- $^-$NRu(III) $\rightarrow$ QO$^\bullet$ --- HNRu(II)

For consistency, we are doing everything in water for the ground state Ru complex (i.e., not the MLCT state in MeCN). We will assume that this reaction occurs at pH=0 and that the redox potentials are calculated relative to SHE, but these two effects will cancel out in the final calculation of the total driving force, which involves both a protonation and a deprotonation, and both an oxidation and a reduction.

Couple 1: $^-$NRu(III) + H$^\bullet \rightarrow$ HNRu(II)

Couple 1a: $^-$NRu(III) + $H^+ \rightarrow$ HNRu(III)

pKa = 3.2
Jon Cape's CV experiment and thermodynamic cycle analysis

$\Delta G^o = -1.368\ (pK_a - pH)$ kcal/mol
$= -4.378$ kcal/mol

at pH = 0

Couple 1b: HNRu(III) + $e^- \rightarrow$ HNRu(II)

$E(Ru^{III/II})$ for protonated species is 0.875 vs SHE
Jon Cape's CV experiment

$\Delta G^o = -23.061\ E$ kcal/mol E is the reduction potential in Volts
$= -20.178$

Couple 2: QOH $\rightarrow$ QO$^\bullet$ + H$^\bullet$

Redox potential is available for the combined electron/proton transfer.
Using Jon Cape's equations, combined with the experimental data from

Table S2 of Supporting Information for J. L. Cape, M. K. Bowman, D. M. Kramer, Phytochemistry 67 (2006) 1781-1788.

$E(UQH^{\bullet}/UQH2) = 0.805$
$E(TMQH^{\bullet}/TMQH2) = 0.869$
in H_2O at pH=0

$\Delta G^o = 23.061\ E$ kcal/mol
= 18.564 kcal/mol for UQH
= 20.040 kcal/mol for TMQ

Driving force for total PCET reaction is the sum for Couples 1a, 1b, and 2:

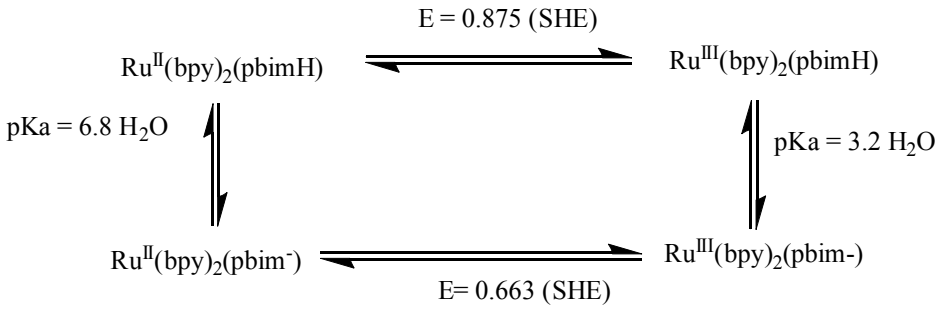
For UQH:
$\Delta G^o = (-4.378 - 20.178 + 18.564)$ kcal/mol
$= -6.0$ kcal/mol

In units of V, E = 0.260 V

For TMQH:
$\Delta G^o = (-4.378 - 20.178 + 20.040)$ kcal/mol
$= -4.5$ kcal/mol

In units of V, E = 0.196 V

<u>Calculation of redox potentials and pKas for Ru complex:</u>
Jon Cape ran the CV for the Ru compound in both 1M triflic acid and in 250 mM Borate buffer (pH 9) to obtain the $Ru^{III/II}$ couples for the protonated and deprotonated forms in aqueous solution. From this he calculated the following cycle: (personal communication, Jon Cape)



<u>Calculation of Redox Potential for Semiquinone:</u>

(1) $Q + 2H \rightarrow QH_2$
(2) $Q + H \rightarrow QH\cdot$

(3) $QH\cdot + H \rightarrow QH_2$

From the Nernst equation:

$$E_1 = E_1^0 + \frac{RT}{2F}\ln\frac{[Q]}{[QH_2]}$$

$$E_2 = E_2^0 + \frac{RT}{F}\ln\frac{[Q]}{[QH\cdot]}$$

$$E_3 = E_3^0 + \frac{RT}{F}\ln\frac{[QH\cdot]}{[QH_2]}$$

At equilibrium $E_1=E_2=E_3$ since all three redox reactions are at the same ambient potential. Therefore, $E_2 + E_3 = 2E_1$ so

$$E_2^0 + \frac{RT}{F}\ln\frac{[Q]}{[QH\cdot]} + E_3^0 + \frac{RT}{F}\ln\frac{[QH\cdot]}{[QH_2]} = 2E_1^0 + \frac{RT}{F}\ln\frac{[Q]}{[QH_2]}$$

so $E_2^0 + E_3^0 = 2E_1^0$

Rearranging, we get: $E_3^0 = 2E_1^0 - E_2^0$.

We can define these redox potentials as follows (assumed to be measured at pH=0):

$$E_1^0 = E(Q/QH_2)$$

$$E_2^0 = E(Q/QH\cdot)$$

$$E_3^0 = E(QH\cdot/QH_2)$$

Now we get another expression for E_2^0. The second reaction can be broken into 2 steps:

$Q + e^- \rightarrow Q\cdot^-$

$Q\cdot^- + H^+ \rightarrow QH\cdot$

$E_2^0 = E(Q/Q\cdot^-) + 0.059(pK_{a,SQ} - pH)$, where pH = 0 here.

We also need to calculate E_1^0, which is at pH=0, from E(Q/QH2) measured at pH=7.

$$E_1^0 = E(Q/QH_2, pH) + 0.059\,pH = E(Q/QH_2, pH = 7) + 0.059(7)$$

$E(QH\cdot/QH_2) = 2E(Q/QH_2,pH=7) + 2(0.059)(7) - E(Q/Q\cdot^-) - 0.059(pK_{a,SQ})$

Using numbers from SI of the Phytochemistry 2006 paper:

UQH:

$E(QH\cdot/QH_2) = 2(0.117) + 2(0.059)(7) - (-0.075) - 0.059\,(5.6) = 0.805$ V

TMQH:

$E(QH\cdot/QH_2) = 2(0.085) + 2(0.059)(7) - (-0.165) - 0.059\,(4.95) = 0.869$ V

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