Supplemetary Information: A key to efficient electron transport is robust excited state energies of quinone radical anions to the local environment

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1 Experimental Details

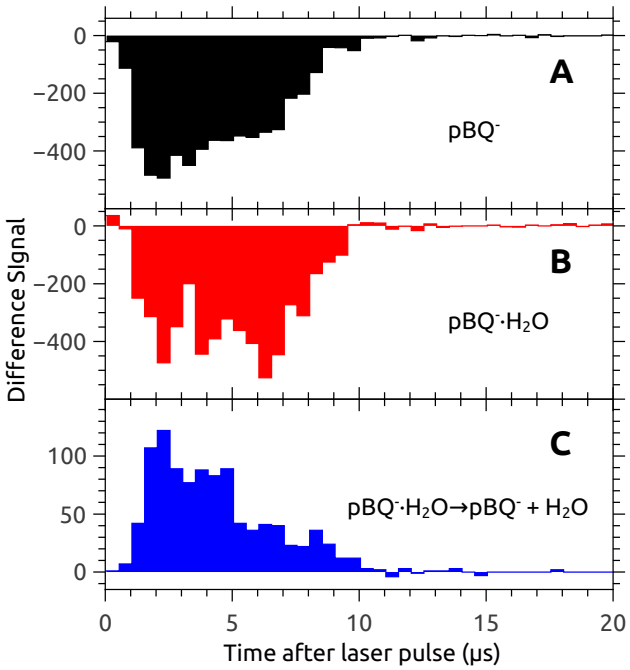

Figure 1: Time profiles of action signals (difference in counts between "laser on" and "laser off") measured at 445 nm. **A** and **B** show depletion of the $p\mathrm{BQ}^-$ and $p\mathrm{BQ}^-\cdot\mathrm{H_2O}$ ion bunches; **C** shows photo-induced dissociation of $p\mathrm{BQ}^-\cdot\mathrm{H_2O}$.

Figure 1 shows the time profiles of the action signals, *i.e.* the change in the number of detected ions when the ion bunch is illuminated with a laser pulse. A negative signal (as in (Figure 1**A** and **B**) is thus indicative of beam depletion, while a positive signal indicated photo-induced dissociation of the parent ion (Figure 1**C**).

In Figure 2, we show the photodissociaton yield of the solvated complex as a function of laser power measured at several laser wavelengths. The laser beam is attenuated using neutral density filters and the full laser power at each wavelength is normalized to 1. At every wavelength measured, the yield is linearly dependent on laser power, indicating that one photon is sufficient to induce dissociation on the microsecond timescale probed by our experiment. Least-squared fits to the function $y = Ax$ have been obtained for each wavelength and the slope A has been divided out of the data in Figure 2 so that all the points are scattered about $y = x$, the solid line in the figure. There is a hint of saturation at full power at 445 nm, the position of the band maximum. However, the near absence of saturation indicates that no (or very few) $p\mathrm{BQ}^-$ ions are lost due to two-photon absorption processes.

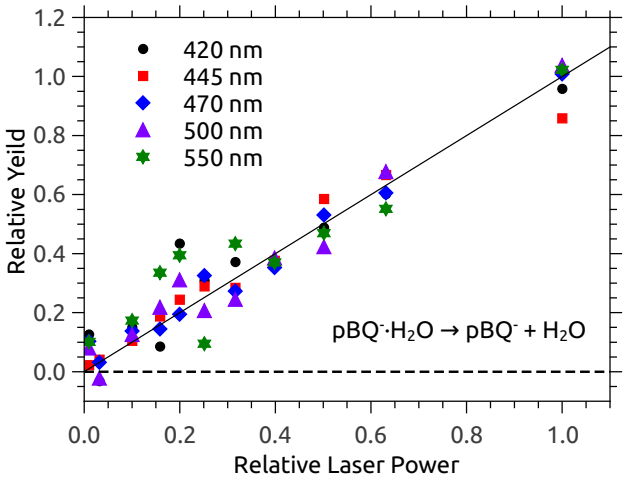

Figure 2: Relative photofragment yield as a function of laser power measured at several laser wavelengths. At each wavelength the power dependence is linear, corresponding to a one-photon process.

2 Theoretical results

Below, we give the coordinates of optimized structures, electronic energies E(in Hartrees), and zero-point kinetic energies ZKE (in Hartrees) calculated at the B3LYP/6-311G(2d,p) level of density functional theory.

2.1 *p*BQ$^-$ anion

C	0	-4.6639903276	-1.54494324	-0.0004210882
C	0	-3.2978672851	-1.5450454791	-0.0002146808
C	0	-2.5148388831	-0.3249952648	-0.00089403
C	0	-3.2976844074	0.8951721139	-0.0018093591
C	0	-4.6638074447	0.8952743605	-0.0020157443
C	0	-5.446835845	-0.3247758589	-0.0013364084
H	0	-5.2285462753	-2.4741008581	0.000101282
H	0	-2.7334506038	-2.4742875855	0.0004781987
H	0	-2.7331284557	1.824329725	-0.0023317381
H	0	-5.2282241279	1.8245164699	-0.0027086028
O	0	-1.2540204223	-0.3250896248	-0.0007040372
O	0	-6.7076543321	-0.3246815098	-0.0015264062

E = -381.6289218 ZKE = 0.082874

2.2 *p*BQ neutral

C	0	-4.6485663463	-1.5924679278	-0.0003874246
C	0	-3.3132983789	-1.5925678512	-0.0001858993
C	0	-2.5415036737	-0.3249932766	-0.0008980415
C	0	-3.3131083881	0.9426968018	-0.001843017
C	0	-4.6483763553	0.942796737	-0.0020445384
C	0	-5.4201710721	-0.3247778435	-0.0013323936
H	0	-5.2378323043	-2.5021111187	0.0001182676
H	0	-2.7241687498	-2.5022992258	0.0004976435
H	0	-2.7238424243	1.85233999	-0.0023487162
H	0	-5.2375059744	1.8525281166	-0.002728071
O	0	-1.3241562927	-0.3250843802	-0.000714417
O	0	-6.6375184501	-0.3246867399	-0.0015160123

E = -381.5630057 ZKE = 0.084805

2.3 *p*BQ neutral, anion geometry

E = -381.5533502

2.4 *p*BQ^{-}·H_2O anion complex

C	0	-4.5434105552	-1.448488443	-0.1700098447
C	0	-3.2682670615	-1.2299105275	-0.6074321893
C	0	-2.6724998709	0.0858633908	-0.604917328
C	0	-3.5140755785	1.151100884	-0.1167651591
C	0	-4.7889247012	0.9320447228	0.3209701942
C	0	-5.3942945412	-0.3852412232	0.3268801353
H	0	-4.9773130827	-2.4446635029	-0.1793052862
H	0	-2.6491242751	-2.0402028649	-0.9802996864
H	0	-3.0775546946	2.1461043617	-0.1132241497
H	0	-5.408356726	1.7464207139	0.6868283114
O	0	-1.4843487101	0.3072466912	-1.0054623227
O	0	-6.5686354261	-0.5889324824	0.7319868138
O	0	-0.0842873875	-1.9720267897	-1.5086980348
H	0	-0.0656350181	-2.2480692486	-0.5867446243
H	0	-0.5703902812	-1.1098942323	-1.4413598196

E = -458.1043335 ZKE = 0.108116

2.5 *p*BQ·H_2O neutral complex

C	0	-0.8324350792	-1.2472117375	-0.0556903321
C	0	0.410692974	-0.7567142152	-0.0490269829
C	0	0.647137111	0.7048704326	0.0010993647
C	0	-0.5319166478	1.5993146643	0.0438713446
C	0	-1.7725706995	1.1052690552	0.0371387985
C	0	-2.0183746611	-0.3582057297	-0.0124197858
H	0	-1.0411090077	-2.3100865447	-0.0928347596
H	0	1.3014542738	-1.3760846847	-0.0791036675
H	0	-0.3196725125	2.6614662561	0.0788574571
H	0	-2.6562465286	1.7319588057	0.0666022157
O	0	1.77890456	1.1713129994	0.0064910697
O	0	-3.1500051119	-0.8067040732	-0.0162844824
O	0	3.6277868902	-1.0949038895	-0.0554530568
H	0	3.9058394767	-1.1519796595	0.8647935337
H	0	3.2282883226	-0.2128999094	-0.1228555568

E = -458.0250729 ZKE = 0.109468

2.6 *p*BQ·H_2O neutral complex, anion geometry

E =-458.0115425

2.7 H_2O

O	0	0.0452134686	-0.4948194408	0.
H	0	1.0065850449	-0.4482513661	0.
H	0	-0.2318019629	0.4269540369	0.

E = -76.448838 ZKE = 0.021359

2.8 OH^{-} anion

O	0	-0.3846519368	0.53383458	0.
H	0	0.5927722368	0.53383458	0.

E = -75.7641716 ZKE = 0.007989

2.9 *p*BQ·H neutral

C	0	-4.5970372675	-1.5312182836	-0.049778242
C	0	-3.2329719799	-1.470237238	-0.1419986386
C	0	-2.5818801573	-0.2214579675	-0.1459865166
C	0	-3.3202619324	0.975989268	-0.055543256
C	0	-4.6821760273	0.9306392548	0.0370744129
C	0	-5.4024342376	-0.3290811495	0.0453737743
H	0	-5.1238289661	-2.4771842342	-0.0444162172
H	0	-2.6409785308	-2.3784333734	-0.2127207131
H	0	-2.7775666442	1.9134922859	-0.0622023936
H	0	-5.2753138185	1.8338508877	0.1077294158
O	0	-6.6472299726	-0.3777771431	0.1297410706
O	0	-1.237381106	-0.1078771043	-0.2348849168
H	0	-0.8389043499	-0.9850626385	-0.2912973291

E = -382.1664072 ZKE = 0.095893