Supporting Information

Microhydration Structures of Protonated Oxazole

Kuntal Chatterjee and Otto Dopfer*

Institut für Optik und Atomare Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

* Corresponding author: dopfer@physik.tu-berlin.de

Figure Captions

Figure S1. Optimized structure of the neutral Ox-W dimer and its linear IR absorption spectrum calculated at the B3LYP-D3/aug-cc-pVTZ level. Binding energy (D_0) and bond lengths are given in cm^{-1} and Å, respectively.

Figure S2. NBO atomic charge distribution (in e) of selected $H^+Ox\text{-}W_{n\leq4}$ structures obtained at the B3LYP-D3/aug-cc-pVTZ level.

Figure S3. Potential energy barrier (E_e) for internal rotation of the W ligand in $H^+Ox\text{-}W(H)$ calculated at the B3LYP-D3/aug-cc-pVTZ level in cm^{-1}. Bond lengths are given in Å.

Figure S4. Optimized structure and linear IR absorption spectrum of the $H^+Ox\text{-}W(C5)$ isomer calculated at the B3LYP-D3/aug-cc-pVTZ level. Binding energy (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parentheses correspond to relative energies and free energies (E_0, G_0) with respect to $H^+Ox\text{-}W(H)$ in cm^{-1}.

Figure S5. Potential energy barrier (E_e) between $H^+Ox\text{-}W_4(b)$ and $Ox\text{-}H^+W_4(1)$ evaluated at the B3LYP-D3/aug-cc-pVTZ level in cm^{-1}.

Figure S6. Orbital interaction between the σ* orbital of the X-H bond (X=N/O/C) and the lone pair of O involved in the XH…O H-bonds of selected $H^+Ox\text{-}W_{n\leq4}$ isomers obtained from the NBO analysis at the B3LYP-D3/aug-cc-pVTZ level. $E^{(2)}$ values given in kJ/mol.

Figure S7. Visualization of the NCI analysis of the XH…O (X=N/O/C) H-bonds in selected $H^+Ox\text{-}W_{n\leq4}$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. ρ* values for the H-bonds are given in a.u.

Figure S8. Experimental proton affinities of W_n clusters (n=1-4) and Ox.

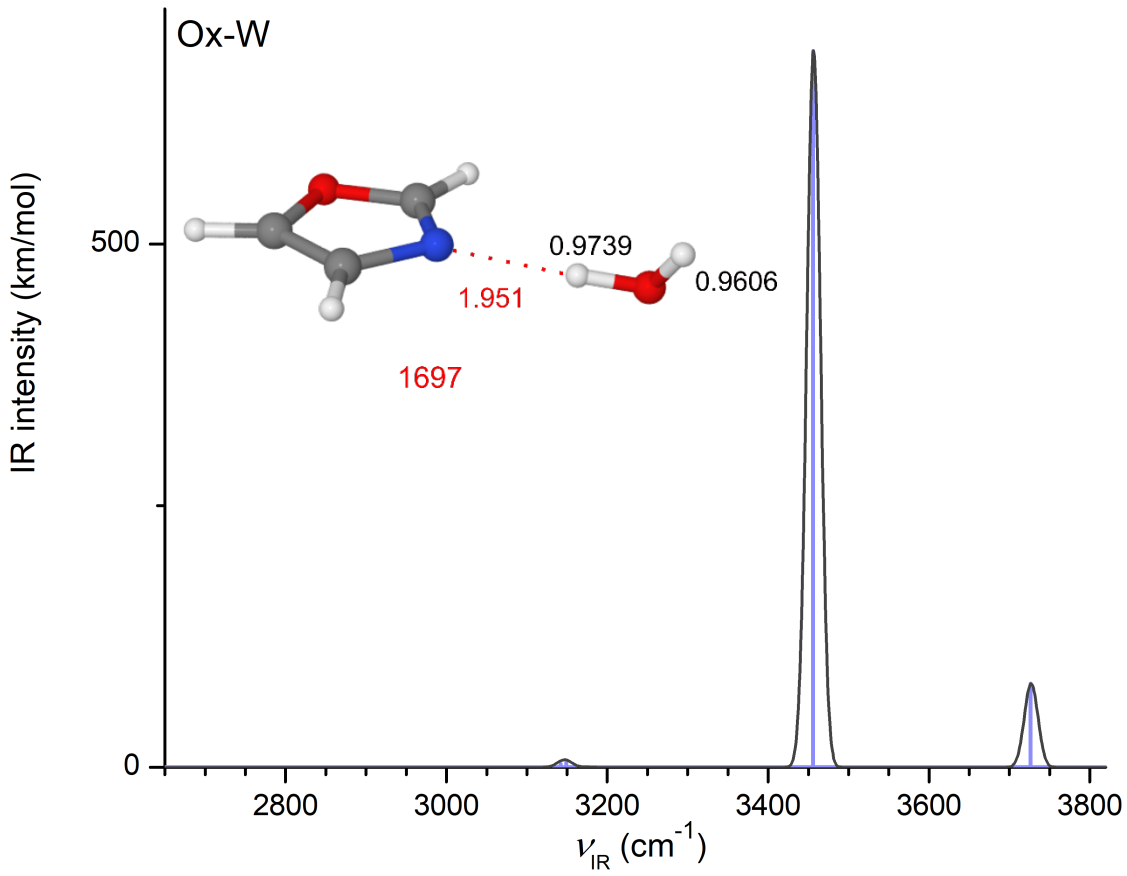
Ox-W
IR intensity (km/mol)
500
0
0.9739
0.9606
1.951
1697
2800
3000
3200
3400
3600
3800
ν_{IR} (cm^{-1})

Figure S1

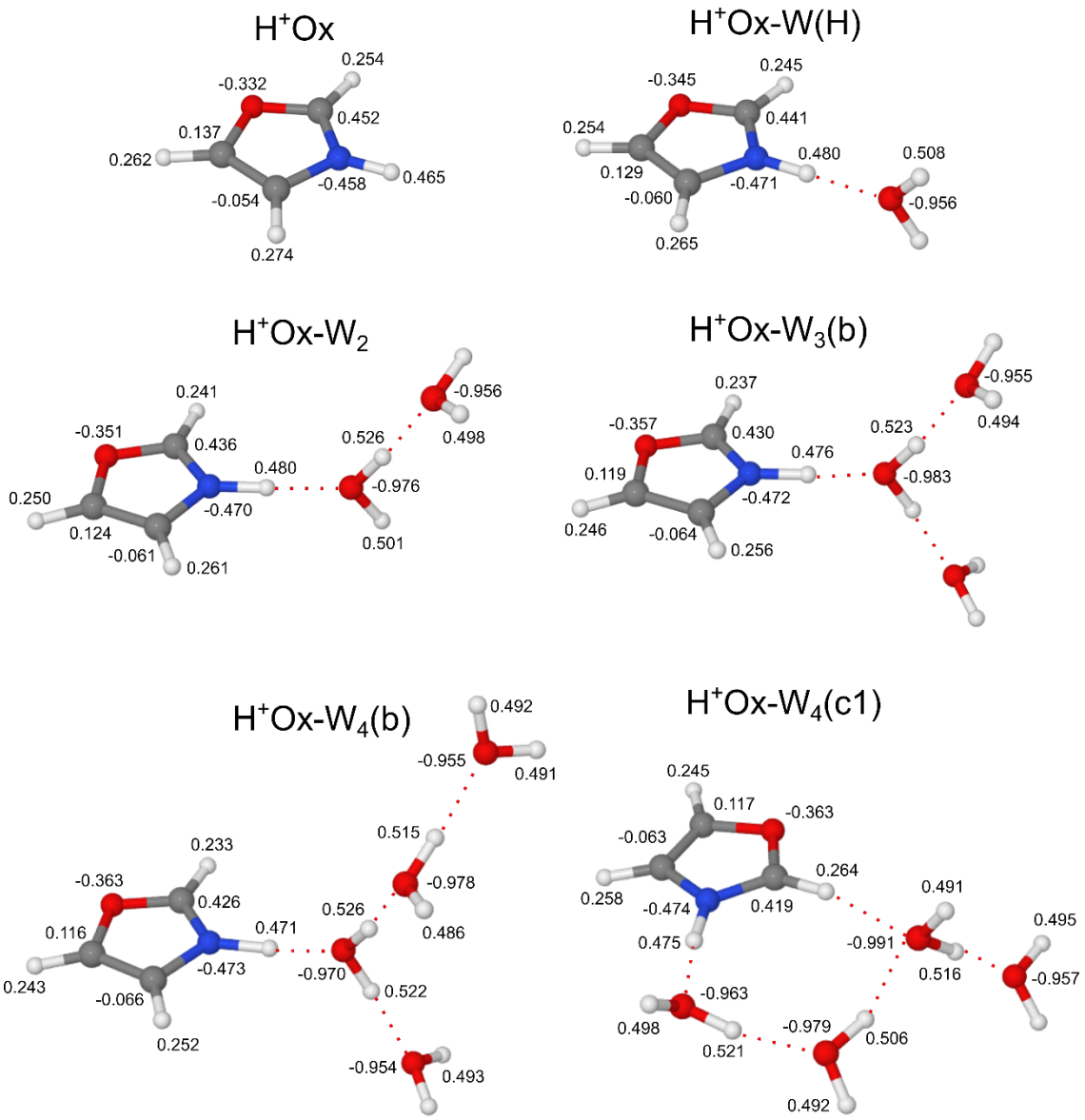
H+Ox
0.254
-0.332
0.452
0.137
0.262
0.465
-0.458
-0.054
0.274
H+Ox-W(H)
0.245
-0.345
0.441
0.254
0.480
0.508
0.129
-0.471
-0.060
-0.956
0.265
H+Ox-W2
0.241
-0.956
-0.351
0.436
0.526
0.498
0.480
-0.976
0.250
-0.470
0.124
0.501
-0.061
0.261
H+Ox-W3(b)
0.237
-0.955
-0.357
0.430
0.523
0.494
0.476
0.119
-0.983
-0.472
0.246
-0.064
0.256
H+Ox-W4(b)
0.492
-0.955
0.491
0.515
0.233
-0.978
-0.363
0.426
0.526
0.471
0.116
0.486
-0.970
-0.473
0.243
0.522
-0.066
0.252
-0.954
0.493
H+Ox-W4(c1)
0.245
0.117
-0.363
-0.063
0.264
0.491
0.258
-0.474
0.419
0.495
0.475
-0.991
0.516
-0.957
-0.963
0.498
-0.979
0.506
0.521
0.492

Figure S2

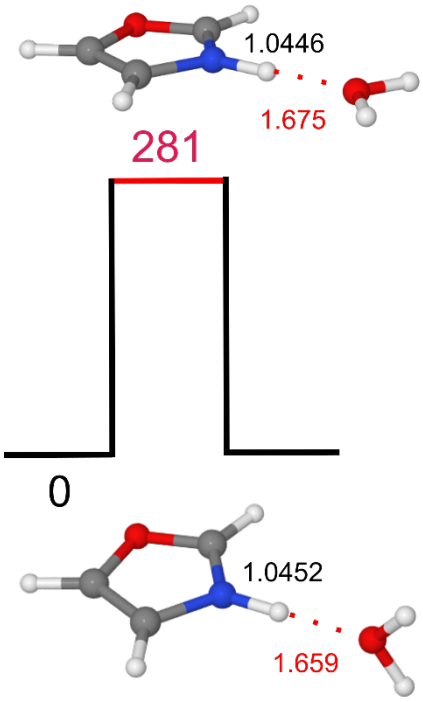

Figure S3

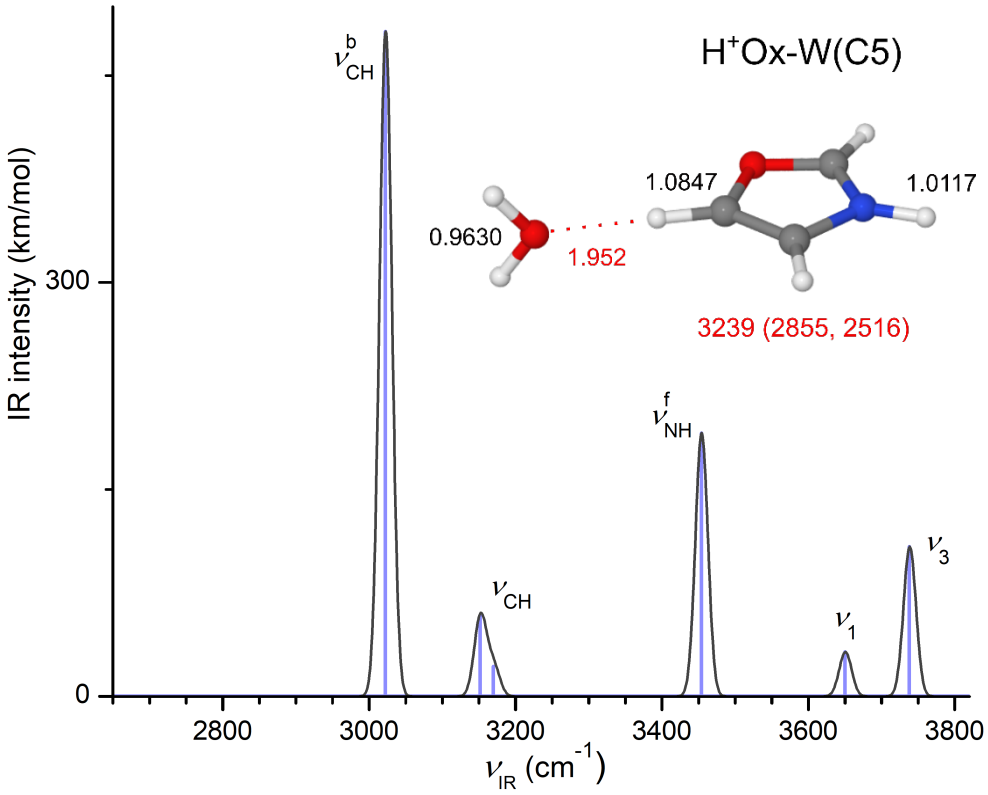
H+Ox-W(C5)
IR intensity (km/mol)
300
0
2800
3000
3200
3400
3600
3800
νIR (cm-1)
νCHb
νCH
νNHf
ν1
ν3
0.9630
1.952
1.0847
1.0117
3239 (2855, 2516)

Figure S4

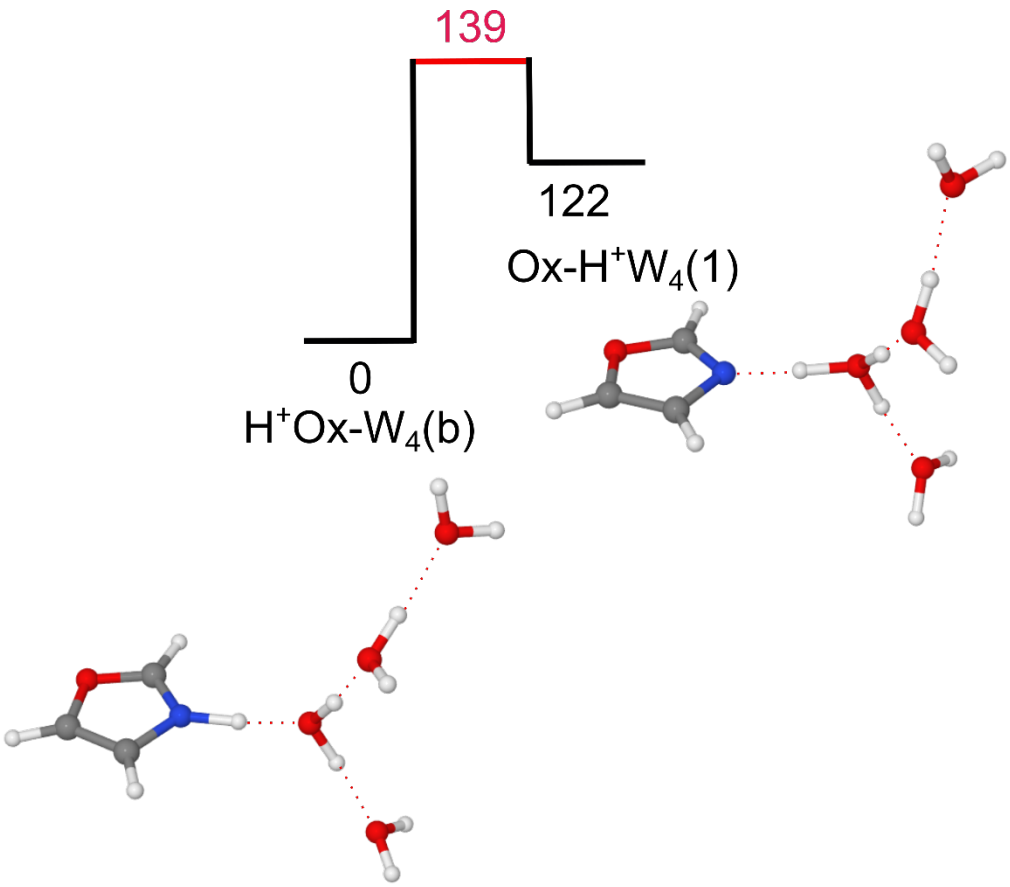

Figure S5

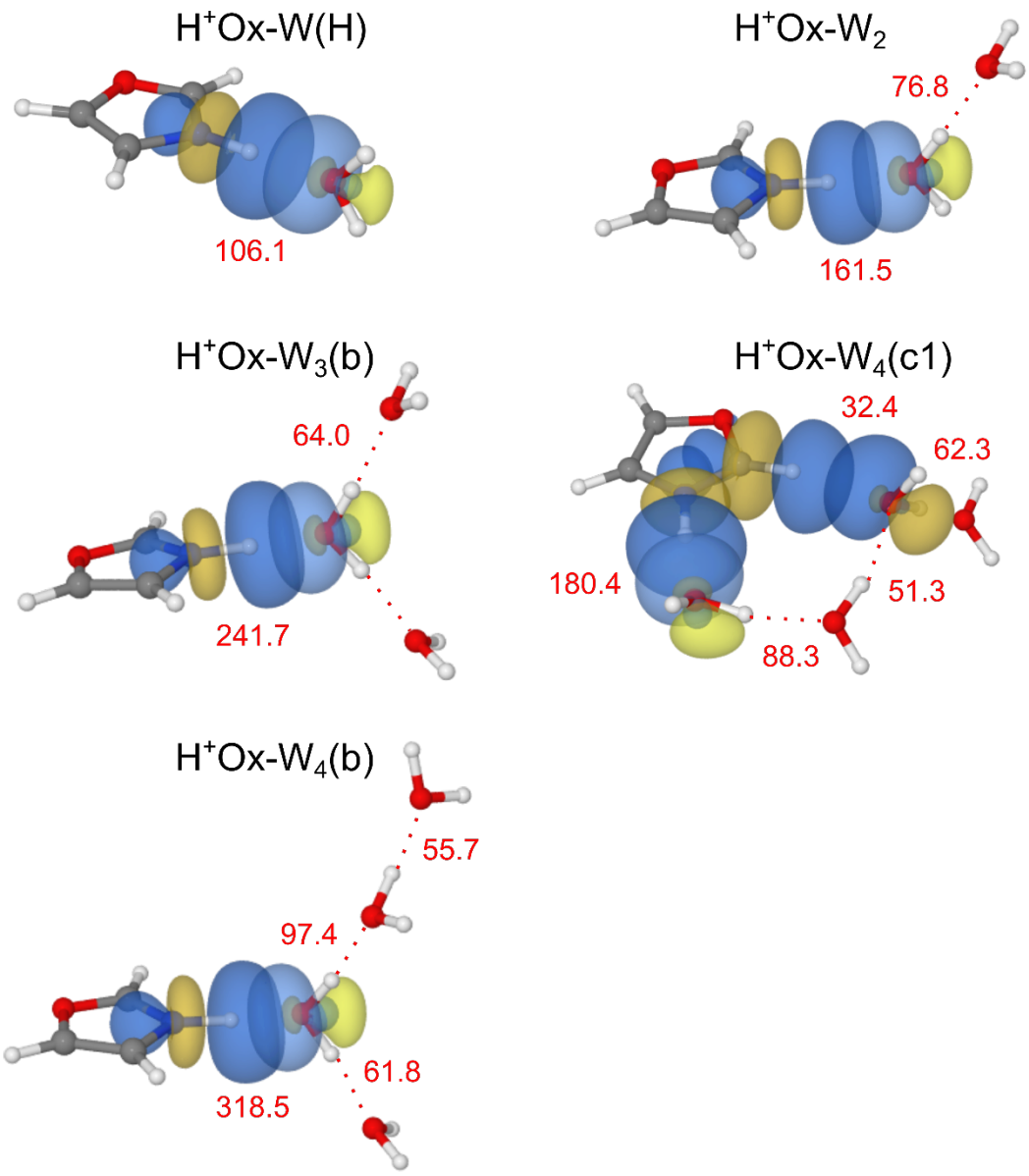
H+Ox-W(H)
106.1
H+Ox-W2
76.8
161.5
H+Ox-W3(b)
64.0
241.7
H+Ox-W4(c1)
32.4
62.3
180.4
51.3
88.3
H+Ox-W4(b)
55.7
97.4
61.8
318.5

Figure S6

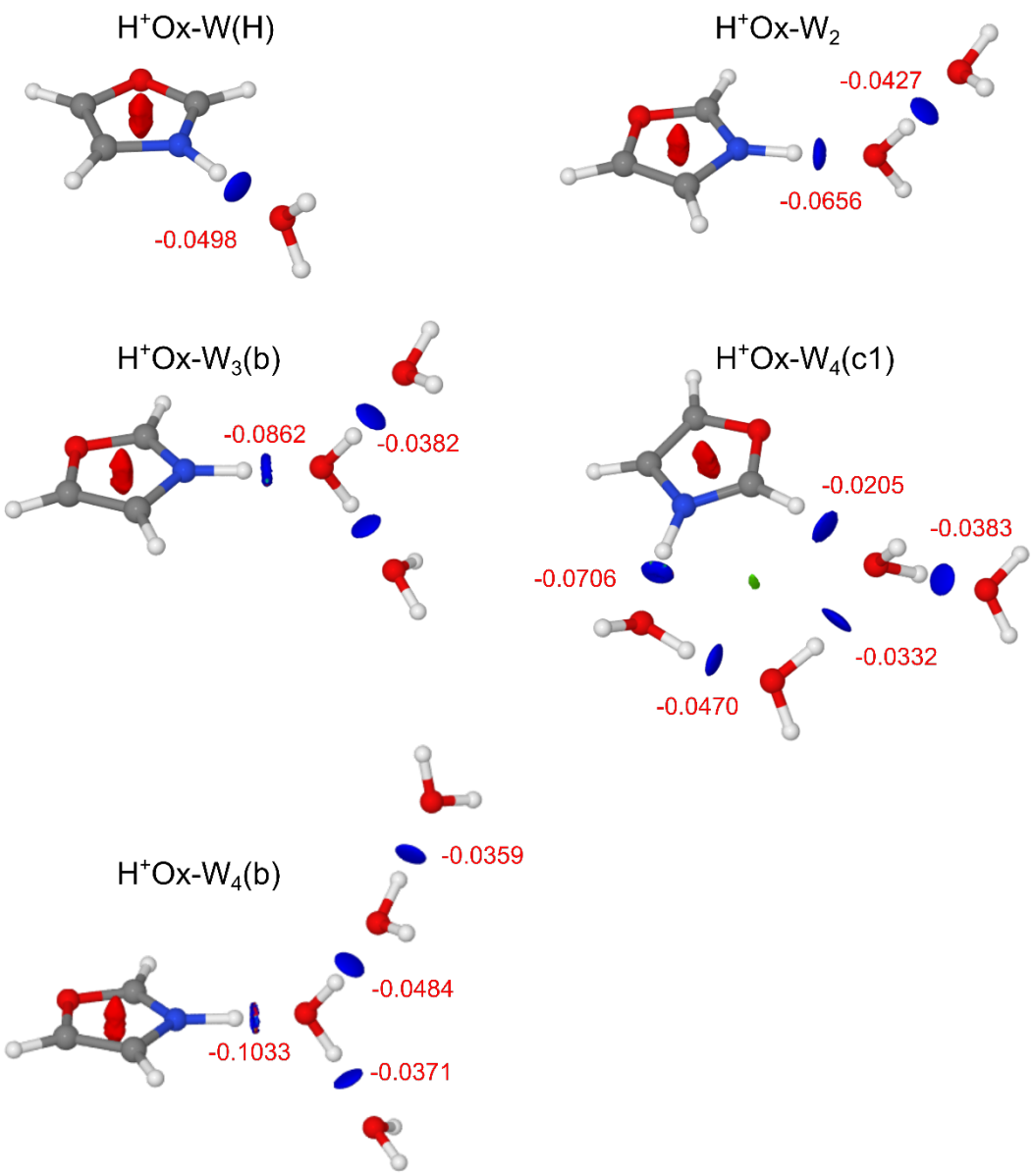
H+Ox-W(H)
-0.0498
H+Ox-W2
-0.0427
-0.0656
H+Ox-W3(b)
-0.0862
-0.0382
H+Ox-W4(c1)
-0.0205
-0.0383
-0.0706
-0.0332
-0.0470
H+Ox-W4(b)
-0.0359
-0.0484
-0.1033
-0.0371

Figure S7

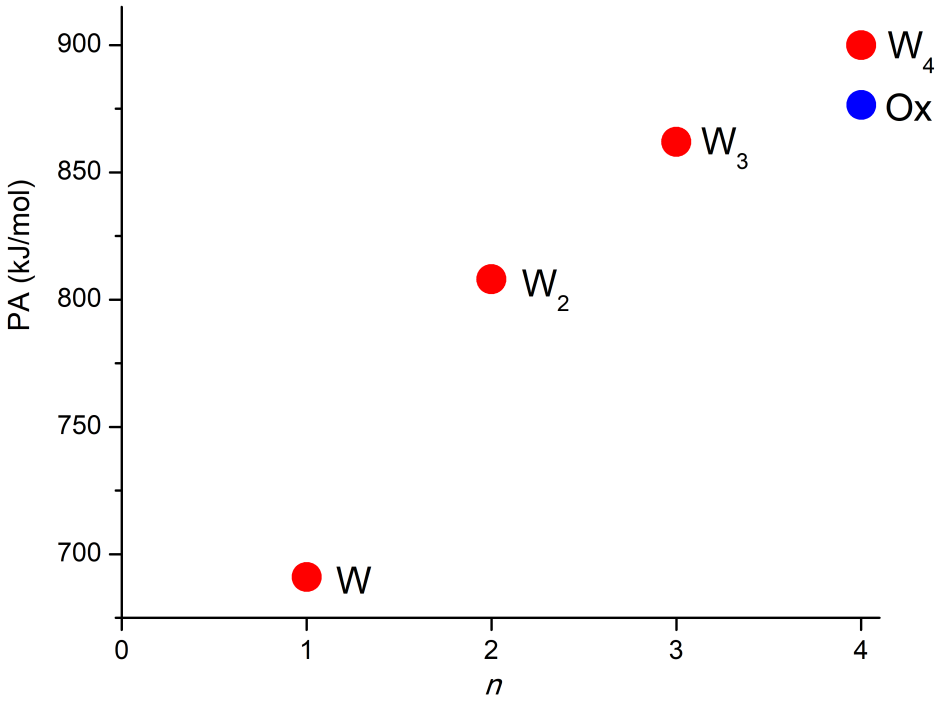

Figure S8