

Supplemental Information

Proton transfer in acetaldehyde–water clusters mediated by a single water molecule

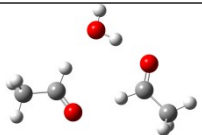
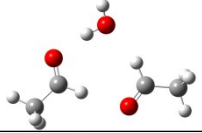
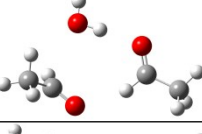
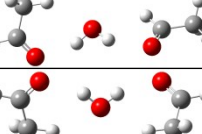
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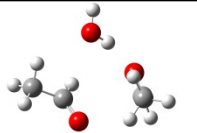
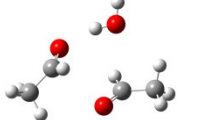
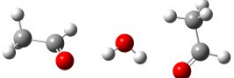
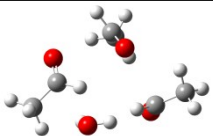
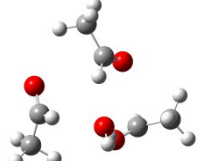
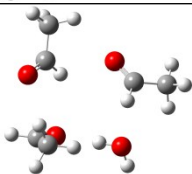
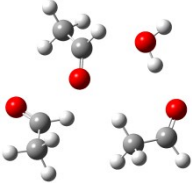
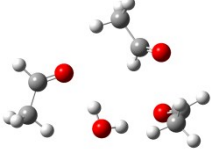
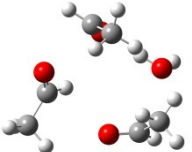
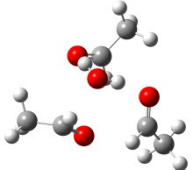
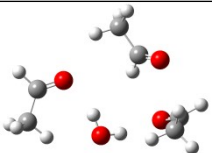
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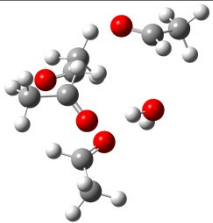
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Table S1

Names of neutral molecules and clusters considered in the paper and their pictures, adiabatic and vertical ionization energies, appearance energy given in eV; energy of neutral (sum of electronic and zero-point energies) is given in Hartree. Three different ionization processes are presented: direct ionization (DI), conventional PT (cPT), and water mediated PT (WmPT).

name	picture	aIE, eV	vIE, eV	AE, eV	Energy of neutral, Hartree	Type of ionization
dimerAwater1		8.434	9.286	8.652	-383.965444	CPT
dimerAwater3b		8.434	9.286	8.652	-383.965443	CPT
dimerBwater2		8.426	9.467	9.166	-383.966343	CPT
dimerBwater3		8.963	9.779	--	-383.963219	DI
dimerCwater2		8.999	9.875	--	-383.964148	DI

dimerCwater4a		8.206	9.613	8.737	-383.966893	WmPT
dimerDwater4		8.439	9.563	9.209	-383.966841	CPT
dimerFwater4		8.962	9.779	--	-383.963220	DI
trimerC1water34		8.220	9.279	8.236	-537.744923	CPT
trimerD1water12		8.018	9.277	8.040	-537.743349	CPT
trimerD1water42a		8.197	9.287	8.185	-537.744111	CPT
trimerD2water42		7.940	9.253	8.329	-537.740470	CPT
trimerG1water2		8.530	9.386	--	-537.743331	DI
trimerG1water4a		8.084	9.281	8.201	-537.744678	CPT
trimerG3water3a		8.511	9.471	8.902	-537.745355	WmPT
trimerG4water1		8.529	9.384	--	-537.743277	DI

trimerG4water2		7.722	9.224	8.066	-537.744707	CPT
tetramerG3water3a		8.322	9.162	8.516	-691.525914	WmPT

Optimized Cartesian coordinates of clusters listed in Table S1

dimerAwater1

C	-2.01025300	-0.35051500	-0.05925400
O	-1.26471000	-1.30328900	-0.07838100
H	-1.60513000	0.67443200	-0.15135400
C	-3.49786800	-0.46513100	0.09077100
H	-3.80502600	-1.50665300	0.18496800
H	-3.81448200	0.10517500	0.96992000
H	-3.98328900	-0.00330400	-0.77503900
C	1.93652000	-0.30351600	-0.00999300
O	2.15377300	0.88450700	0.09408800
H	0.90064700	-0.67435100	-0.11934200
C	3.01331000	-1.34123500	0.00089300
H	3.99509800	-0.88944900	0.13974400
H	2.80753900	-2.06469700	0.79586400
H	2.98047800	-1.89631800	-0.94227000
O	-0.22707400	2.39002000	-0.00888500
H	0.64909900	1.97427200	0.04973900
H	-0.07109200	3.27338200	-0.34131400

dimerAwater3b

C	2.01066200	-0.35012500	0.06019300
O	1.26464100	-1.30252800	0.07899500
H	1.60624300	0.67495500	0.15393800
C	3.49803200	-0.46545000	-0.09162000
H	3.80430400	-1.50697900	-0.18854900
H	3.81438500	0.10685000	-0.96955100
H	3.98451700	-0.00617500	0.77496500
C	-1.93669800	-0.30341300	0.01032400
O	-2.15452100	0.88452600	-0.09338000
H	-0.90068400	-0.67372200	0.12013500
C	-3.01294700	-1.34167500	-0.00172200
H	-3.99482900	-0.89031100	-0.14128300
H	-2.80614900	-2.06493400	-0.79659100
H	-2.98069100	-1.89687100	0.94139800
O	0.22696500	2.38971300	0.00839300
H	-0.64928400	1.97411000	-0.04973000
H	0.07121400	3.27336700	0.34015700

dimerBwater2

C	-1.95907700	-0.70131300	-0.45692600
O	-1.01830900	-1.44851600	-0.33202400
H	-2.13205400	-0.18460100	-1.41940900
C	-2.94540200	-0.39423200	0.62450100
H	-2.75688700	-1.00054500	1.51043100
H	-2.84363100	0.66860100	0.86248200
H	-3.96289900	-0.55776100	0.25649100

C	1.94639600	-0.15181800	-0.01171200
O	1.75130600	1.03436900	0.13847900
H	1.10686500	-0.81986800	-0.27277300
C	3.28938000	-0.79167400	0.14215800
H	4.04952200	-0.05568400	0.40215900
H	3.22928200	-1.56610500	0.91337800
H	3.55335200	-1.29897600	-0.79129200
O	-0.90598800	1.97255900	-0.15219500
H	-0.86645600	2.88028200	-0.45191800
H	0.01904400	1.70158400	-0.03175600

dimerBwater3

C	-3.61620200	-0.26084300	-0.17265400
O	-2.78547300	-1.12416800	-0.31628300
H	-4.68682100	-0.50835000	-0.32406700
C	-3.32488900	1.15899200	0.20020200
H	-2.25686600	1.32213300	0.34657900
H	-3.70818300	1.81629800	-0.58743900
H	-3.87891900	1.40587400	1.11198300
C	2.93572800	0.11777300	-0.11788300
O	2.49827100	-0.66049800	0.69457800
H	2.23488700	0.71763600	-0.73060400
C	4.39471400	0.34152900	-0.36686000
H	5.00476900	-0.29522200	0.27299100
H	4.61433200	0.14324000	-1.42071600
H	4.63034000	1.39549000	-0.18772200
O	-0.20178600	0.12633600	0.09903300
H	-0.90556600	-0.51515200	-0.05808900
H	0.52782000	-0.36002600	0.50163100

dimerCwater2

C	-3.43224700	0.23563800	0.18921800
O	-2.60903900	0.99322000	0.64141700
H	-4.50868400	0.43776200	0.36473600
C	-3.12374900	-0.98976200	-0.61274200
H	-3.61860000	-0.90653200	-1.58619200
H	-2.04920100	-1.12233500	-0.74102200
H	-3.56134900	-1.85982700	-0.11219400
C	3.43224400	0.23563900	-0.18923900
O	2.60902700	0.99322000	-0.64142300
H	4.50867800	0.43775900	-0.36478400
C	3.12376100	-0.98975500	0.61273600
H	2.04921400	-1.12232600	0.74103500
H	3.56135300	-1.85982500	0.11218900
H	3.61862600	-0.90651500	1.58617700
O	0.00000100	-0.10917000	0.00002800
H	0.71535900	0.46656100	-0.29745200
H	-0.71536700	0.46655700	0.29749400

dimerCwater4a

C	-1.43498800	-0.59255600	-0.42077800
O	-0.78799800	-1.53642800	-0.03547000
H	-1.07130600	0.01129000	-1.27485600
C	-2.71383900	-0.12735400	0.19595900
H	-3.48360300	-0.02688400	-0.57513800
H	-3.04372500	-0.80796700	0.98058500
H	-2.52733500	0.87111100	0.60421400
C	1.88618100	-0.48230200	-0.41086100
O	1.53743000	0.49528700	-1.03433000
H	2.22240700	-1.38136500	-0.95930900
C	1.92812100	-0.57231400	1.07934300
H	1.36479000	-1.45414300	1.39416400
H	2.96827800	-0.71299000	1.39294500
H	1.51261600	0.32328700	1.54158200
O	-0.27243500	2.16259700	0.34587400
H	-0.18702000	3.10394900	0.19726100
H	0.43607300	1.74922500	-0.17202400

dimerDwater4

C	-1.75241700	0.19311200	0.29357900
O	-1.44036400	1.05948500	-0.49337800
H	-1.28083500	0.16069900	1.29181100
C	-2.76343400	-0.86880900	0.01593400
H	-3.19924200	-0.74634200	-0.97514000
H	-2.26359400	-1.83804800	0.09788400
H	-3.54403800	-0.83821800	0.78237600
C	1.32468100	-0.80102400	-0.35160600
O	0.51674400	-1.46997900	0.24735800
C	2.77920100	-0.72363600	-0.02016500
H	3.37413600	-0.93781700	-0.91329100
H	2.98608800	0.31111500	0.26999000
H	3.03802700	-1.40944000	0.78614000
H	0.99799400	-0.16861300	-1.19963900
O	1.05844400	2.11892400	0.24780600
H	0.15153200	1.92886400	-0.04181100
H	1.13315300	3.07250600	0.26094600

dimerFwater4

C	-2.93571700	0.11775200	-0.11791000
O	-2.49828700	-0.66054800	0.69454200
H	-2.23484000	0.71756300	-0.73063300
C	-4.39469800	0.34157900	-0.36683300
H	-5.00474000	-0.29516800	0.27303700
H	-4.63028700	1.39554100	-0.18765500
H	-4.61437900	0.14331900	-1.42068000
C	3.61622000	-0.26083000	-0.17267900

O	2.78549400	-1.12416400	-0.31625700
H	3.87903700	1.40588800	1.11194800
C	3.32490700	1.15898900	0.20023400
H	3.70808100	1.81631500	-0.58745000
H	2.25689500	1.32208800	0.34672800
H	4.68683000	-0.50831200	-0.32420000
O	0.20172500	0.12633800	0.09902200
H	-0.52786100	-0.36004600	0.50163200
H	0.90552600	-0.51513400	-0.05806300

trimerC1water34

C	2.07530200	-1.02581100	0.38204000
O	1.87706700	-1.28829900	-0.78327900
H	1.28304600	-1.20681300	1.13058600
C	3.35710800	-0.47757900	0.91324200
H	3.75814500	-1.16659100	1.66363500
H	4.08167700	-0.32995000	0.11293800
H	3.14128500	0.46758500	1.41796500
C	0.19664400	2.09414900	0.05836400
O	0.75857800	1.41924100	0.89061500
H	-0.44310600	2.93783100	0.37462400
C	0.33111300	1.89923900	-1.41964300
H	0.93887700	1.02383300	-1.64779400
H	-0.66722800	1.79567400	-1.85102900
H	0.78678400	2.79553000	-1.85441900
C	-3.19372800	-1.11246700	0.82005100
C	-2.15038900	-0.05839200	0.63008200
O	-2.32030500	0.97665100	0.03228900
H	-1.16801400	-0.26464200	1.09784000
H	-4.12955200	-0.82908200	0.33843700
H	-2.80827700	-2.04452600	0.39860800
H	-3.35447400	-1.27208100	1.89122200
O	-0.83499200	-1.89746700	-1.16125300
H	-1.08395800	-1.74715800	-2.07310600
H	0.12571200	-1.75546400	-1.13129600

trimerD1water12

C	-2.22726000	-0.51661100	0.04040700
O	-2.44160700	0.60113300	-0.36299300
H	-1.72698000	-0.66856000	1.01681900
C	-2.57795300	-1.76566000	-0.70685700
H	-3.10422700	-1.53438300	-1.63288900
H	-1.64620400	-2.29884200	-0.92030700
H	-3.18856900	-2.41547600	-0.07211200
C	1.71392200	-1.03054300	-0.95302700
O	0.78823500	-1.55674700	-0.37136600
C	3.03395500	-0.72726100	-0.32062000
H	3.41332100	0.22681900	-0.68742200
H	2.94919000	-0.71462700	0.76668800
H	3.74050200	-1.51046800	-0.61977600
H	1.62078300	-0.80690300	-2.02869500
C	-0.34801900	3.07948500	0.36384900
C	0.35885000	1.78625500	0.12112000
O	1.10835900	1.58230100	-0.80604300
H	0.15958800	0.98549700	0.85851700
H	-0.03536500	3.83873900	-0.35256500
H	-1.42175200	2.88791900	0.27454700
H	-0.16044100	3.41361100	1.38875100

O	0.36608000	-1.03014400	2.32854800
H	0.52665800	-1.72029300	2.97151300
H	0.58399200	-1.40936300	1.46252900

trimerD1water42a

C	-1.49818300	1.50083400	-0.34155000
O	-2.23215900	0.90499700	0.41127400
H	-0.87596700	0.93659800	-1.06210100
C	-1.36121300	2.98845300	-0.38556500
H	-2.02408400	3.46455700	0.33660300
H	-0.31748100	3.23743300	-0.17703700
H	-1.58419600	3.34160700	-1.39746900
C	2.17298600	0.61117200	0.62013900
O	1.37290100	1.47034100	0.33995700
C	3.54335500	0.50272900	0.03227100
H	3.59588100	-0.45490700	-0.49291600
H	3.74475900	1.32792400	-0.65069200
H	4.28753400	0.48007600	0.83448100
H	1.90888300	-0.17548600	1.35217900
C	-1.40603200	-2.00926000	1.25274400
C	-1.82933600	-1.71139400	-0.14982000
O	-1.07409500	-1.64721900	-1.09666400
H	-2.91200200	-1.57659900	-0.30989700
H	-0.32350900	-2.11888600	1.32492000
H	-1.75464800	-1.20002300	1.89833300
H	-1.89822700	-2.93003500	1.58325800
O	1.65611900	-2.08188200	-0.59231500
H	1.90821700	-2.88045900	-1.05558400
H	0.73324800	-1.91689700	-0.85141600

trimerD2water42

C	2.75908100	-1.59993300	-0.18151300
O	3.13749300	-0.51631700	-0.55654500
H	3.38977700	-2.48872400	-0.38359700
C	1.47959800	-1.85997300	0.54341800
H	1.69709000	-2.39076200	1.47596800
H	0.93062500	-0.94167400	0.75355900
H	0.86759400	-2.53662400	-0.06334600
C	-0.51803200	1.84885800	0.96323800
O	-0.60211500	0.66636400	1.20425700
C	-1.23830800	2.54141800	-0.14709600
H	-1.75193700	3.42544000	0.24290600
H	-0.47913600	2.88693600	-0.85530400
H	-1.94429100	1.87675500	-0.64471800
H	0.13284100	2.48938000	1.58640000
C	-2.24612200	-2.04921300	0.43322300
C	-2.12859000	-1.03436500	-0.66405700
O	-3.05536800	-0.42826400	-1.13686700

H	-1.10032000	-0.85980400	-1.03991400
H	-3.28929200	-2.20116900	0.70978200
H	-1.80136500	-2.99608500	0.10967500
H	-1.67458500	-1.68932300	1.29328200
O	1.94356000	2.08813900	-0.47034600
H	2.66626300	2.66863600	-0.70821400
H	2.32240600	1.19688300	-0.48375900

trimerG1water2

C	2.80147300	-0.98380900	-0.27846800
O	2.01811800	-1.11169000	-1.19312600
C	2.60339400	-1.54095800	1.09500300
H	3.35760800	-2.31736800	1.26579400
H	2.77424300	-0.74913200	1.82784000
H	1.60346900	-1.96015700	1.21032000
H	3.75601300	-0.45380600	-0.45043200
C	-3.40363400	0.22906600	0.17931000
O	-2.26529300	0.61712800	0.05958500
C	-3.83429300	-1.20075800	0.12574200
H	-4.30907100	-1.45700700	1.07894400
H	-4.60436700	-1.30838700	-0.64522100
H	-2.99614400	-1.86888600	-0.07355600
H	-4.21072300	0.97098100	0.34513100
C	0.16863800	2.95885900	-0.13825500
C	1.02412900	1.73452400	-0.19741500
O	1.95325500	1.50999900	0.53949700
H	0.75995700	0.99759200	-0.98244600
H	0.51325200	3.64311600	0.63674200
H	0.18026600	3.45282000	-1.11508700
H	-0.86330000	2.64573100	0.04905500
O	-0.62922100	-1.78860400	-0.27463300
H	-0.95655600	-0.88604800	-0.18807200
H	0.22223600	-1.70565400	-0.72509100

trimerG1water4a

C	-2.13153500	-0.35799200	-0.27785500
O	-2.25778200	0.44334800	0.61761100
C	-2.90158200	-1.63439000	-0.38376100
H	-3.41062500	-1.67210100	-1.35197300
H	-2.18478200	-2.45958300	-0.36148200
H	-3.62226400	-1.72715900	0.42836500
H	-1.40334200	-0.16530700	-1.08867000
C	-0.35480700	2.31573200	0.11946400
O	-0.01046100	2.02500900	-1.00639600
C	0.41333800	1.96534700	1.35375700
H	0.65240200	2.88394000	1.89922500
H	-0.22851800	1.35789100	1.99646600
H	1.32902700	1.42640000	1.11000900

H	-1.27835400	2.89794400	0.27164200
C	2.28803000	-1.49148400	1.12979600
C	1.49796600	-1.91258500	-0.06977000
O	0.29435400	-1.99428900	-0.10051600
H	2.09426800	-2.16563000	-0.96612300
H	1.63019600	-1.25342800	1.96606100
H	2.97607100	-2.29582300	1.41008300
H	2.89213400	-0.62434300	0.84937700
O	2.38622200	0.59427800	-1.26742000
H	1.54924300	1.09040800	-1.26820200
H	2.83741100	0.85223700	-2.07079400

trimerG3water3a

C	-1.63605700	-1.16643200	-0.00053500
O	-0.79560400	-1.58163400	-0.76768800
C	-3.07738500	-0.98244700	-0.35463600
H	-3.69357500	-1.59891200	0.30784300
H	-3.34551600	0.06151000	-0.17203700
H	-3.26306400	-1.24660100	-1.39566800
H	-1.35699200	-0.89921900	1.03594800
C	-0.09691500	1.61621100	-0.92895800
O	-1.05677100	1.63321600	-0.19511200
C	0.92198300	2.70484300	-1.01626400
H	1.06295300	2.99813300	-2.06075500
H	0.63356700	3.56413800	-0.41136600
H	1.87271100	2.29550900	-0.65971400
H	0.07425500	0.73726700	-1.58057900
C	2.41404700	-1.91315800	-0.68297500
C	1.74394700	-1.20612100	0.44764900
O	1.82344500	-0.01473000	0.64972100
H	1.15439400	-1.84069900	1.13369100
H	2.99256600	-1.21919000	-1.29250500
H	3.06571000	-2.69749000	-0.28506700
H	1.64168900	-2.40063300	-1.28366200
O	-0.25384300	0.71763900	2.54419900
H	0.56104000	0.57588600	2.04392800
H	-0.75527700	1.31699600	1.98530100

trimerG4water1

C	2.79962400	-0.98641100	-0.27744600
O	2.01655300	-1.11305600	-1.19250700
C	2.59887100	-1.54106200	1.09665300
H	3.35164100	-2.31830000	1.26992800
H	2.76987100	-0.74815900	1.82830300
H	1.59815400	-1.95855700	1.21133900
H	3.75587700	-0.45947800	-0.44936400
C	1.02595500	1.73404800	-0.19788300
O	1.95609600	1.51058800	0.53806600

C	0.17146400	2.95918600	-0.14014300
H	0.18371200	3.45183400	-1.11765200
H	-0.86081900	2.64756800	0.04762800
H	0.51690000	3.64421900	0.63380900
H	0.76020600	0.99577600	-0.98110600
C	-3.83676600	-1.19562300	0.12507600
C	-3.40122700	0.23270500	0.17956500
O	-2.26095700	0.61619400	0.06356100
H	-4.20599300	0.97776700	0.34246500
H	-4.60577200	-1.30093400	-0.64722400
H	-3.00015900	-1.86610600	-0.07270600
H	-4.31386000	-1.45040900	1.07752000
O	-0.63178400	-1.79283700	-0.27726400
H	-0.95665500	-0.88983700	-0.18593400
H	0.22010700	-1.70954700	-0.72679500

trimerG4water2

C	-2.53410700	0.11296300	0.29275900
O	-2.17642600	-1.02980500	0.47801600
C	-3.11696600	0.60969100	-0.98753800
H	-4.09999200	1.05116800	-0.79604100
H	-2.46782500	1.40610900	-1.36163600
H	-3.19746800	-0.19369300	-1.71925600
H	-2.44464100	0.85804400	1.10207100
C	0.79527200	1.56892500	0.45183400
O	-0.25665300	1.71262900	-0.13208700
C	1.99687400	2.42964800	0.23110700
H	2.32239900	2.85383300	1.18629400
H	2.80520900	1.78723400	-0.13014400
H	1.78622100	3.22290400	-0.48617700
H	0.90484700	0.75402600	1.19069500
C	0.66403500	-1.52184000	-1.44767200
C	1.88412000	-1.56874800	-0.58079400
O	2.68959000	-0.67585900	-0.48614900
H	2.03044400	-2.50974200	-0.01678400
H	0.56264800	-0.54860500	-1.92812700
H	0.74180700	-2.30794800	-2.20685000
H	-0.22285700	-1.73896100	-0.84677100
O	0.20163000	-1.39658400	1.88996100
H	0.19282300	-1.92811500	2.68547200
H	-0.71410300	-1.37313700	1.57115400

tetramerG3water3a

C	-0.15906800	0.59287400	-1.71609500
O	0.69019200	-0.18385200	-2.08917800
C	-0.63894400	1.76376800	-2.51253400
H	-1.71926200	1.67156300	-2.66261900
H	-0.46544500	2.67325000	-1.93022400
H	-0.12797700	1.82438900	-3.47329500
H	-0.64132200	0.45924200	-0.73242500
C	2.36523700	1.30256000	0.28701600
O	1.37648600	1.99882700	0.26877000
C	3.16442700	1.00137300	1.51157800
H	4.22429200	1.19494700	1.32205600
H	2.81312400	1.58186000	2.36442300
H	3.05461800	-0.06832600	1.71864100
H	2.70789300	0.82262000	-0.64960300
C	1.51253200	-3.01440300	-0.70427900
C	0.65450200	-2.07201800	0.07169600
O	1.04925300	-1.42672600	1.02188000
H	-0.39697600	-1.98258200	-0.25145600
H	2.50325800	-3.10430900	-0.25867800
H	1.02697600	-3.99340100	-0.75778100
H	1.58674200	-2.62990500	-1.72546200
O	-0.66452400	0.68996400	1.93473800
H	-0.09995200	-0.07787800	1.75872900
H	-0.14849800	1.42943900	1.59799500
C	-3.71110500	0.72053800	0.88258100
C	-2.97561100	-0.57958800	0.80757400
O	-2.59231200	-1.09353600	-0.21601300
H	-2.79811100	-1.07672300	1.78018400
H	-3.84829500	1.15213400	-0.10911400
H	-4.68292200	0.56224900	1.36119900
H	-3.13272700	1.39339800	1.52062700