Electronic Supplementary Material for PCCP
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Characterization of the bond between hydrogen and the non-nuclear attractor in anionic water clusters

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Supplementary Information

Structural coordinates for the optimized anionic water clusters

Tetramer, $(H_2O)_4^-$

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	-1.49754000	-0.42692600	-0.15214100
H	-0.42692600	1.49754000	-0.15214100
H	1.49754000	0.42692600	-0.15214100
H	0.42692600	-1.49754000	-0.15214100
O	-1.40132500	-1.40132500	-0.08800200
O	-1.40132500	1.40132500	-0.08800200
O	1.40132500	1.40132500	-0.08800200
O	1.40132500	-1.40132500	-0.08800200
H	-1.52811800	-1.56364600	0.85615400
H	-1.56364600	1.52811800	0.85615400
H	1.52811800	1.56364600	0.85615400
H	1.56364600	-1.52811800	0.85615400

Hexamer, $(H_2O)_6^-$

	Coordinates (Angstroms)		
Atom	X	Y	Z
O	1.80705500	-1.68015600	2.35652600
H	1.99080800	-1.29078200	1.49323900
H	0.98350800	-2.17833600	2.20336400
H	-1.17488300	-2.19353800	1.29120700
O	-0.94082600	-2.43701600	2.19485400
H	-0.96902000	-1.58514000	2.66748900
H	-0.36561300	0.67894500	2.69525200
O	-0.21240300	0.04384900	3.40505600
H	0.64598600	-0.35125800	3.16645600
H	-2.00045400	1.25494200	-1.51079500
O	-1.82325400	1.61998200	-2.38600200
H	-1.32572600	0.90683600	-2.82618300
O	0.89105400	2.47769100	-2.16993900
H	1.14523800	2.21776700	-1.27636800
H	-0.08257000	2.44464300	-2.14106100
H	0.74781600	0.76325000	-3.07006700
O	0.27837500	-0.02435000	-3.40049400
H	0.40490500	-0.66733100	-2.69253400

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Octamer, $(H_2O)_8^-$

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	3.11304700	1.40958800	0.63181600
H	3.11261700	-0.63185400	1.40939300
H	3.11301800	-1.40959200	-0.63181900
H	3.11261400	0.63184800	-1.40939500
O	3.07587700	1.95428800	-0.18365200
O	3.07437700	0.18367700	1.95391100
O	3.07584400	-1.95429300	0.18365000
O	3.07435800	-0.18368200	-1.95391500
H	2.16445700	2.26592300	-0.20110400
H	2.16242100	0.20097300	2.26401200
H	2.16441800	-2.26591100	0.20110700
H	2.16239800	-0.20096700	-2.26400500
O	-3.07504900	-1.22875500	1.53047700
O	-3.07516900	-1.53050000	-1.22876600
O	-3.07518100	1.53050300	1.22876800
O	-3.07505700	1.22875700	-1.53047500
H	-3.11284900	1.52457200	0.24815200
H	-3.11281100	0.24814500	-1.52456400
H	-3.11283000	-1.52456900	-0.24814900
H	-3.11280900	-0.24814300	1.52456700
H	-2.16334400	1.41429900	-1.78041900
H	-2.16351100	1.78054000	1.41438900
H	-2.16333700	-1.41429300	1.78042700
H	-2.16349900	-1.78053300	-1.41439300

Decamer, $(H_2O)_{10}^-$

	Coordinates (Angstroms)		
Atom	X	Y	Z
O	0.73377300	2.22355100	3.14024600
O	1.88797400	1.38497500	-3.14024600
O	-1.88797400	1.38497500	3.14024600
O	-1.90060500	-1.36759000	3.14024600
O	0.71333600	-2.23019100	3.14024600
O	2.34147100	-0.01074500	3.14024600
O	1.90060500	-1.36759000	-3.14024600
O	-0.71333600	-2.23019100	-3.14024600
O	-2.34147100	-0.01074500	-3.14024600
O	-0.73377300	2.22355100	-3.14024600
H	-0.20265700	1.93068000	3.19090500
H	-1.89881000	0.40387500	3.19090500
H	-0.97087200	-1.68107200	3.19090500
H	1.29877800	-1.44283400	3.19090500
H	1.77356100	0.78935100	3.19090500
H	0.81531600	2.55765600	2.24185300
H	-2.18052900	1.56577100	2.24185300
H	-2.16295700	-1.58995600	2.24185300
H	0.84374800	-2.54841800	2.24185300
H	2.68442200	0.01494800	2.24185300
H	1.89881000	0.40387500	-3.19090500
H	0.97087200	-1.68107200	-3.19090500
H	-1.29877800	-1.44283400	-3.19090500

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H	-1.77356100	0.78935100	-3.19090500
H	0.20265700	1.93068000	-3.19090500
H	2.18052900	1.56577100	-2.24185300
H	2.16295700	-1.58995600	-2.24185300
H	-0.84374800	-2.54841800	-2.24185300
H	-2.68442200	0.01494800	-2.24185300
H	-0.81531600	2.55765600	-2.24185300