Supporting Information

Ionic-charge dependence of the intermolecular Coulombic decay time-scale for aqueous ions probed by the core-hole clock

W. Pokapanich,[†] N. V. Kryzhevoi,[*,‡] N. Ottosson,[†] S. Svensson,[†] L. S. Cederbaum,[‡] G. Öhrwall,[¶] and O. Björneholm[*,†]

Department of Physics and Astronomy, Uppsala University, P.O. Box 516, SE-751 20 Uppsala, Sweden, Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany, and MAX-lab, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden

E-mail: nikolai.kryzhevoi@tc.pci.uni-heidelberg.de; olle.bjorneholm@fysik.uu.se

TABLE I: The geometrical coordinates (atomic units) and the energies (Hartrees) of the $Ca^{2+}(H_2O)_n$ clusters obtained at the MP2/6-311++G(2d,2p) level of theory.

$Ca^{2+}(H_2O)_1$	Energy:	-752.8344603	
ca	0.000000	0.000000	0.000000
o	0.000000	0.000000	4.279369
h	1.444559	0.000000	5.407312
h	-1.444559	0.000000	5.407312

$Ca^{2+}(H_2O)_2$	Energy:	-829.2278038	
ca	0.000000	0.000000	0.000000
o	0.000000	0.000000	4.368234
o	0.000000	0.000000	-4.368234
h	1.441230	0.000000	5.494592
h	-1.441230	0.000000	5.494592
h	0.000000	-1.441230	-5.494592
h	0.000000	1.441230	-5.494592

$Ca^{2+}(H_2O)_4$	Energy:	-981.9922268	
ca	0.000000	0.000000	0.000000
o	0.000000	0.000000	4.436510
o	4.182781	0.000000	-1.478837
o	-2.091391	-3.622395	-1.478837
o	-2.091391	3.622395	-1.478837
h	0.365978	-1.393569	5.554623
h	-0.365978	1.393569	5.554623
h	4.773664	0.379838	-3.161909
h	5.700234	-0.379838	-0.541173
h	-3.667038	-4.324033	-0.886220
h	-1.569911	-4.746629	-2.816862
h	-1.472604	5.337764	-1.506494
h	-3.764345	3.732897	-2.196589

$Ca^{2+}(H_2O)_6$	Energy:	-1134.7250197	
ca	0.000000	0.000000	0.000000
o	0.000000	0.000000	-4.537232
o	0.000000	-4.537232	0.000000
o	0.000000	0.000000	4.537232
o	0.000000	4.537232	0.000000
o	-4.537232	0.000000	0.000000
o	4.537232	0.000000	0.000000
h	0.000000	-1.443211	-5.644831
h	0.000000	1.443211	-5.644831
h	0.000000	1.443211	5.644831
h	0.000000	-1.443211	5.644831
h	-1.443211	-5.644831	0.000000
h	1.443211	-5.644831	0.000000
h	1.443211	5.644831	0.000000
h	-1.443211	5.644831	0.000000
h	5.644831	0.000000	1.443211
h	5.644831	0.000000	-1.443211
h	-5.644831	0.000000	-1.443211
h	-5.644831	0.000000	1.443211

TABLE II: The geometrical coordinates (atomic units) and the energies (Hartrees) of the $K^+(H_2O)_n$ clusters obtained at the MP2/6-311++G(2d,2p) level of theory.

$K^+(H_2O)_1$		Energy:	-675.6363000
k	0.000000	0.000000	0.000000
o	0.000000	0.000000	4.984719
h	1.430101	0.000000	6.102970
h	-1.430101	0.000000	6.102970

$K^+(H_2O)_2$		Energy:	-751.9789279
k	0.000000	0.000000	0.000000
o	0.000000	0.000000	5.055962
o	0.000000	0.000000	-5.055962
h	1.430222	0.000000	6.172622
h	-1.430222	0.000000	6.172622
h	0.000000	-1.430222	-6.172622
h	0.000000	1.430222	-6.172622

$K^+(H_2O)_4$		Energy:	-904.6562700
k	0.000000	0.000000	0.000000
o	0.000000	0.000000	5.127582
o	4.834331	0.000000	-1.709194
o	-2.417166	-4.186654	-1.709194
o	-2.417166	4.186654	-1.709194
h	0.374536	-1.381216	6.240970
h	-0.374536	1.381216	6.240970
h	5.422898	0.366251	-3.384639
h	6.345188	-0.366251	-0.776008
h	-3.989157	-4.879492	-1.129123
h	-1.894886	-5.311969	-3.031524
h	-1.808276	5.894458	-1.727208
h	-4.075767	4.297004	-2.433439

$K^+(H_2O)_6$		Energy:	-1057.3241931
k	0.000000	0.000000	0.000000
o	0.000000	0.000000	-5.216400
o	0.000000	-5.216400	0.000000
o	0.000000	0.000000	5.216400
o	0.000000	5.216400	0.000000
o	-5.216400	0.000000	0.000000
o	5.216400	0.000000	0.000000
h	0.000000	-1.433975	-6.324408
h	0.000000	1.433975	-6.324408
h	0.000000	1.433975	6.324408
h	0.000000	-1.433975	6.324408
h	-1.433975	-6.324408	0.000000
h	1.433975	-6.324408	0.000000
h	1.433975	6.324408	0.000000
h	-1.433975	6.324408	0.000000
h	6.324408	0.000000	1.433975
h	6.324408	0.000000	-1.433975
h	-6.324408	0.000000	-1.433975
h	-6.324408	0.000000	1.433975