Supplementary Information

Title: Structural transitions in ion coordination driven by changes in competition for ligand binding

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Supplementary Figures

Figure S1: Optimized structures of gas-phase Na^+-water coordination complexes. The Na^+-O distances depicted next to the dashed lines connecting the atom centers are in Ångstrom units. Note a natural increase in ion-ligand distance occurs with increase in coordination number. The 6-31G(d) basis set was used to describe Na^+ ions, while the O and H atoms were described using the 6-31++G(d,p) basis set.

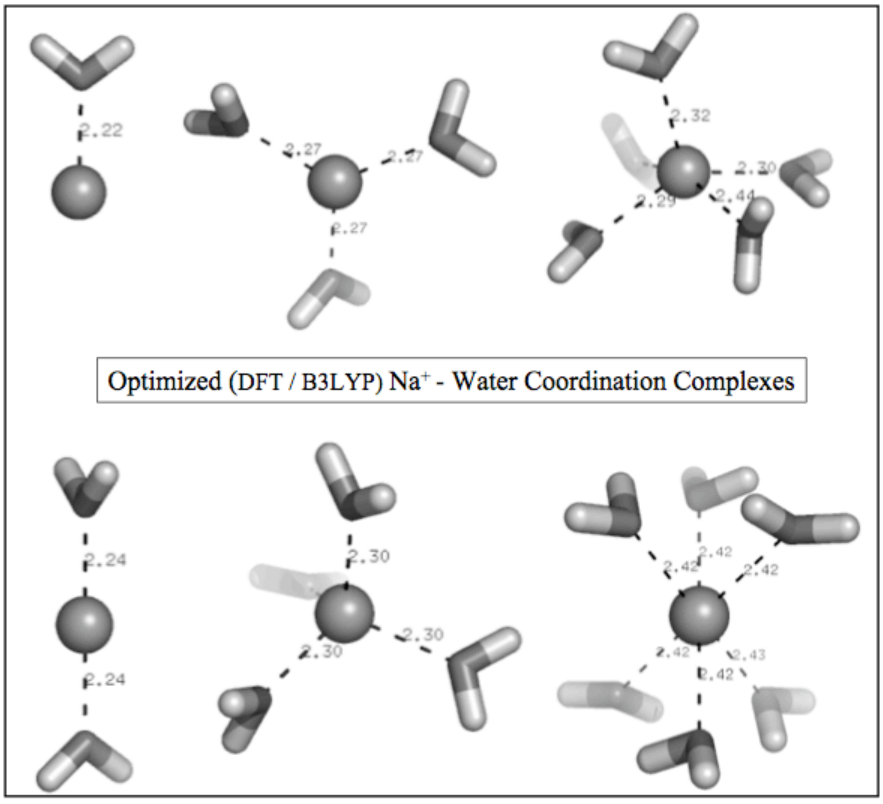
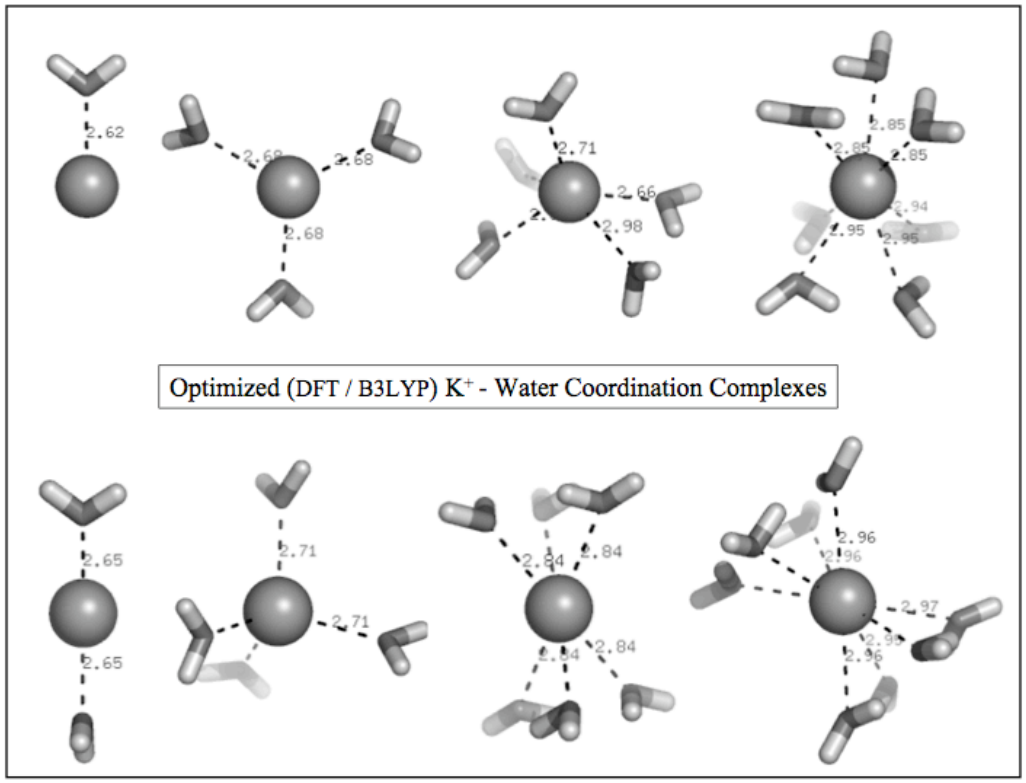


Figure S2: Optimized structures of gas-phase K^+-water coordination complexes. The K^+-O distances depicted next to the dashed lines connecting the atom centers are in Ångstrom units. Note as in Na^+ clusters, there is a natural increase in ion-ligand distance with increase in coordination number. The 6-311+G(2d) basis set was used to describe K^+ ions, while the O and H atoms were described using the 6-31++G(d,p) basis set.



Reference 36 in main manuscript cited in full: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., Gaussian 03. In Gaussian, Inc., Wallingford CT: 2004.