

Supporting Information:
**Nanometer Patterning of Water by Tetraanionic
Ferrocyanide Stabilized in Aqueous Nanodrops**

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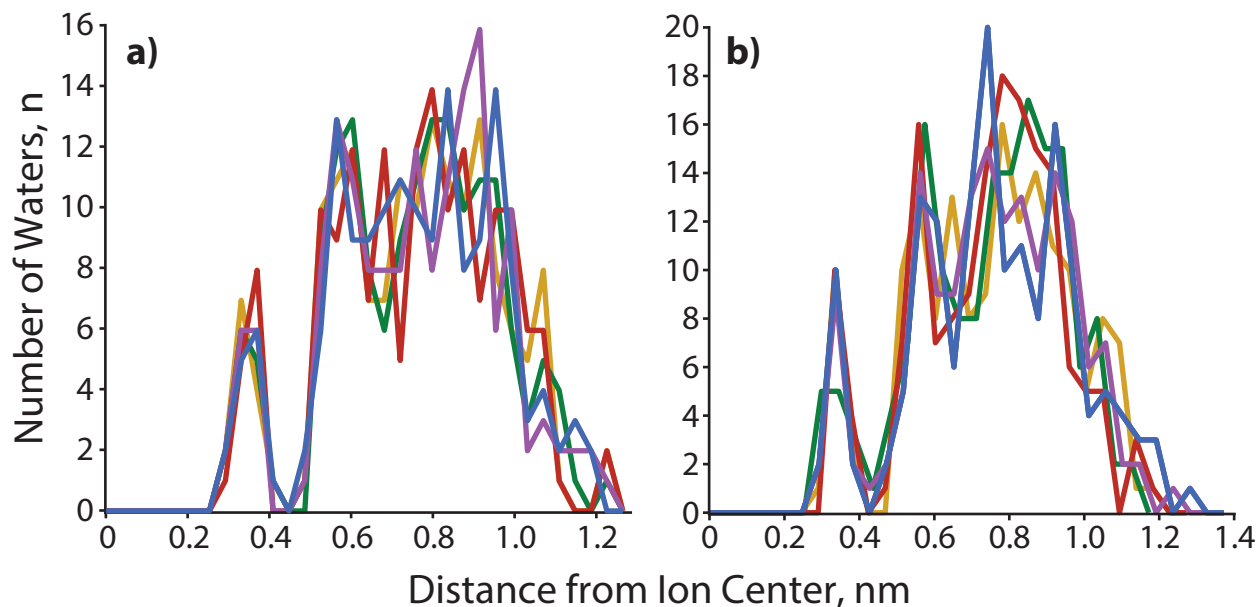


Figure 1: [Figure S1] Comparison of the radial distribution functions for five individual structures of $\text{Fe}(\text{CN})_6^{4-}(\text{H}_2\text{O})_{160}$, each plotted as a different color and taken from (a) 20 ps separations within the final 1 ns of a single annealing cycle and (b) the final structure within the last 1 ns of five separate annealing cycles. These plots illustrate that although the RMS displacement of a single water molecule at 133 K during the last 1 ns of a single cycle is $\sim 0.78 \pm 0.24 \text{ \AA}$, there is still an appreciable change to the overall nanodrop within this 20 ps timescale. The use of a simulated annealing cycle increases the RMS displacement for a single water molecule to $\sim 10.07 \pm 1.95 \text{ \AA}$, which indicates the potential energy of the system is sufficient to overcome local minima and exchange water molecules between hydration shells. The structure of a fourth solvation shell is apparent in the single distributions, which were used to calculate an average center of $\sim 1.10 \text{ nm}$ (Figure 7).

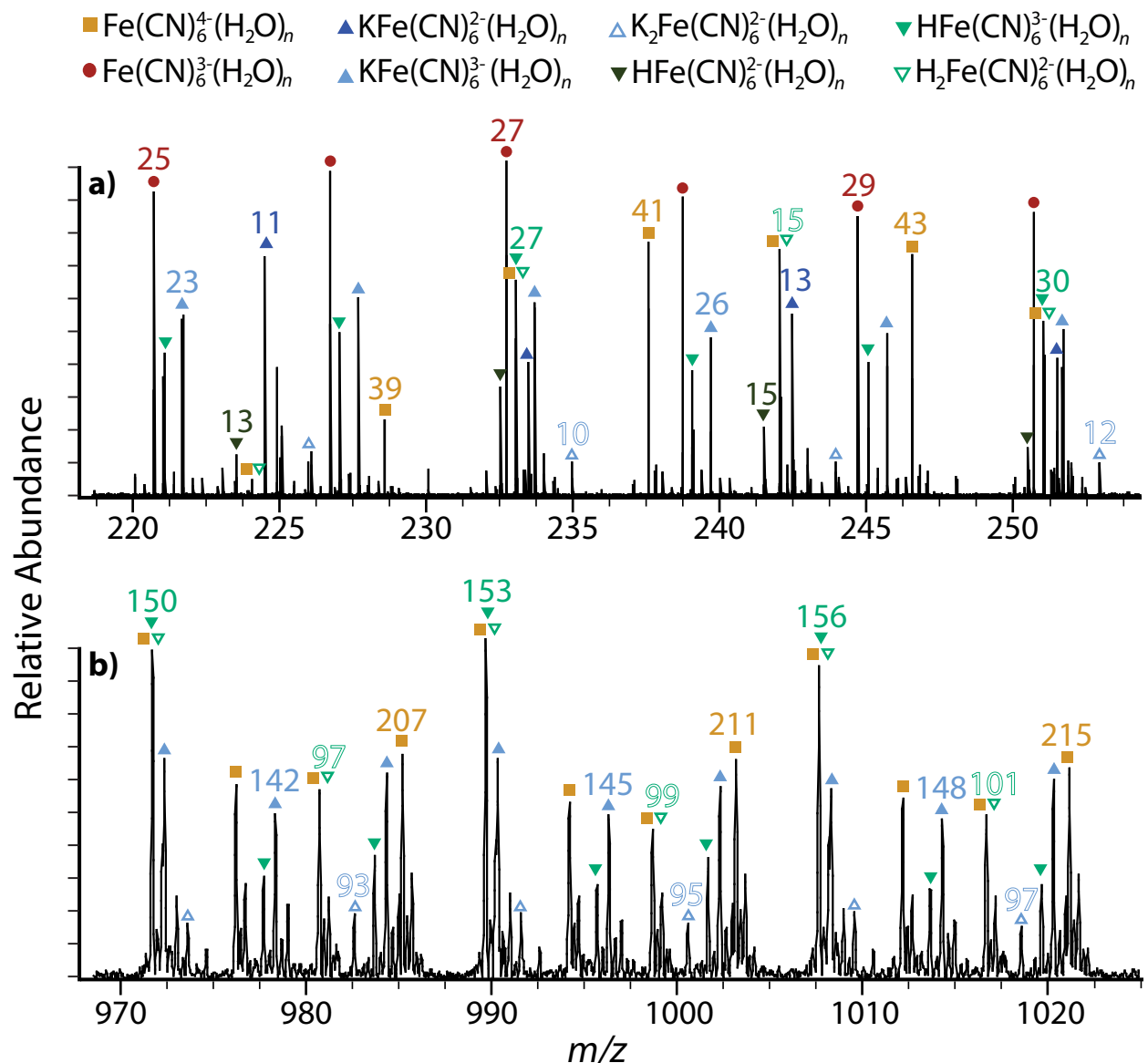


Figure 2: [Figure S2] Expanded regions from Figure 1 are shown to illustrate (a) the onset of ferrocyanide clusters and (b) the absence of trianion ferricyanide and associated adducts at large cluster sizes. Overlapping peaks are present for every second ferrocyanide cluster size with $\text{H}_2\text{Fe}(\text{CN})_6^{2-}(\text{H}_2\text{O})_n$ and every fourth ferrocyanide cluster size with $\text{HFe}(\text{CN})_6^{3-}(\text{H}_2\text{O})_n$.

Full Citation for Reference 6:

E. Harris, B. Sinha, D. Pinxteren, A. Tilgner, K. W. Fomba, J. Schneider, A. Roth, T. Gnauk, B. Fahlbusch, S. Mertes, T. Lee, J. Collett, S. Foley, S. Borrmann, P. Hoppe, H. Herrmann, *Science*, 2013, **340**, 727-730.

Full Citation for Reference 43:

P. J. Faustino, Y. Yang, J. J. Progar, C. R. Brownell, N. Sadrieh, J. C. May, E. Leutzinger, D. A. Place, E. P. Duffy, F. Houn, S. A. Loewke, V. J. Mecozzi, C. D. Ellison, M. A. Khan, A. S. Hussain, R. C. Lyon, *J. Pharm. Biomed. Anal.*, 2008, **47**, 114-125.

Full Citation for Reference 52:

Y. Shao, L. F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, R. A. DiStasio, R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C. P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, B. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer, J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2006, **8**, 3172-3191.

Full Citation for Reference 54:

J. A. Fournier, C. T. Wolke, C. J. Johnson, M. A. Johnson, N. Heine, S. Gewinner, W. Schllkopf, T. K. Esser, M. R. Fagiani, H. Knorke, K. R. Asmis, *Proc. Natl. Acad. Sci. USA*, 2014, **111**, 18132-18137.

Cartesian Coordinates for Lowest Energy $\text{Fe}(\text{CN})_6^{4-}(\text{H}_2\text{O})_{160}$ Structure from Simulated Annealing Molecular Dynamics in Figure 7:

Fe: 0.00000 0.00000 0.00000	O: -3.08480 -6.69080 0.97330
N: -0.00510 3.14710 0.00380	H: -3.33990 -5.79680 0.60470
C: 0.01300 1.99980 0.01390	H: -2.82540 -6.59350 1.93410
N: -3.15440 0.01050 -0.00130	O: 8.00100 4.28760 7.30150
C: -1.99620 -0.02470 0.01410	H: 7.57260 3.73160 8.01380
N: 0.00820 -0.00530 3.14030	H: 7.30130 4.82930 6.83560
C: -0.05410 -0.01190 1.98160	O: -5.34000 3.20140 4.30030
N: 0.00620 -3.15810 0.02200	H: -5.81090 3.41170 5.15710
C: 0.02040 -1.98050 -0.01120	H: -5.19310 4.04550 3.78480
N: 3.17960 0.00640 -0.00140	O: -0.72030 -8.90910 -5.19220
C: 1.99950 -0.02870 0.00300	H: -0.99440 -8.44310 -6.03340
N: 0.00440 0.00230 -3.15960	H: -0.72680 -8.25810 -4.43310
C: -0.00130 0.01500 -1.98770	O: 8.58060 2.64640 5.28710
O: 3.42240 -5.45580 5.01600	H: 8.60520 3.31130 6.03360
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O: -2.43350 1.45330 10.23120	H: 7.68160 -5.78760 -5.54250
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