Deuteronium deuteroxide. The why of pD 7.435.

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Earlier, I constructed a possible model of hydronium hydroxide, or $H3O^+.OH^-$ One way of assessing the quality of the model is to calculate the free energy difference between it and two normal water molecules and compare the result to the measured difference. Here I apply a further test of the model using isotopes.

Pure water has pH 7, which means both $[H3O^+]$ and $[OH^-]$ are 10^{-7}M. Converting this to a free energy one gets ΔG 298 19.088 kcal/mol. Now the pD of pure deuterium oxide is reported as 7.435, equivalent to ΔG 298 20.274, an isotope effect on the free energy of ΔΔG 298 1.186 kcal/mol. How does the theoretical model (ωB97XD/Def2-TZVPPD/SCRF=water ‡) previously reported[1],[2] do? The value obtained is 1.215,[3] an apparent error of only 0.029 kcal/mol. I am quite pleased with the close correspondence; at least the model is capable of reporting good isotope effects on the ionisation equilibrium of pure water!

Finally, with some confidence assured, one might apply this to tritonium tritoxide. Tritiated water is so radioactive it would boil in an instant, probably well before its pT could be measured. ΔΔG 298 is calculated as 1.798 kcal/mol. Will this estimate ever be challenged by experiment?

‡ It is assumed no isotope effect acts on the dielectric constant of water and hence the continuum model used here to model it.

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REFERENCES

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