How reliable is the hard-soft acid-base principle? An assessment from numerical simulations of electron transfer energies

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By computing the electron-transfer energies for two million simulated double acid-base exchange reactions, we assess the reliability of the global hard-soft acid-base (HSAB) principle. We find that the HSAB principle is often thwarted by the tendency of strong acids to prefer strong bases. We define the strong-weak and hard-soft driving forces to characterize the strength of these two competing effects, and assess the reliability of the HSAB principle for different strengths and directions of the hard-soft and strong-weak driving forces. We provide a series of probability tables for making informed predictions about the preferred products of double acid-base exchange reactions.