

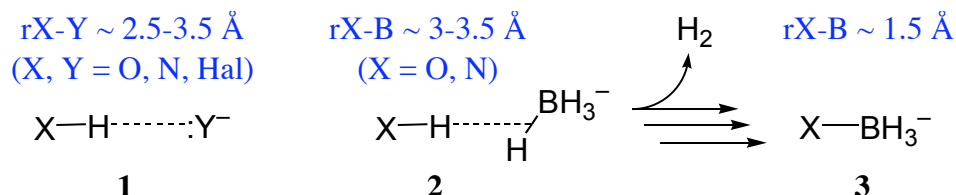
From H-bonding Hydrides to Organic Electrides

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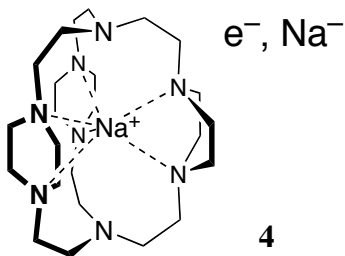
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Unlike classical $X-H \cdots Y^-$ hydrogen bonds **1**, those of type **2** between protonic and hydridic hydrogens $X-H \cdots H-M$ (AKA dihydrogen bonds) can react via proton transfer from $X-H$ to $H-M$ (X electronegative; M electropositive, e.g. B), triggering irreversible H_2 loss and formation of new $X-M$ bonds **3**. Study of the reaction and crystal engineering consequences of this difference (see Radu Custelcean's *Chem. Rev.* **2001**, *101*, 1963-1980) called for molecular crystals designed to allow the solid state H-bond to covalent switch while maintaining crystalline order--i.e. synthesis of networks primed to cross-link into crystalline covalent 3D structures via a crystal-to-crystal reaction (see Custelcean & Vlassa's *Chem. Eur. J.* **2002**, *8*, 302-308.)

In the hydrogen loss reaction $X-H \cdots H-M \rightarrow H_2 + X-M$ the elements that move most are both hydrogens, light atoms capable of quantum mechanical tunneling. Ab Initio modeling of the dynamics in this process are encouraging (see Simona Marincean's *J. Phys. Chem. A* **2004**, *108*, 5521-5526.) More recent simulations suggest that such processes may be relevant in the context of biological hydride transfer reactions as well.



Among unusual and reactive anions, beyond hydrides lie alkalides and electrides. In collaboration with J. L. Dye, synthetic studies (see Misha Redko's *Synthesis* **2006**, 759-761) guided by ab initio modeling have recently enabled construction of the first room-temperature-stable organic electride and its isostructural sodide salts **4** (see M. Redko's *J. Am. Chem. Soc.* **2005**, *127*, 12416-12422).