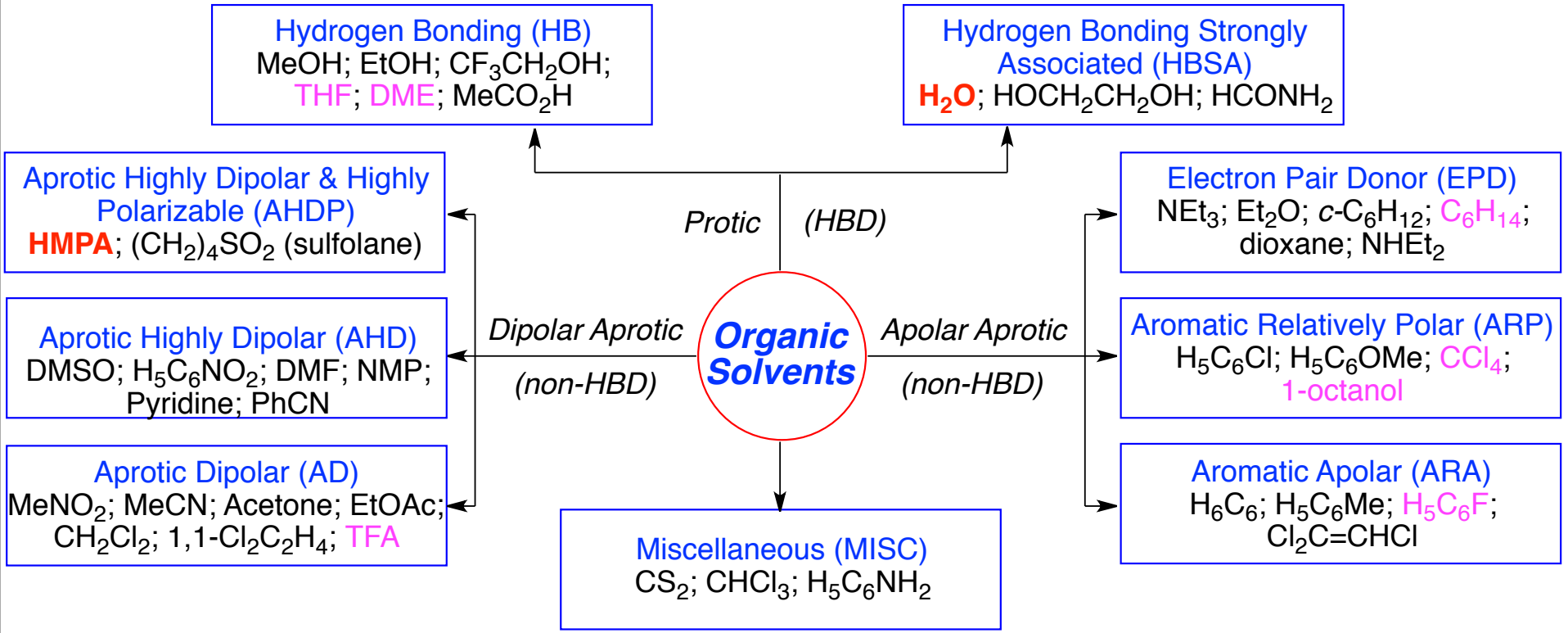
Solvent Effects



This classification is based on a basis set of 8 solvent physiochemical variables (the Kirkwood function, molecular refraction (MR), molecular dipole moment, the delta parameter of Hildebrand, index of refraction, boiling point, and the energies of HOMO and LUMO) by a nonhierarchical multivariate statistical method. This classification is based on the representation of 83 solvents as points in an eight-dimensional space, solvent similarity being measured from the distance between two points within this space. The original eight-dimensional space may be reduced to a three-dimensional subspace with only an 18% loss of information. This subspace is defined by the principal components, F1- (strongly correlated with molecular refraction, refractive index, and HOMO energy), F2- (strongly correlated with the Kirkwood function, dipole moment, and boiling point), and F3- (strongly correlated with LUMO energy). The 83 solvents may be grouped into 9 classes by their clustering of component values.

Chastrette et al. *JACS* ***1985****, 107,* 1; Katritzky, A. R. et al. *Chem. Rev.* **2004**, *104*, 175; Reichardt, C.; Welton T. *"Solvents and Solvent Effects in Organic Chemistry; 4th Ed., Wiley 2011.*