Thermodynamic modeling of binary mixtures of ethylenediamine with water, methanol, ethanol, and 2-propanol by association theory

Hossein Jalaei Salmani [a], Hamed Karkhanechi [a*], Mohammad Reza Moradi [b],

Hideto Matsuyama [c]

[a] Department of Chemical Engineering, Faculty of Engineering, Ferdowsi University of

Mashhad, Mashhad, 91779-48974, Iran

[b] LUT School of Engineering Science, LUT University, P.O.Box 20, 53850 Lappeenranta,

Finland

[c] Research Center for Membrane and Film Technology, Department of Chemical Science and

Engineering, Kobe University, 1-1 Rokkodai, Nada-ku, Kobe 657-8501, Japan

Schemes

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[*] Corresponding Author: Email: karkhanechi@um.ac.ir

The studied schemes are presented in Figures S1 to S2 where Figure S1 shows 4C scheme for EDA; it should be stated that both graphical representations in Figure S1 are equivalent while format "a" was selected in this study for other representations. What matters is that in this scheme only 4 association sites can form the hydrogen bond; two lone electron pairs (electron donor) and only two hydrogen atoms (electron acceptor). In fact, among four hydrogen atoms only two of them are allowed to form the hydrogen bond. In case of 2B scheme for EDA, only one electron pair and only one hydrogen atom participate in the bond formation; in other words, among two amin groups one group is ignored to form the hydrogen bond and only one hydrogen atom in another group participates in the bond formation. As can be seen in Figure S3, four distinct association sites on water are able to form the hydrogen bonds. However, according to Figure S4 two suitable sites belong to alcohols for the hydrogen bond formation.

Regarding a mixture containing two associating compounds such as EDA-water binary mixture, it is evident that the lone electron pairs (electron donor) and hydrogen atoms (electron acceptor) that were previously designated as a candidate can form the hydrogen bond
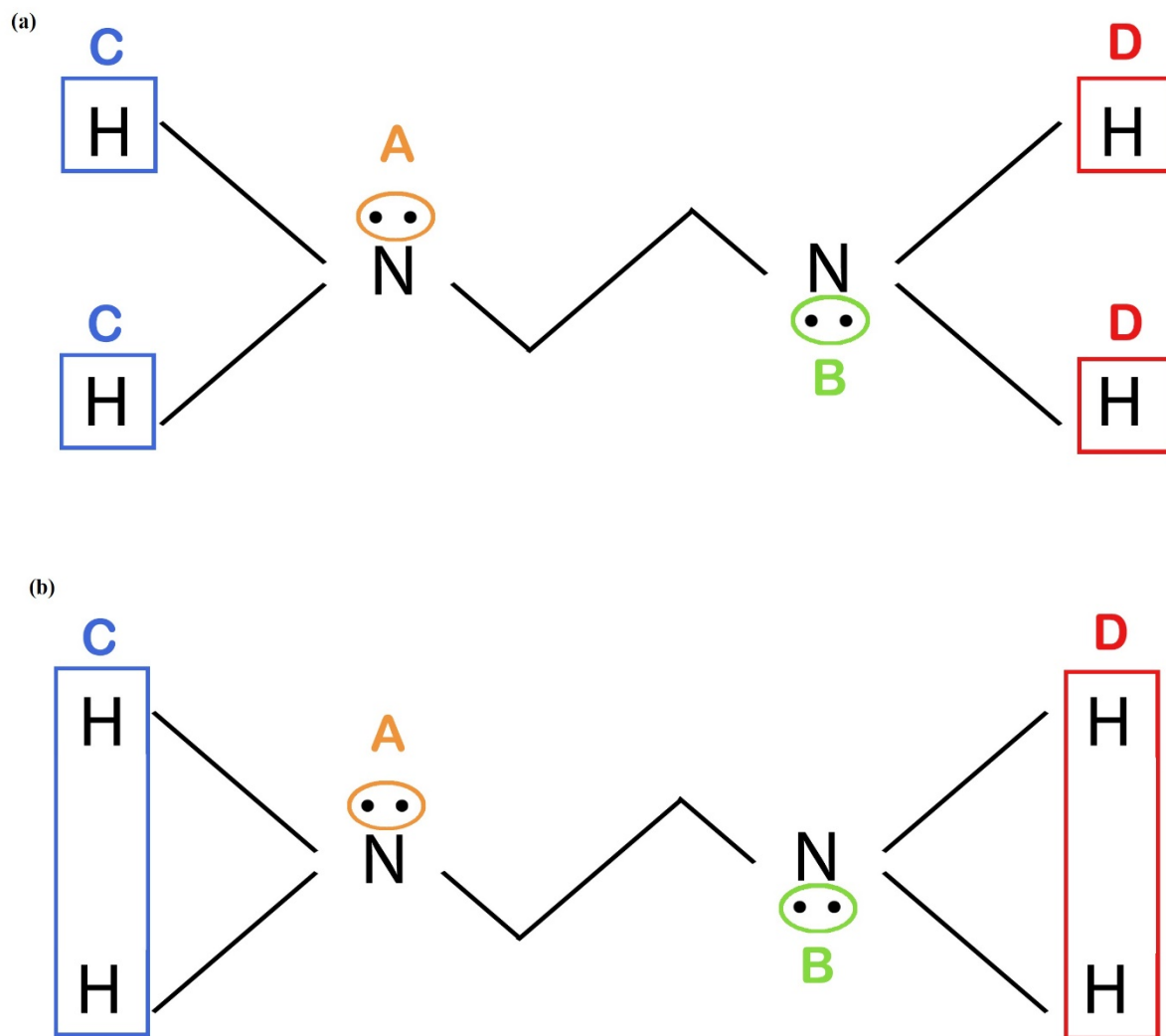
Figure S1: Graphical representation of 4C scheme for EDA (both graphical representations (a and b) are equivalent)
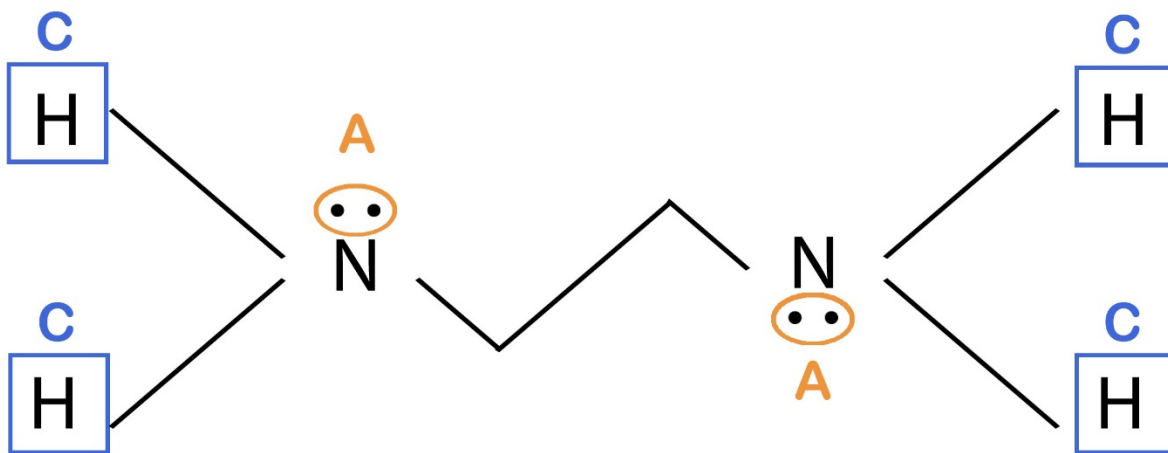
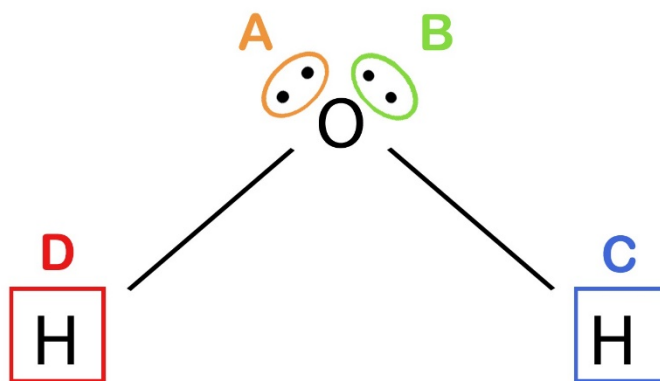**Figure S2: Graphical representation of 2B scheme for EDA**

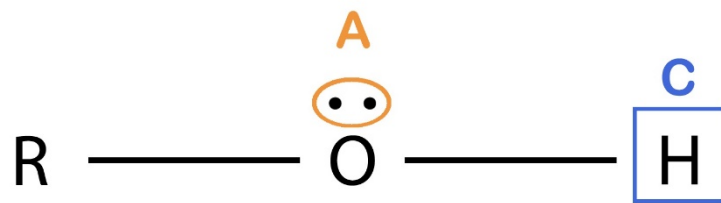**Figure S3: Graphical representation of 4C scheme for water**

Figure S4: Graphical representation of 2B scheme for alcohols