Supporting information

Intradiffusion, Density and Viscosity Studies in Binary Liquid Systems of Acetylacetone + Alkanols at 303.15 K

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^{1}H NMR spectrum. Keto-enol tautomerism is regarded as a slow exchange process compared to NMR time scale [1-2] so that the individual NMR spectrum for two tautomer states can be distinguished for further diffusion measurement. For example in our experiment, the NMR spectrum for mixture of AcAc and ethanol (x_1=0.3) shows in Figure 1S.

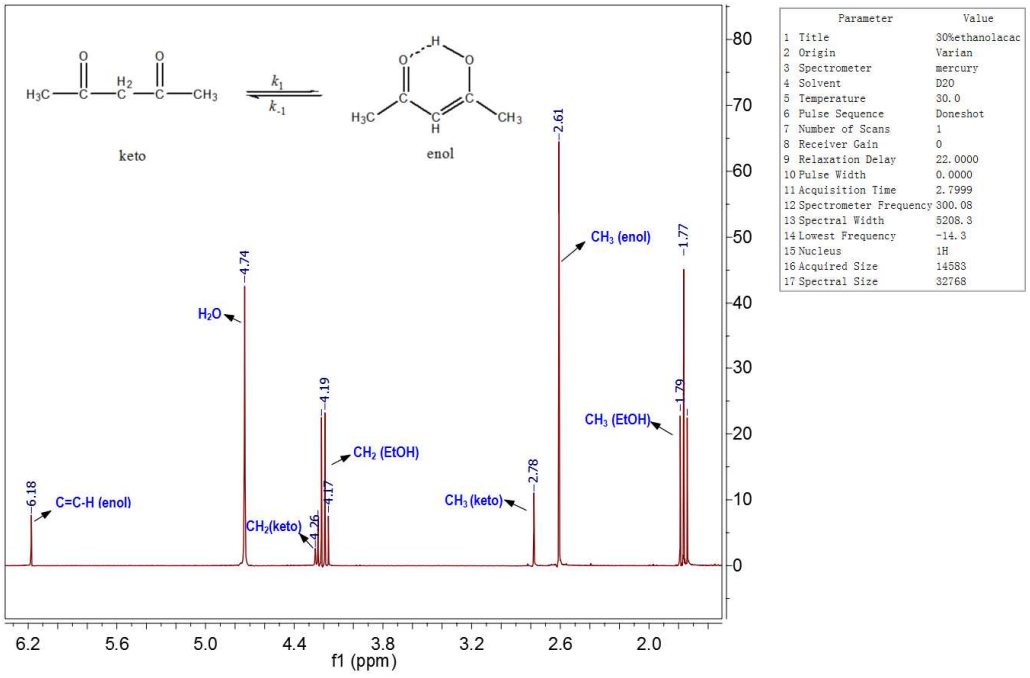

Figure 1S. NMR spectrum of mixture of AcAc+ethanol (x_1=0.3)

Effect of interconversion rate on diffusion measurement. It is measured that the conversion rate (k_1) from keto to enol form of AcAc in methanol solution to be 8.11×10^{-3} s^{-1} at 30 □,[3] and the conversion rate (k_{-1}) from enol to keto be 2.43×10^{-3} s^{-1}. The mean lifetime of keto and enol is thus estimated from reciprocal proportion of k_1 and k_{-1}, respectively,[4] to be 123 s and 411 s or so. Compared with δ value applied in our NMR experiment (1-3 ms), the conversion rate of the tautomerism is sufficiently slow so that the diffusion measurement can be carried out during the application of the pulse gradient.

^{1}H DOSY PFG NMR experimental details. Diffusion coefficients are calculated according to the Tejskal-Tanner formula[5] or its modification (please see the main article). Pulse sequence "doneshot" was applied in experiment (Figure 2S).[6] Before setting up the DOSY experiment, record a normal s2pul spectrum on the nucleus to be observed, then choose the values of DOSY parameters for a given sample involves determining the proper relationship among three parameters: encoding gradient duration gt1, its strength gzlvl1 and the diffusion delay del. It may be useful to set gt1=0.002, del=0.05 s and to array the gradient strength: gzlvl1=50, 500, 1000, 1500, 2000 for our experiment system. For the maximum gradient power used in the DOSY experiment, select the gzlvl1 value which attenuates the signal intensities to 5%-15 % of the intensities obtained with the weakest gradient pulse. After having determined suitable values for gt1, del and the maximum gradient power, call the setup_dosy macro, then 12 arrayed gradient levels are exerted on all signals which results in signal attenuation (Figure 3S). After the acquisition and data processing, the special DOSY spectrum with diffusion coefficients on the vertical axis and chemical shifts on the horizontal axis will be obtained.[7]

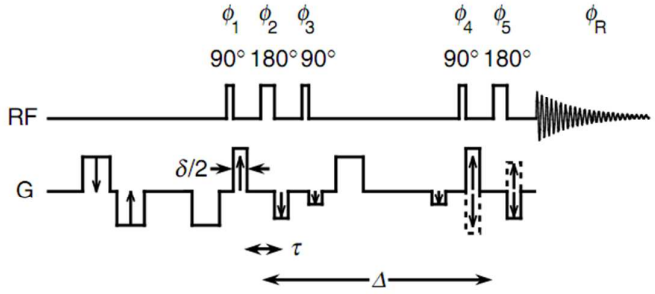

Figure 2S. Doneshot pusle sequence

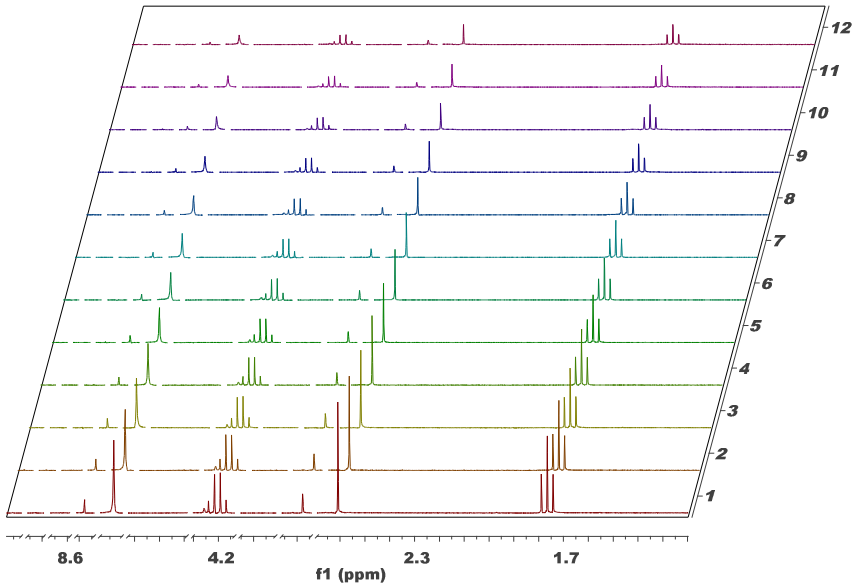

Figure 3S. The attenuation of signal with increasing gradient strength

Calculation of keto-enol equilibrium constant. As for equilibrium constant of keto-enol tautomerism, the ratio of concentration of keto to enol (i.e. K_e = [keto]/[enol]) is used to derive this value. It is shown in Figure 4S that the concentration of keto and enol can be easily obtained from the integration of signal concerned, and the result is below: K_e=[keto]/[enol]=1/3.78=0.26.

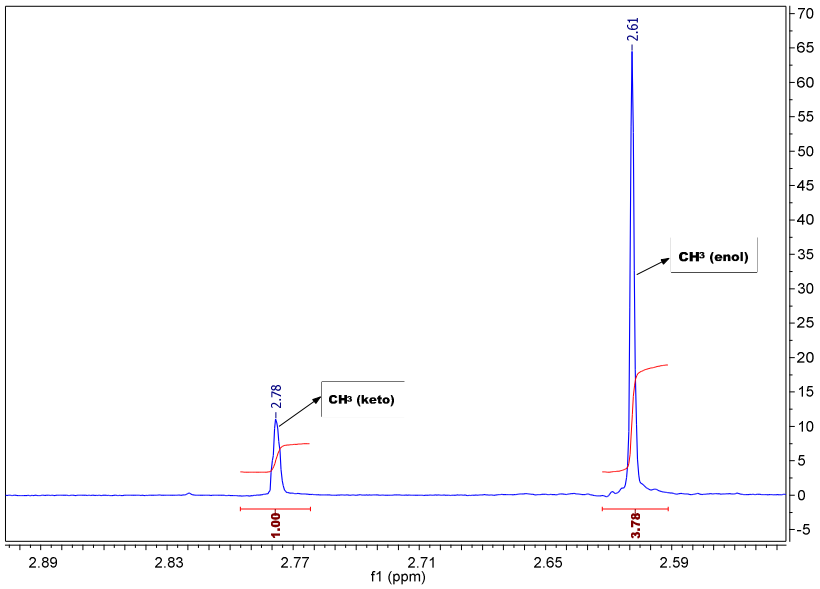

Figure 4S. Integration of signal of keto and enol of AcAc

Reference：

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