

Excited-State Tautomerization of 7-Azaindole in Non-polar Solution: A Theoretical Study  
Based on Liquid-Phase Potential Surfaces of Mean Force

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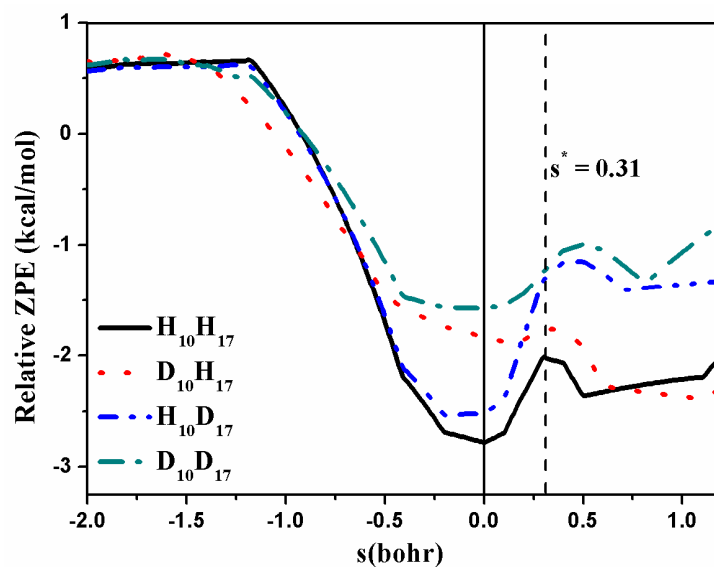
**Table S1.** Excited-state dipole moments  $\mu$ (Debye) of reactant, TS, and product for 7AI-CH<sub>3</sub>OH and 7AI-C<sub>2</sub>H<sub>5</sub>OH complexes at the CASSCF(10,9) level in the gas phase and in heptane with the IEFPCM and SMD models.

		R(L <sub>b</sub> )	TS(L <sub>a</sub> )	P
7AI-CH <sub>3</sub> OH	GAS	1.55	4.87	1.75
	IEFPCM	1.83	5.84	1.95
	SMD	1.92	5.95	2.03
7AI-C <sub>2</sub> H <sub>5</sub> OH	GAS	1.46	5.16	1.66
	IEFPCM	1.72	6.18	1.86
	SMD	1.79	6.37	1.88

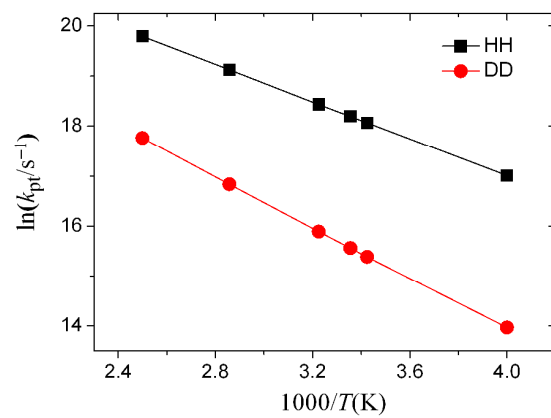
**Table S2** Alcohol-dependent ESDPT rate constants,  $k_{pt}$  (ps<sup>-1</sup>) in n-heptane, and Kamlet-Taft acidity ( $\alpha$ ) and basicity ( $\beta$ ) values for methanol and ethanol. <sup>a</sup>

	$k_{pt}$ (ps <sup>-1</sup> )	$\alpha$	$\beta$
7AI-CH <sub>3</sub> OH	(88) <sup>-1</sup>	0.93	0.62
7AI-C <sub>2</sub> H <sub>5</sub> OH	(95) <sup>-1</sup>	0.83	0.77

a) Ref. 1. Acidity ( $\alpha$ ) and basicity ( $\beta$ ) constants for methanol and ethanol measured from the bulk alcohol, since the values of the monomeric alcohol show similar trends to those of the bulk alcohol.



**Figure S1.** Relative zero-point energies in terms of the corresponding reactant values along the MEP of isotopically substituted 7Al-CH<sub>3</sub>OH complexes calculated at the MRPT2//SMD/CASSCF(10,9) /6-31G(d,p) level in heptane. The vertical solid and dashed lines represent conventional TSs at the CASSCF and MRPT2 levels, respectively.



**Figure S2.** Arrhenius plots of HH and DD rate constants for 7Al-CH<sub>3</sub>OH complexes in heptane

1. Kwon, O. H.; Lee, Y. S.; Park, H. J.; Kim, Y. H.; Jang, D. J. *Angew. Chem. Int. Ed.* **2004**, *43*, 5792-5796.