Supplementary Information

Theoretical investigation on DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline and α,β-unsaturated aldehyde to construct 3-sulfonyl α-carboline

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Table S1. Calculated relative energies (all in kcal mol^{-1}, relative to isolated species) for the ZPE-corrected Gibbs free energies (ΔG_{gas}), Gibbs free energies for all species in solution phase (ΔG_{sol}) at 423 K by M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) method and difference between absolute energy.

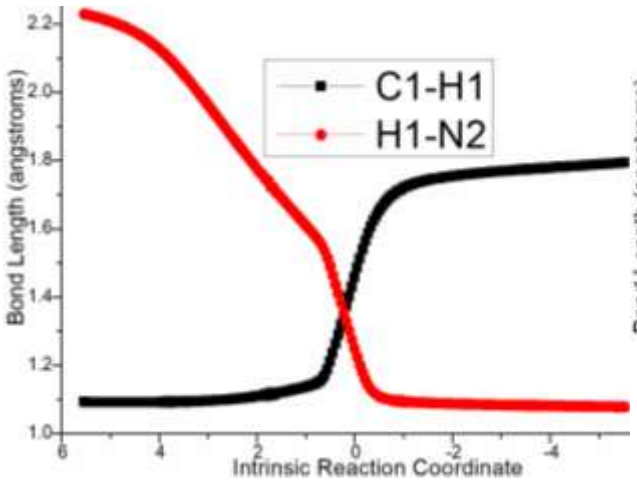
Species	ΔG_{gas}	$\Delta G_{sol(DMF)}$
1+dabco	0.00	0.00
i1	-11.77	-6.33
ts-i12	1.54	8.81
i2	-3.11	-0.94
1-h	0.00	0.00
1i	25.44	-12.99
1+2-h	0.00	0.00
i3	5.36	-20.84
ts-i3A	34.06	3.50
A	23.13	-14.29
ts-AB	43.04	3.42
B	21.71	-15.21
ts-Bi4	44.61	5.79
i4	15.42	-22.60
1+2	0.00	0.00
C	-7.34	-18.09
ts-CD	22.91	8.86
D	-28.54	-44.20
ts-Di5	4.63	-15.78
i5	-28.20	-32.90
1+2-h2o	0.00	0.00
E	-17.60	-13.39
1+2-h2o-2h	0.00	0.00
3	25.42	18.33

Table S2. The activation energy (local barrier) (in kcal mol^{-1}) of all reactions in the gas, solution phase calculated with M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) method.

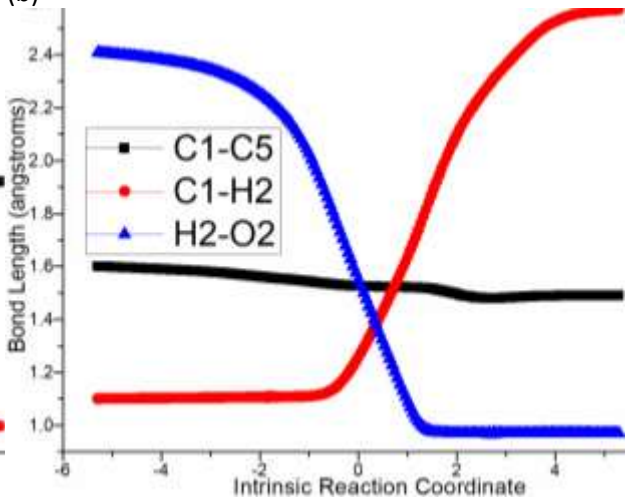
TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i12 (918i)	13.31	15.14
ts-i3A (167i)	28.70	24.34
ts-AB (156i)	19.91	17.71
ts-Bi4 (106i)	22.90	21.00
ts-CD (1586i)	30.25	26.95
ts-Di5 (1383i)	33.17	28.42

Figure S1. Evolution of bond lengths along the IRC for (a) **ts-i12** (b) **ts-CD** (c) **ts-Di5** at M06-2X/6-311++G(d,p) level.

(a)



(b)



(c)