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Z/E(C=C)-isomerization of coumarin enamines induced by organic solvents

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Table 1S ^{13}C NMR chemical shifts in ppm of imines **1** and **2**.

№, atom	Imine 1		Imine 2	
	2	163.6	165.3	163.7
3	98.37	98.39	97.09	97.01
4	181.6	178.5	181.2	178.4
5	125.7	126.4	125.5	126.2
6	124.7	124.3	123.8	124.0
7	134.6	134.5	134.2	134.4
8	117.3	117.4	117.1	117.1
9	154.6	153.2	162.1	160.5
4a	120.3	120.6	120.3	120.6
8a	154.2	154.9	154.7	154.5
10	137.6	134.5	134.2	134.4
11,15	118.3	118.4	127.5	127.5
12,14	130.6	130.6	129.1	129.1
13	135.2	135.2	128.6	128.6
CH ₃ (3) CH ₂ (4)	20.3	20.9	54.4	54.3

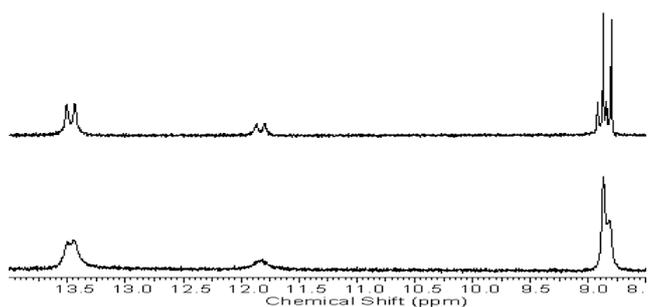


Figure 1S Spectra ^1H NMR of the compound **1** in DMSO-d_6 after solution preparation (down) and after 4 hours (up).

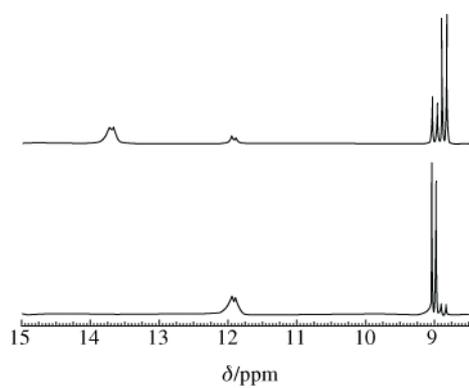


Figure 2S Spectra ^1H NMR of compound **1** in CDCl_3 recorded immediately after solution preparation (bottom) and after 25 h (top).

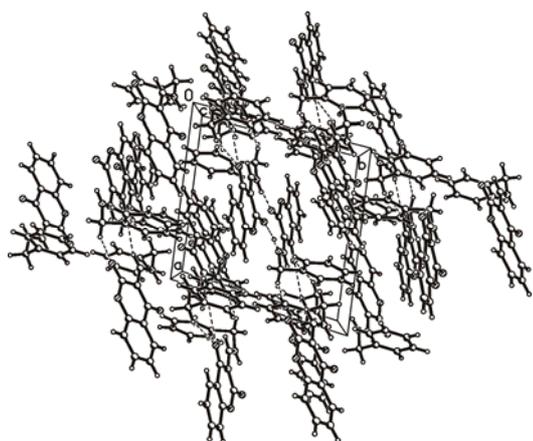


Figure 3S Crystal structure of imine **2**.

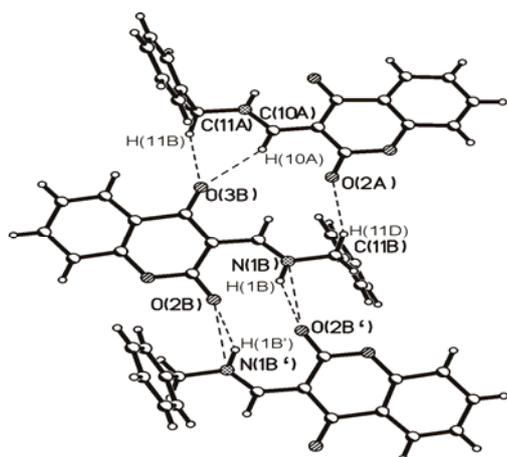


Figure 4S Intermolecular bonding of E- and Z-ketoenamines molecules of **2** in crystal.

Table 2S Selected bond distances ($\alpha/\text{\AA}$) and angles (ω°) of imine **2**.

O(1A)-C(1A)	1.380(4)	O(1B)-C(1B)	1.335(4)
O(2A)-C(1A)	1.208(4)	O(2B)-C(1B)	1.252(4)
O(3A)-C(3A)	1.238(4)	O(3B)-C(3B)	1.211(4)
N(1A)-C(10A)	1.295(4)	N(1B)-C(10B)	1.255(4)
C(1A)-C(2A)	1.440(5)	C(1B)-C(2B)	1.411(5)
C(2A)-C(3A)	1.432(5)	C(2B)-C(3B)	1.444(5)
C(2A)-C(10A)	1.389(4)	C(2B)-C(10B)	1.410(5)
C(1A)-O(1A)-C(9A)	121.5(3)	C(1B)-O(1B)-C(9B)	119.8(3)
C(10A)-N(1A)-C(11A)	124.4(3)	C(10B)-N(1B)-C(11B)	125.1(3)
O(2A)-C(1A)-O(1A)	115.0(3)	O(2B)-C(1B)-O(1B)	114.2(4)
O(2A)-C(1A)-C(2A)	126.5(3)	O(2B)-C(1B)-C(2B)	124.1(4)
O(1A)-C(1A)-C(2A)	118.5(3)	O(1B)-C(1B)-C(2B)	121.7(4)
C(10A)-C(2A)-C(1A)	116.5(3)	C(10B)-C(2B)-C(1B)	120.6(3)
C(10A)-C(2A)-C(3A)	121.9(3)	C(10B)-C(2B)-C(3B)	117.8(3)
C(1A)-C(2A)-C(3A)	121.6(3)	C(1B)-C(2B)-C(3B)	121.5(3)
O(3A)-C(3A)-C(2A)	122.3(3)	O(3B)-C(3B)-C(2B)	123.7(4)
O(3A)-C(3A)-C(4A)	121.5(3)	O(3B)-C(3B)-C(4B)	122.7(4)
C(2A)-C(3A)-C(4A)	116.1(3)	C(2B)-C(3B)-C(4B)	113.6(3)
N(1A)-C(10A)-C(2A)	124.2(3)	N(1B)-C(10B)-C(2B)	129.8(4)
N(1A)-C(11A)-C(12A)	111.0(3)	N(1B)-C(11B)-C(12B)	111.7(3)

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