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# The mechanism of two reversible phase transitions and dielectric anomalies in a single-component organic molecule 1-sulfo-4-dimethylamino-pyridinium

Zihong Yu,[a] Xiuli You,[b] Wenqing Du,[a] Ziqin Peng,[a] Wenjing Guo,[a] Zhenhong Wei[a,*]

[a] College of chemistry, Nanchang University, Nanchang, 330031, P. R. China.

[b] Jiangxi key laboratory of organic chemistry, Jiangxi science and technology normal university, Nanchang, 330013, China.

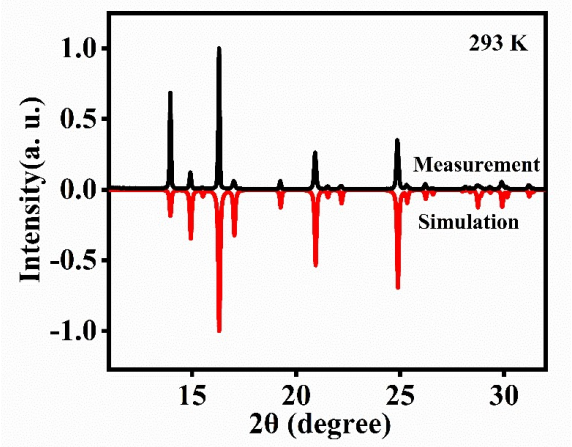


**Figure S1.** The powder X-ray diffraction pattern of compound **1** with the simulated one in red and the experimental one in black.

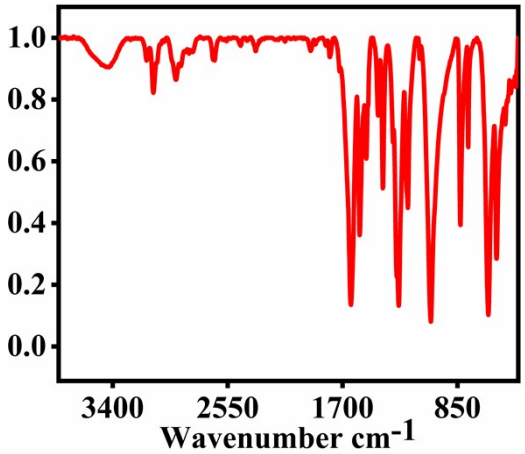


**Figure S2.** Infrared diagram of **1**.

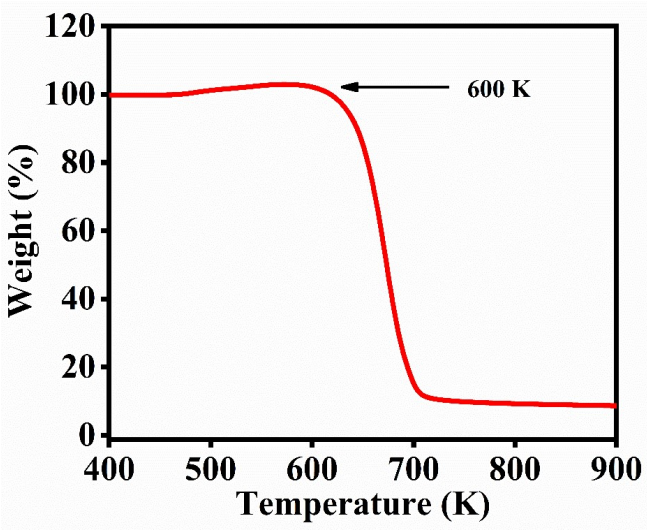


**Figure S3.** Thermogravimetric (TGA) curve of **1**.

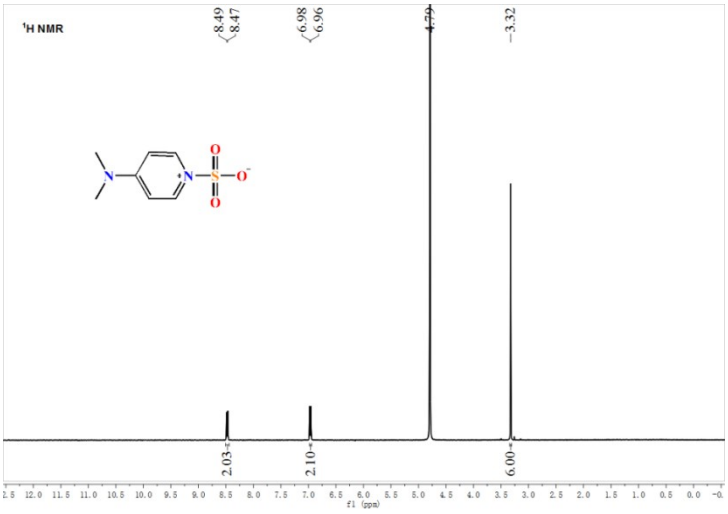


**Figure S4.** $^{1}$H NMR diagram of **1**.

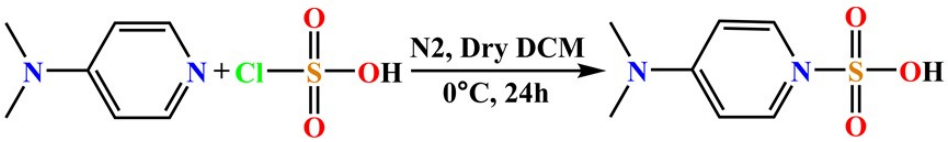


**Figure S5.** Synthesis and structural diagram of **1**.

**Table S1.** Bond lengths [Å] and angles [°] for **1** (243 K).

| | | | |
|---|---|---|---|
| S1-O1 | 1.419(2) | N2-C7 | 1.458(3) |
| S1-O3 | 1.4278(18) | N2-C6 | 1.459(3) |
| S1-O2 | 1.429(2) | C1-C2 | 1.349(3) |
| S1-N1 | 1.7697(19) | C2-C3 | 1.427(3) |
| N1-C1 | 1.362(3) | C3-C4 | 1.425(3) |
| N1-C5 | 1.361(3) | C4-C5 | 1.350(3) |
| N2-C3 | 1.334(3) | | |
| O1-S1-O3 | 116.22(13) | C3-N2-C6 | 121.2(2) |
| O1-S1-O2 | 117.08(14) | C7-N2-C6 | 117.28(19) |
| O3-S1-O2 | 113.15(12) | C2-C1-N1 | 121.9(2) |
| O1-S1-N1 | 102.05(10) | C1-C2-C3 | 120.5(2) |
| O3-S1-N1 | 102.72(10) | N2-C3-C4 | 122.3(2) |
| O2-S1-N1 | 102.58(10) | N2-C3-C2 | 121.6(2) |
| C1-N1-C5 | 119.16(19) | C4-C3-C2 | 116.1(2) |
| C1-N1-S1 | 121.63(15) | C5-C4-C3 | 120.3(2) |
| C5-N1-S1 | 118.86(15) | C4-C5-N1 | 122.1(2) |
| C3-N2-C7 | 121.46(19) | | |

**Table S2.** Bond lengths [Å] and angles [°] for **1**(293 K)

| | | | |
|---|---|---|---|
| S1-N1 | 1.756(4) | N1-C1 | 1.363(3) |
| S1-O2$^{1}$ | 1.449(5) | N1-C1$^{1}$ | 1.363(3) |
| S1-O2 | 1.449(5) | N2-C3 | 1.328(5) |
| S1-O1$^{1}$ | 1.477(5) | N2-C4 | 1.464(4) |
| S1-O1 | 1.477(5) | N2-C4$^{1}$ | 1.464(4) |
| S1-O2A$^{1}$ | 1.457(8) | C3-C2$^{1}$ | 1.420(3) |
| S1-O2A | 1.457(8) | C3-C2 | 1.420(3) |
| S1-O1A | 1.409(7) | C1-C2 | 1.344(5) |
| S1-O1A$^{1}$ | 1.409(7) | | |
| O2$^{1}$-S1-N1 | 102.0(3) | O1A$^{1}$-S1-N1 | 109.2(7) |
| O2-S1-N1 | 102.0(3) | O1A-S1-O2A | 59.1(9) |
| O2-S1-O2$^{1}$ | 108.2(6) | O1A$^{1}$-S1-O2A | 122.6(11) |
| O2$^{1}$-S1-O1$^{1}$ | 89.4(4) | O1A-S1-O1A$^{1}$ | 140.9(13) |
| O2-S1-O1$^{1}$ | 147.4(4) | C1-N1-S1 | 120.90(18) |
| O2$^{1}$-S1-O1 | 147.4(4) | C1$^{1}$-N1-S1 | 120.90(18) |
| O2-S1-O1 | 89.4(4) | C1-N1-C1$^{1}$ | 117.9(4) |
| O2$^{1}$-S1-O2A$^{1}$ | 22.0(8) | C3-N2-C4 | 121.5(2) |
| O2-S1-O2A$^{1}$ | 88.7(9) | C3-N2-C4$^{1}$ | 121.5(2) |
| O1$^{1}$-S1-N1 | 100.7(2) | C4-N2-C4$^{1}$ | 116.9(4) |
| O1-S1-N1 | 100.7(2) | N2-C3-C2 | 122.16(18) |

| | | | |
|---|---|---|---|
| O1-S1-O1[1] | 63.5(6) | N2-C3-C2[1] | 122.15(18) |
| O2A[1]-S1-N1 | 97.0(9) | C21-C3-C2 | 115.7(4) |
| O2A-S1-N1 | 97.0(9) | C2-C1-N1 | 122.5(3) |
| O1A-S1-N1 | 109.2(7) | C1-C2-C3 | 120.7(3) |

**Table S3.** Bond lengths [Å] and angles [°] for **1** (328 K)

| | | | |
|---|---|---|---|
| S1-N1 | 1.776(3) | N1-C1 | 1.349(3) |
| S1-O2 | 1.478(6) | N1-C1[1] | 1.349(3) |
| S1-O2[1] | 1.478(6) | N2-C3 | 1.326(5) |
| S1-O1[1] | 1.480(5) | N2-C4[1] | 1.455(3) |
| S1-O1 | 1.480(5) | N2-C4 | 1.455(3) |
| S1-O2A | 1.466(12) | C3-C2 | 1.419(3) |
| S1-O2A[1] | 1.466(12) | C3-C2[1] | 1.419(3) |
| S1-O1A | 1.311(9) | C1-C2 | 1.347(4) |
| S1-O1A[1] | 1.311(9) | O2A-O1A | 1.382(18) |
| S1-N1 | 1.776(3) | N1-C1 | 1.349(3) |
| O2[1]-S1-N1 | 101.4(3) | O1A1-S1-O2A | 121.7(9) |
| O2-S1-N1 | 101.4(3) | O1A-S1-O1A[1] | 143.8(11) |
| O2-S1-O2[1] | 107.1(5) | C1-N1-S1 | 120.19(16) |
| O2-S1-O1[1] | 149.2(4) | C1[1]-N1-S1 | 120.19(16) |
| O2-S1-O1 | 89.4(4) | C1-N1-C1[1] | 119.4(3) |
| O2[1]-S1-O1 | 149.2(4) | C3-N2-C4[1] | 121.44(19) |
| O2[1]-S1-O1[1] | 89.4(4) | C3-N2-C4 | 121.44(19) |
| O1-S1-N1 | 100.5(2) | C41-N2-C4 | 117.0(4) |
| O1[1]-S1-N1 | 100.5(2) | N2-C3-C2[1] | 122.14(16) |
| O1-S1-O1[1] | 65.5(5) | N2-C3-C2 | 122.15(16) |
| O2A-S1-N1 | 98.1(8) | C2-C3-C2[1] | 115.7(3) |
| O2A[1]-S1-N1 | 98.1(8) | C2-C1-N1 | 121.8(2) |
| O1A[1]-S1-N1 | 107.7(5) | C1-C2-C3 | 120.6(2) |
| O1A-S1-N1 | 107.7(5) | O1A-O2A-S1 | 54.7(6) |
| O1A-S1-O2A | 59.4(7) | S1-O1A-O2A | 65.9(7) |