

Supporting Information

Switchable Dielectric Constant in an Inclusion Compound Bis(Thiourea) Imidazolium Chloride

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Table S1. Hydrogen bonds of **1** at 293 K, 143K and 123 K.

	<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	∠ <i>D</i> –H··· <i>A</i>
293 K	N(1)–H(1A)···Cl(1)#1	0.86	2.56	3.346(3)	152
	N(1)–H(1B)···S(1)#2	0.86	2.55	3.403(3)	175
143 K	N(1)–H(1A)···Cl(1)#3	0.86	2.57	3.345(4)	150
	N(1)–H(1B)···S(1)#4	0.86	2.52	3.379(4)	173
	N(2)–H(2A)···Cl(1)#3	0.86	2.52	3.304(4)	153
	N(2)–H(2B)···S(1)#5	0.86	2.54	3.393(4)	174
	N(3)–H(3B)···Cl(1)#6	0.90	2.42	3.308(13)	169
	N(4)–H(4B)···S(1)	0.90	2.58	3.463(12)	168
123 K	N(1)–H(1A)···Cl(1)	0.86	2.49	3.284(3)	155
	N(1)–H(1B)···S(2)#7	0.86	2.53	3.381(3)	171
	N(2)–H(2A)···Cl(1)	0.86	2.61	3.377(3)	150
	N(2)–H(2B)···S(2)#8	0.86	2.54	3.394(3)	171
	N(3)–H(3A)···Cl(1)	0.86	2.53	3.311(3)	152
	N(3)–H(3B)···S(1)#9	0.86	2.52	3.373(3)	172
	N(4)–H(4A)···Cl(1)	0.86	2.54	3.318(3)	152
	N(4)–H(4B)···S(1)#10	0.86	2.54	3.397(3)	176
	N(5)–H(5B)···Cl(1)	0.86	2.39	3.244(3)	172
	N(6)–H(6A)···S(2)#11	0.86	2.51	3.352(3)	168

Symmetry codes: #1 *x*, *y*–1, *z*; #2 –*x*+3/2, –*y*+1/2, *z*+1/2; #3 *x*–1/2, *y*–1/2, *z*; #4 –*x*+3/2, –*y*+3/2, *z*+1/2; #5 –*x*+3/2, –*y*+3/2, *z*–1/2; #6 –*x*+2, –*y*+1, *z*+1/2; #7 *x*+1/2, –*y*+3/2, –*z*+2; #8 *x*+1/2, –*y*+3/2, –*z*+1; #9 *x*–1/2, –*y*+3/2, –*z*+2; #10 *x*–1/2, –*y*+3/2, –*z*+1; #11 *x*+1/2, –*y*+1/2, –*z*+2.

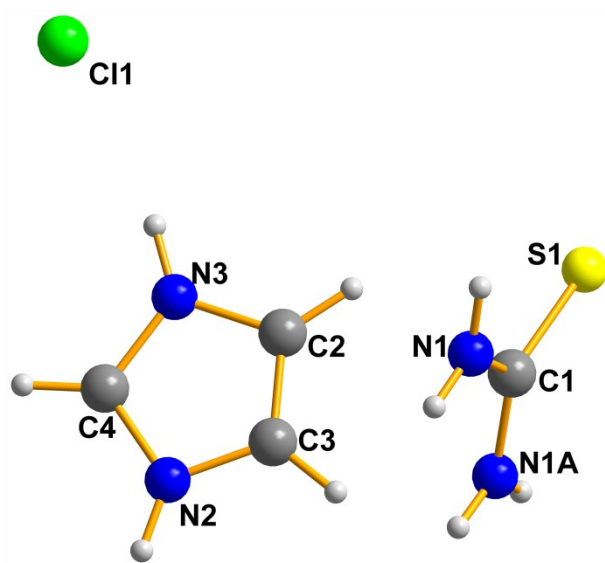


Fig. S1 Asymmetric structure unit of **1** at 293 K. The N1A atom is generated by a symmetry operator: $x, y, 1.5-z$.

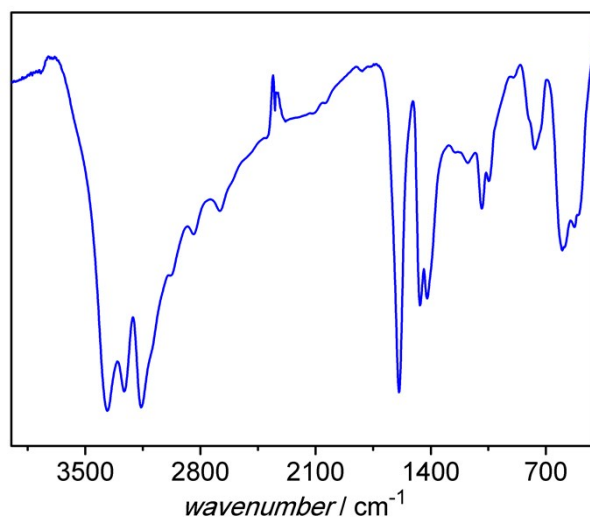


Fig. S2 Infrared spectrum of **1** measured at room temperature.

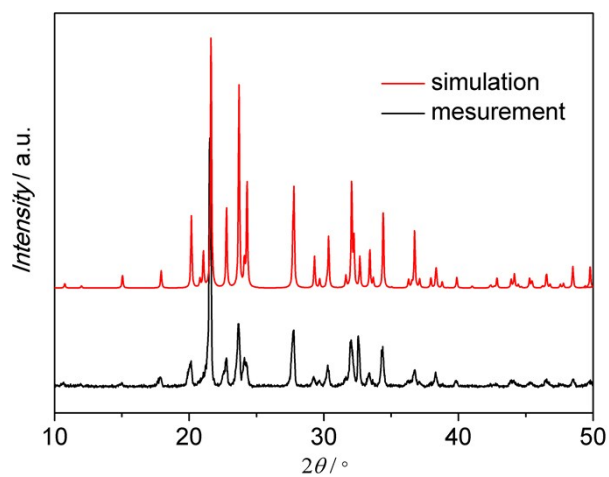


Fig. S3 PXRD pattern for the as-prepared samples of **1** and the simulated one based on the single crystal structure at 293 K.

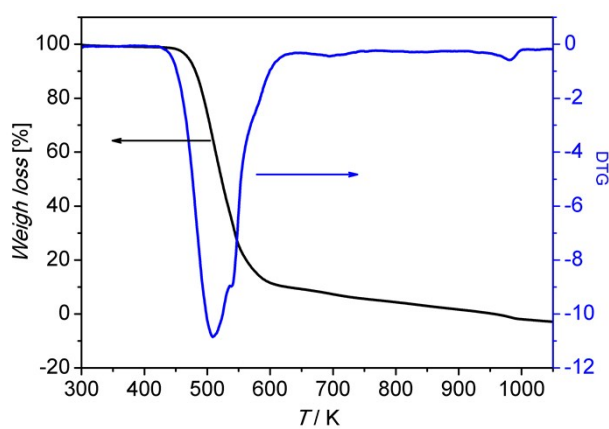


Fig. S4 TGA measurement of **1** in the temperature range 300–920 K.

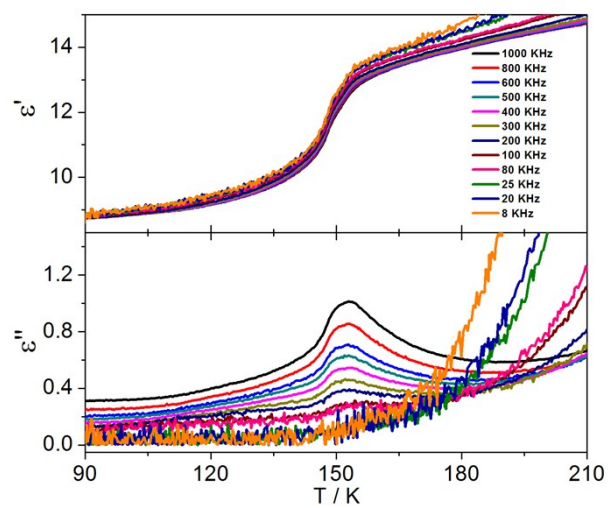


Fig. S5 Complex dielectric permittivity of **1** as a function of temperature at different frequencies on cooling.