Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Electrical property and Schottky behavior of a flexible Schiff-base compound: X-ray structure and stabilization of 1D water chain

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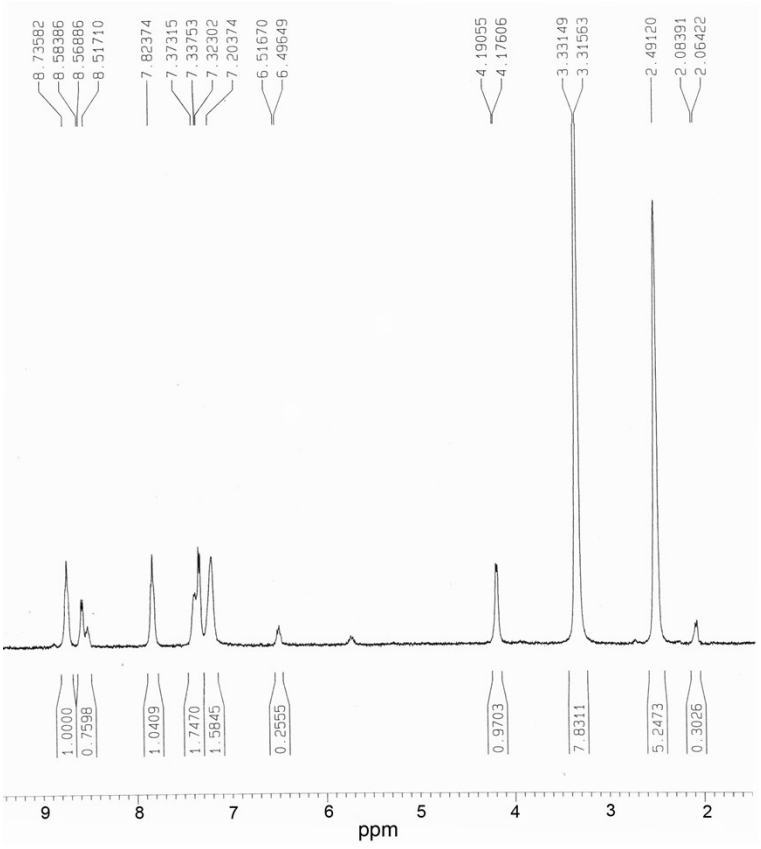

Fig. S1 NMR Spectrum of compound **1** in [D_6]DMSO solvent.

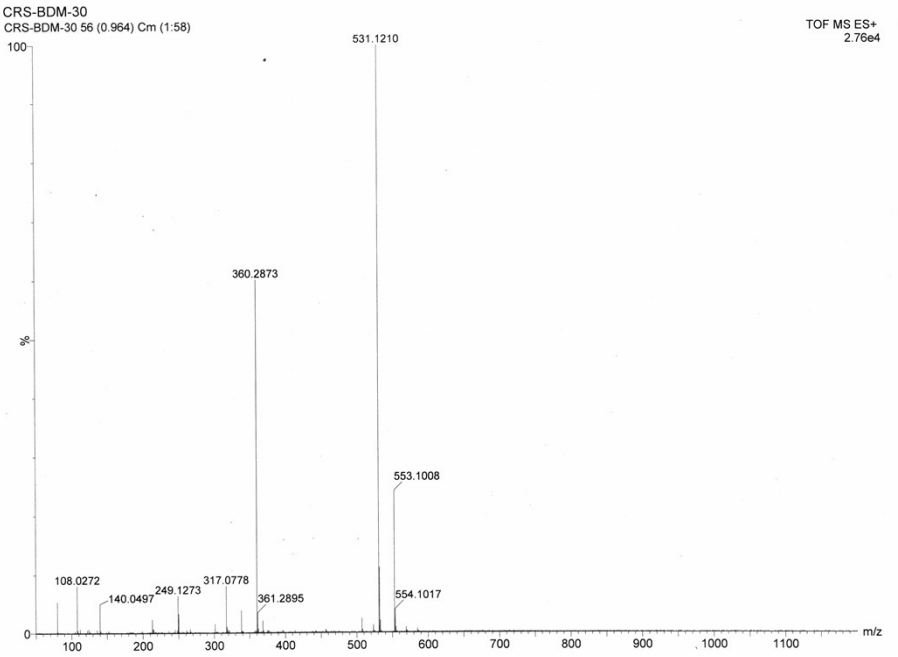

Fig. S2 Mass spectrum of compound **1**.

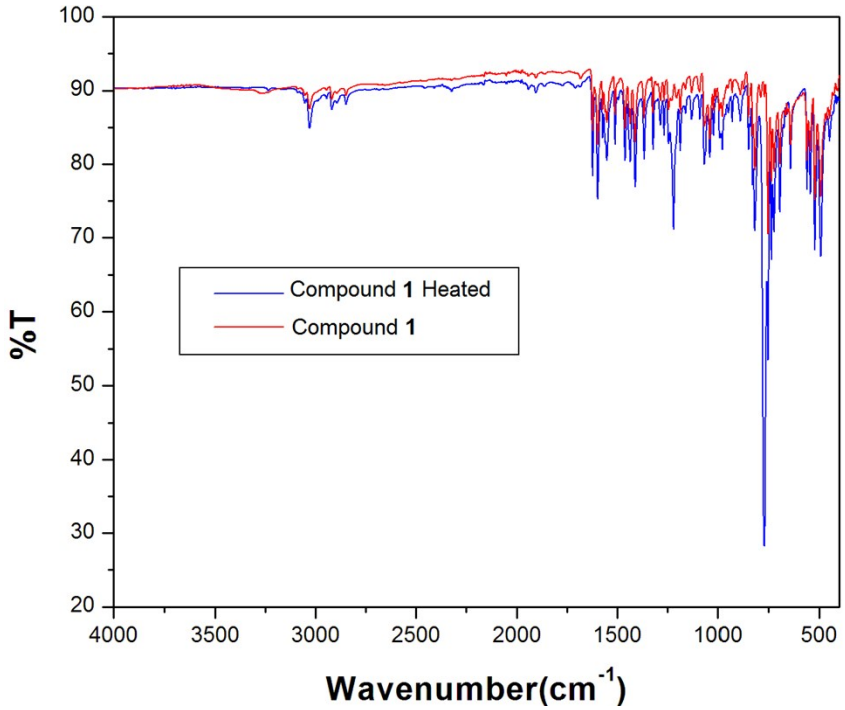

Fig. S3 IR Spectra of compound **1** at room temperature (red) and heating at 100 °C (blue).

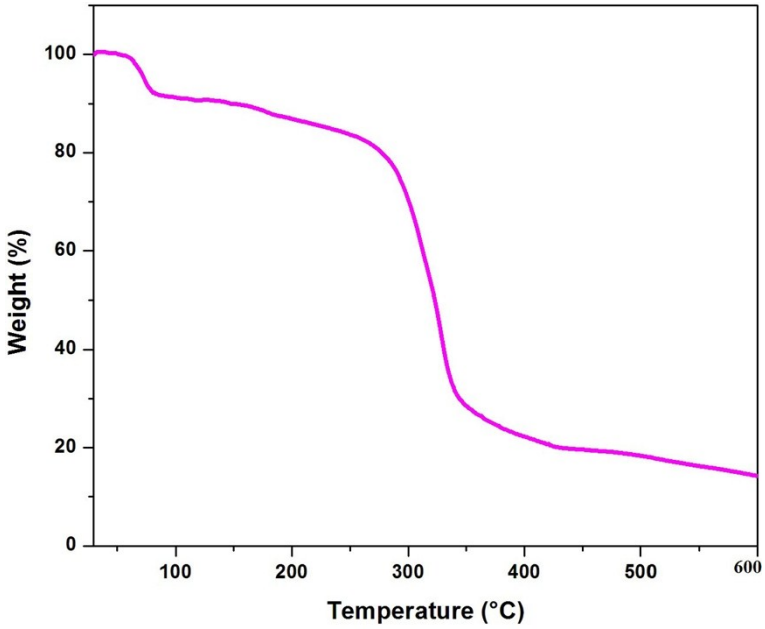

Fig. S4 TGA plot of compound **1** measured under N_2 atmosphere.

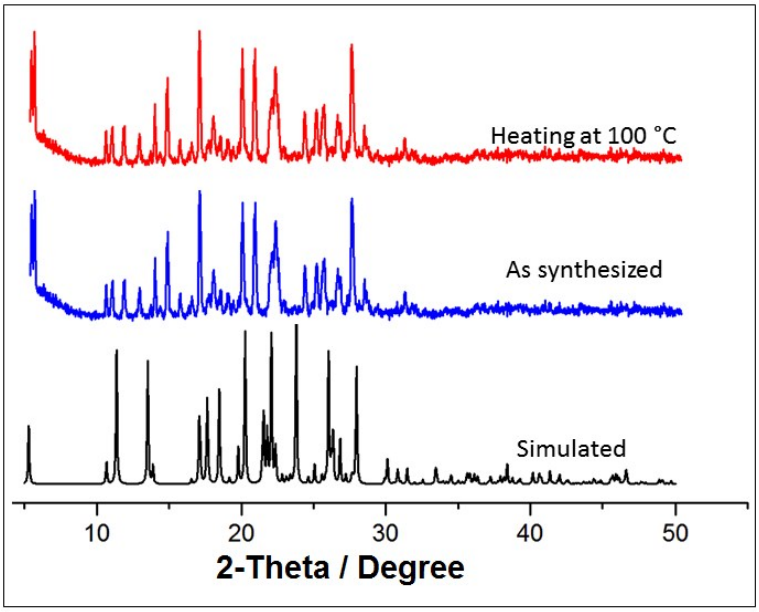

Fig. S5 Powder X-ray diffraction patterns of simulated **1** (black), as-synthesized **1** (blue) and heating at 100 °C (red).

Table S1 Crystal data and refinement parameters for compound **1**.

Formula	$C_{32}H_{28}N_4O_2S_2$
Fw	564.70
crystsyst	triclinic
space group	$P\bar{1}$
a (Å)	5.4376(2)
b (Å)	8.0683(4)
c (Å)	17.0332(9)
α(deg)	77.328(3)
β(deg)	84.635(3)
γ (deg)	80.612(3)
V (Å^3)	718.02(6)
Z	1
D_{calcd}(g/cm^3)	1.306
μ(mm^{-1})	0.222
λ(Å)	0.71073
data[$I > 2\sigma(I)$]/params	2565/187
GOF on F^2	1.044
final R indices[$I > 2\sigma(I)$][a,b]	$R1$ = 0.0552 $wR2$ = 0.1625

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles in **1**

S(1)-C(12)	1.764(3)	C(1)-N(1)-C(5)	113.9(3)
N(2)-C(6)	1.246(4)	N(2)-C(6)-C(3)	123.7(3)
S(1)-C(13)	1.812(3)	S(1)-C(12)-C(11)	124.5(2)
N(2)-C(7)	1.422(4)	C(6)-N(2)-C(7)	120.9(3)
N(1)-C(1)	1.303(5)	N(2)-C(7)-C(8)	124.5(3)
N(1)-C(5)	1.329(6)	C(1)-N(1)-C(5)	113.9(3)
C(12)-S(1)-C(13)	102.31(14)	C(13)-C(16)-C(15)a	120.4(3)
N(1)-C(1)-C(2)	125.4(4)	S(1)-C(13)-H(13A)	110
N(1)-C(5)-C(4)	125.8(4)	S(1)-C(13)-H(13B)	110
N(2)-C(7)-C(12)	116.6(3)	N(2)-C(6)-H(6)	118
S(1)-C(12)-C(7)	116.9(2)	N(1)-C(5)-H(5)	117
S(1) -C(13)-C(16)	109.5(2)	C(16)-C(14)-H(14)	120
N(2)-C(6)-C(3)	123.7(3)	N(1)-C(1)-H(1)	117

Symmetry transformations used to generate equivalent atoms: a = 2-x, -y, 1-z

Table S3 DFT table of the compound **1**

Compound **1**				
MO	Energy (eV)	S	N	Other
LUMO+10	0.48	1	27	72
LUMO+9	-0.37	2	3	94
LUMO+8	-0.42	0	1	99
LUMO+7	-0.49	1	6	93
LUMO+6	-0.54	1	2	96
LUMO+5	-0.76	4	1	94
LUMO+4	-0.88	0	0	100
LUMO+3	-0.89	0	0	100
LUMO+2	-1.22	14	2	84
LUMO+1	-2.34	0	35	65
LUMO	-3.25	0	34	65
HOMO	-6.10	44	13	43
HOMO-1	-6.14	46	14	40
HOMO-2	-6.59	36	4	59
HOMO-3	-6.68	33	15	52
HOMO-4	-6.71	10	12	78
HOMO-5	-7.05	0	70	30
HOMO-6	-7.05	0	70	30
HOMO-7	-7.13	3	0	97
HOMO-8	-7.29	14	0	86
HOMO-9	-7.45	9	0	90
HOMO-10	-7.62	0	20	80

ILCT : Intra ligand charge transfer transition

Table S4 Calculated transitions and their assignments of the compound **1**

Excitation energy (eV)	Wave length Thro. (nm)	Oscillation frequency (f)	Key Transitions	Nature of transitions
4.6854	264.62	0.2408	(24%) HOMO-2→LUMO+2	ILCT
4.5935	269.91	0.0304	(20%)HOMO→LUMO+3	ILCT
4.3889	282.49	0.0454	(53%) HOMO-8→LUMO+1	ILCT
3.7969	326.54	0.0267	(49%) HOMO-2→LUMO	ILCT
3.5675	347.54	0.0834	(40%) HOMO-3→LUMO+1	ILCT
2.9760	416.62	0.0608	(52%) HOMO→LUMO	ILCT
4.2004	295.17	0.1128	(78%) HOMO →LUMO+2	ILCT