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SUPPORTING INFORMATION FOR

Thionine dye confined in zeolite L: synthesis location and optical properties

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Figure S1. Observed and calculated diffraction patterns and final difference curve from Rietveld refinements of the pure ZL and of the ZL/0.15Th, ZL/0.27Th composites. The inset shows a zoom (the 2Θ range 2–10°) of the collected patters of ZL and of the ZL/0.15Th, ZL/0.27Th composites.

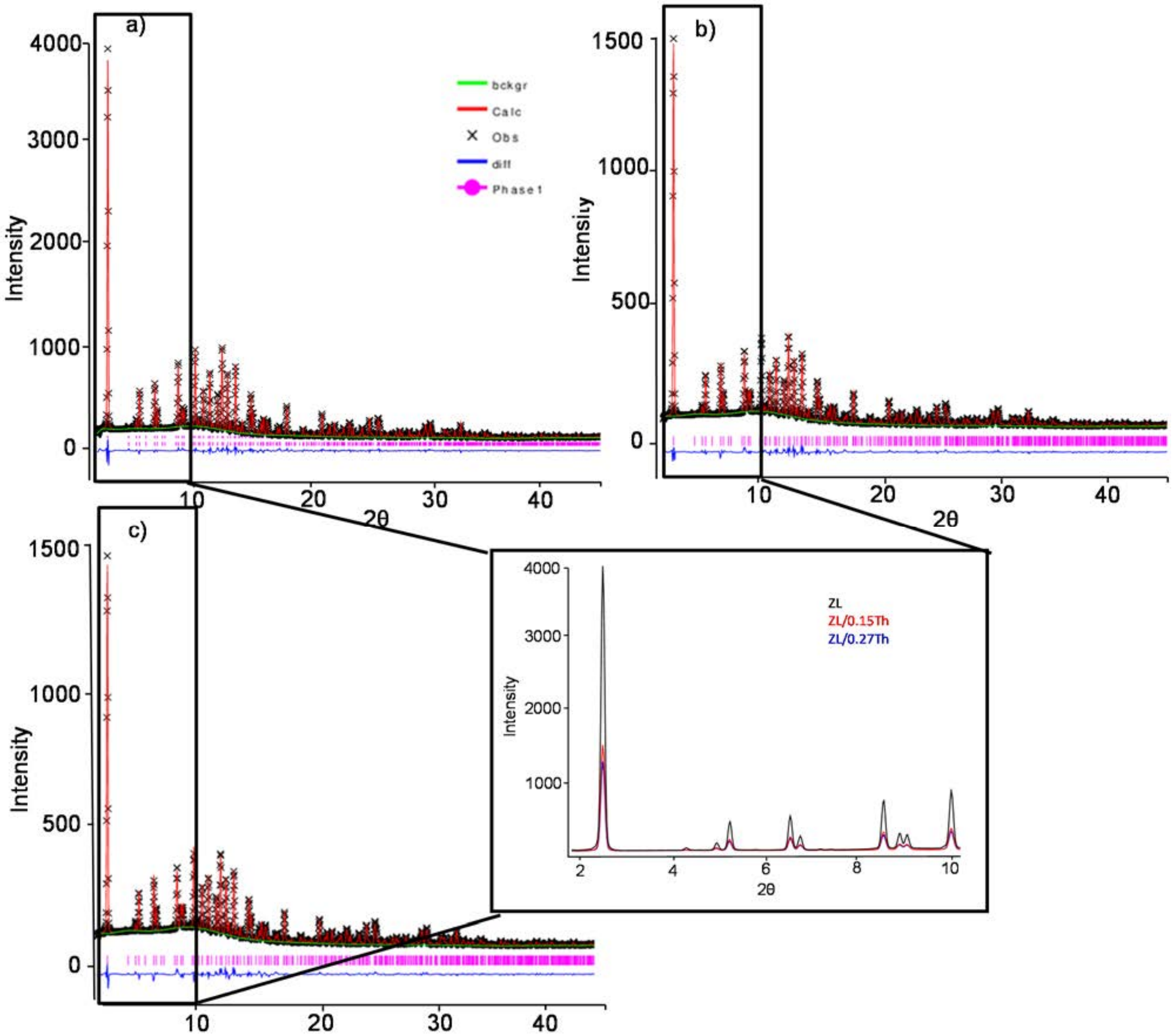

Table S1. Atomic coordinates, occupancy factors and thermal displacement parameters for the structures of the ZL/0.15Th, ZL/0.27Th composites.

Atom	x/a	y/b	z/c	Occ.	U_{iso}
			ZL/0.15Th		
T1	0.0922(2)	0.3559(2)	0.5	1	0.010(5)
T2	0.1651(2)	0.4971(1)	0.2105(2)	1	0.010(5)
O1	0	0.2707(4)	0.5	1	0.013(3)
O2	0.1638(3)	0.3276(5)	0.5	1	0.013(3)
O3	0.2638(2)	0.5276(4)	0.2507(5)	1	0.013(3)
O4	0.1015(3)	0.4128(2)	0.3250(5)	1	0.013(3)
O5	0.4230(1)	0.8460(3)	0.2744(9)	1	0.013(3)
O6	0.1447(4)	0.4777(4)	0	1	0.013(3)
KB	0.33333	0.66667	0.5	1	0.011(2)
KC	0.5	0	0.5	1	0.032(2)
KD	0.2999(3)	0	0	0.779(5)	0.065(3)
WH	0.1278(1)	0	0.3027(1)	0.484(5)	0.114(3)
WF	0.0994(3)	0	0	0.281(2)	0.124(3)
W3	0.2465(3)	0.1103(2)	0.0776(3)	0.261(2)	0.099(3)
W4	0.1533(4)	0.0469(4)	0.5	0.166(2)	0.135(3)
			Th		
S	0.1450(6)	0.0725(2)	0	0.032(1)	0.12(1)
C1	0.0803(4)	0.0401(2)	0.1780(5)	0.032(1)	0.12(1)
C2	0.0106(3)	0.0106(3)	0.1481(5)	0.032(1)	0.12(1)
N1	0.0496(6)	0.0248(2)	0	0.032(1)	0.12(1)
C3	0.1099(6)	0.0550(3)	0.3501(1)	0.032(1)	0.12(1)
C4	0.0409(1)	0.0205(6)	0.4723(9)	0.032(1)	0.12(1)
C5	0.0636(5)	0.0318(2)	0.2909(1)	0.032(1)	0.12(1)
C6	0.0491(1)	0.0245(7)	0.4844(1)	0.032(1)	0.12(1)
N2	0.0699(2)	0.0349(1)	0.3492(1)	0.032(1)	0.12(1)
			ZL/0.27Th		
T1	0.0921(2)	0.3561(2)	0.5	1	0.010(5)
T2	0.1653(2)	0.4971(1)	0.2105(2)	1	0.010(5)
O1	0	0.2707(5)	0.5	1	0.013(3)
O2	0.1642(3)	0.3284(5)	0.5	1	0.013(3)
O3	0.2642(2)	0.5284(4)	0.2485(9)	1	0.013(3)
O4	0.1013(3)	0.4131(2)	0.3245(5)	1	0.013(3)
O5	0.4209(1)	0.8418(5)	0.2735(1)	1	0.013(3)
O6	0.1443(4)	0.4795(4)	0	1	0.013(3)
KB	0.33333	0.66667	0.5	1	0.011(2)
KC	0.5	0	0.5	1	0.032(2)
KD	0.3002(3)	0	0	0.758(5)	0.065(3)
WH	0.1292(1)	0	0.2982(1)	0.364(5)	0.058(3)
WF	0.0986(3)	0	0	0.270(2)	0.163(3)
W3	0.2432(3)	0.1059(2)	0.0775(3)	0.265(2)	0.079(3)
W4	0.1561(4)	0.0397(4)	0.5	0.206(2)	0.100(3)
			Th		
S	0.1450(6)	0.0724(2)	0	0.051(1)	0.12(1)
C1	0.0803(4)	0.0401(2)	0.1780(5)	0.051(1)	0.12(1)

C2	0.0106(3)	0.0106(3)	0.1481(5)	0.051(1)	0.12(1)
N1	0.0496(6)	0.0248(2)	0	0.051(1)	0.12(1)
C3	0.1101(6)	0.0550(3)	0.3501(1)	0.051(1)	0.12(1)
C4	0.0406(1)	0.0203(6)	0.4724(9)	0.051(1)	0.12(1)
C5	0.0635(5)	0.0317(2)	0.2911(1)	0.051(1)	0.12(1)
C6	0.0493(1)	0.0246(7)	0.4845(1)	0.051(1)	0.12(1)
N2	0.0704(2)	0.0352(1)	0.3491(1)	0.051(1)	0.12(1)

Table S2. Extraframework bond distances < 3.2 Å for ZL/0.15Th, ZL/0.27Th composites.

		ZL/0.15Th	ZL/0.27Th			ZL/0.15Th	ZL/0.27Th			ZL/0.15Th	ZL/0.27Th
KB-	**O3 [x6]**	2.902(6)	2.905(7)		**WF[x2]**	2.62(2)	2.65(2)	**W3-**	**KD**	2.72(7)	2.69(3)
KC-	**O5 [x4]**	2.930(8)	3.043(7)		**W4[x2]**	1.83(6)	1.91(3)		**KD**	3.17(7)	3.23(3)
KD-	**O4 [x4]**	3.151(5)	3.146(5)		**W4[x2]**	2.24(6)	2.58(3)		**S**	1.73(2)	1.69(1)
	O6 [x2]	3.012(6)	3.025(7)		**W4[x2]**	2.67(8)	2.79(3)		**N1**	3.19(2)	3.15(1)
	W3[x4]	2.604(5)	2.772(5)	**WH-**	**O1**	3.01(3)	3.01(2)		**C2[x2]**	2.31(6)	2.30(5)
S-	**WH[x2]**	2.57(3)	2.55(2)		**C6[x2]**	2.19(3)	2.23(2)		**C2[x2]**	1.98(5)	1.97(4)
	WF[x2]	1.16(1)	1.169(8)		**C6[x2]**	2.82(3)	2.87(2)		**C1[x4]**	2.60(5)	2.59(4)
	WF[x2]	2.95(4)	2.93(3)		**C6[x2]**	2.95(3)	2.99(2)		**C1[x4]**	1.65(3)	1.64(2)
	W3[x4]	1.73(2)	1.69(1)		**C6[x2]**	2.35(3)	2.38(2)		**C3[x4]**	2.796(7)	2.794(6)
C1-	**WH[x2]**	1.68(3)	1.68(2)		**S[x2]**	2.57(3)	2.55(2)		**C5[x4]**	2.44(3)	2.43(2)
	WH[x2]	2.83(2)	2.84(2)		**N1[x2]**	2.85(3)	2.83(2)		**C5[x4]**	3.03(4)	3.02(3)
	WF[x2]	1.65(3)	1.64(2)		**C2[x2]**	2.54(3)	2.55(2)		**N2[x4]**	2.82(2)	2.81(2)
	WF[x2]	2.60(5)	2.59(4)		**C2[x2]**	2.71(3)	2.72(2)		**WF[x2]**	1.83(7)	1.81(5)
	W3[x2]	2.76(2)	2.71(1)		**C2**	2.79(3)	2.81(2)		**WF[x2]**	3.17(1)	3.14(9)
	W4[x2]	2.74(4)	2.79(2)		**C2**	2.44(3)	2.47(3)		**W3[x4]**	2.50(5)	2.46(3)
	W4[x2]	3.07(5)	3.07(2)		**C1[x2]**	1.68(3)	1.68(2)		**W3[x4]**	2.75(3)	2.64(3)
C2-	**WH[x2]**	2.54(3)	2.55(2)		**C1[x2]**	2.83(2)	2.84(2)	**W4-**	**O1**	2.69(9)	2.55(4)
	WH[x2]	2.71(3)	2.72(2)		**C3[x2]**	1.26(2)	1.28(2)		**O2**	2.83(7)	2.83(4)
	WH	2.44(3)	2.47(3)		**C3[x2]**	2.95(2)	2.98(2)		**C6[x2]**	1.75(7)	1.84(3)
	WH	2.79(3)	2.81(2)		**C3[x2]**	2.87(3)	2.91(2)		**C6[x2]**	2.39(8)	2.51(3)
	WF[x2]	2.07(6)	2.05(4)		**C4[x2]**	2.21(3)	2.26(2)		**C6[x2]**	3.09(7)	3.19(3)
	WF[x2]	2.23(6)	2.22(4)		**C4[x2]**	2.75(3)	2.79(2)		**C6[x2]**	2.84(7)	2.88(3)
	WF	1.98(5)	1.97(4)		**C4[x2]**	3.19(3)	3.16(3)		**C6[x2]**	2.06(7)	2.09(3)
	WF	2.31(6)	2.30(5)		**C4[x2]**	2.96(3)	3.00(2)		**C1[x2]**	2.74(4)	2.79(1)
C3-	**WH[x2]**	1.26(2)	1.28(1)		**C4[x2]**	2.48(3)	2.52(2)		**C1[x2]**	3.07(5)	3.07(2)
	WH[x2]	2.95(2)	2.98(2)		**C5[x2]**	1.56(2)	1.58(2)		**C3[x2]**	1.43(5)	1.51(2)
	WH[x2]	2.87(3)	2.91(2)		**C5[x2]**	2.56(2)	2.58(2)		**C3[x2]**	2.82(9)	2.96(3)
	WF[x2]	2.796(7)	2.794(6)		**N2[x2]**	1.53(2)	1.56(2)		**C3[x2]**	2.16(7)	2.12(3)
	W3[x2]	2.99(3)	2.96(2)		**N2[x2]**	2.62(2)	2.65(2)		**C4[x2]**	1.88(7)	1.98(3)
	W4[x2]	1.43(5)	1.51(2)		**N2[x2]**	3.01(3)	3.05(2)		**C4[x2]**	2.40(8)	2.51(3)
	W4[x2]	2.16(7)	2.12(3)		**WH[x2]**	2.35(3)	2.37(2)		**C4[x2]**	2.99(7)	2.97(7)
	W4[x2]	2.82(9)	2.96(4)		**WH**	2.97(6)	3.04(5)		**C4[x2]**	3.15(7)	3.08(3)
C4-	**WH[x2]**	2.21(3)	2.26(2)		**WF[x2]**	3.12(3)	3.10(2)		**C4[x2]**	2.78(7)	2.82(3)
	WH[x2]	2.75(3)	2.79(2)		**WF**	2.33(3)	2.32(2)		**C4[x2]**	2.13(7)	2.17(3)
	WH[x2]	3.19(3)	3.16(3)		**W3[x2]**	2.65(2)	2.54(2)		**C5[x2]**	2.19(5)	2.26(2)
	WH[x2]	2.96(3)	3.00(2)		**W3[x2]**	2.95(1)	2.76(1)		**C5[x2]**	2.87(7)	2.98(3)
	WH[x2]	2.48(3)	2.52(2)		**W4[x2]**	1.67(2)	1.75(2)		**C5[x2]**	2.52(6)	2.53(2)
	W4[x2]	1.88(7)	1.98(3)		**W4[x2]**	2.35(2)	2.48(1)		**N2[x2]**	1.83(6)	1.91(3)
	W4[x2]	2.13(7)	2.17(3)	**WF-**	**S[x2]**	1.16(1)	1.169(8)		**N2[x2]**	2.67(8)	2.79(3)
	W4[x2]	2.78(7)	2.75(7)		**S[x2]**	2.95(4)	2.93(3)		**N2[x2]**	2.24(6)	2.58(3)
	W4[x2]	3.15(7)	3.08(3)		**N1[x2]**	1.21(6)	1.20(5)		**WH[x2]**	1.66(5)	1.65(2)
	W4[x2]	2.99(7)	2.82(3)		**N1[x2]**	1.99(6)	1.98(5)		**WH[x2]**	2.31(8)	2.46(3)
	W4[x2]	2.40(8)	2.51(3)		**N1[x2]**	2.54(7)	2.53(5)		**W4[x2]**	2.50(7)	2.58(3)

C5-	**WH[x2]**	1.56(3)	1.58(1)	**C2[x4]**	2.07(6)	2.05(4)	**W4**	1.50(2)	1.41(8)
	WH[x2]	2.56(3)	2.58(1)	**C2[x4]**	2.23(6)	2.22(4)	**W4**	1.09(2)	1.27(8)
	WF[x2]	2.44(3)	2.43(2)	**C2[x2]**	2.31(6)	2.30(5)			
	WF[x2]	3.03(4)	3.02(3)	**C2[x2]**	1.98(5)	1.97(4)			
	W4[x2]	2.19(5)	2.26(2)	**C1[x4]**	2.60(5)	2.59(4)			
	W4[x2]	2.52(6)	2.53(3)	**C1[x4]**	1.65(3)	1.64(2)			
	W4[x2]	2.87(7)	2.98(3)	**C3[x4]**	2.796(7)	2.794(6)			
N1-	**WH[x4]**	2.85(3)	2.83(2)	**C5[x4]**	2.44(2)	2.43(2)			
	WF[x2]	1.21(6)	1.20(5)	**C5[x4]**	3.03(4)	3.02(3)			
	WF[x2]	1.99(6)	1.98(5)	**N2[x4]**	2.82(2)	2.81(1)			
	WF[x2]	2.54(7)	2.53(5)	**WF[x2]**	1.83(7)	1.81(5)			
	W3[x4]	3.19(2)	3.15(1)	**WF[x2]**	3.17(2)	3.14(9)			
N2-	**WH[x2]**	1.53(2)	1.56(2)	**W3[x4]**	2.50(5)	2.46(3)			
	WH[x2]	3.01(3)	3.05(2)	**W3[x4]**	2.75(3)	2.64(2)			

Table S3. Assignment of the main signals present in the spectra shown in Figure 4

Frequency (cm^{-1})	Assignment	References
Thionine (Th; acetate salt, in ZL)		
3352, 3235	$\nu_{asym}NH_2$, $\nu_{sym}NH_2$ (observable in Th in ZL)	N.B. Ref 48, p. 321
3200-2800 (range)	νNH_3^+ (Th in the acetate salt)*	N.B. Ref 48, p. 324
2950	νCH_3 (acetate ions)	N.B. Ref 48, p. 223
1650	$\delta_{asym}NH_3^+$ (Th in the acetate salt)*	N.B. Ref 48, p. 324
1645	δNH_2 (Th in ZL, contribution to the peak, together with δH_2O)	N.B. Ref 48, p. 321
1608	δNH_2 (Th in the acetate salt, contribution to the peak, togheter with a skeletal ring mode, see below)	N.B. Ref 48, p. 321
1544	$\nu_{asym}COO^-$ (acetate ions)	Ref 49, p. 232
1608[a], 1604[b], 1486[a,b], 1464[a,b], 1320[a,b]	ring modes of polycyclic compounds; [a]: Th in the acetate salt; [b]: Th in ZL	N.B. Ref 48, p. 270
1425-1340 (range, complex signal)	$\nu C{=}N$ in the ring (thionine)[c] and $\nu_{sym}COO^-$ (acetate ions)[d]	[c] Ref 50 [d] Ref 49, p. 232
1222	$\nu C{-}NH_2$ (both acetate salt and in ZL)	Ref 51, p. 287
Zeolite (including water in the channels)		
3700-3000 (range)	νH_2O	Ref 52
1645	δH_2O (contribution to the peak, together with δNH_2 of Th)	Ref 52
1001	νT-O-T (T= Si, Al)	Ref 52
764, 718	δT-O-T (T= Si, Al)	Ref 52

* likely resulting from the salification by reaction with CH_3COOH of some $–NH_2$ groups