ZINC METAL COMPLEX AS SENSOR FOR SIMULTANEOUS DETECTION OF FLUORIDE AND HSO_4^- IONS

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Table 1. Crystal data and refinement parameters of N17

Compound	**N17**
Empirical Formula	$C_{62}\ H_{60}\ N_{18}\ O_{18}\ Zn_3$
M_w	1541.39
Temperature [K]	293(2)
Crystal System	Triclinic
Space group	$P\bar{1}$
a / [Å]	14.0738(8)
b / [Å]	14.4682(9)
c / [Å]	18.1303(11)
α/ [º]	82.254(3)
β / [º]	81.010(3)
γ/ [º]	68.154(2)
V [Å^3]	3372.7(4)
Z	2
D_c [Mg m^{-3}]	1.518
μ / [mm^{-1}]	1.143
Reflections collected	112098
Data / restraints / parameters	13246 / 0 / 957
Unique reflections, [R_{int}]	13246 [0.0397]
GOF = S_{all}	1.047
Final *R* indices	
R_1, wR_2 [I>2σI]	0.0343, 0.0808
R_1, wR_2 (all data)	0.0542, 0.0861
Δρmax/Δρmin [Å^3]	0.392/-0.316

Table 2. Selected bond lengths and angles (Å,°) for N17

Bond lengths(Å)					
Zn(1)-N(4)	2.0881(17)	Zn(2)-O(16)	2.0710(14)	Zn(3)-N(11)	2.0970(16)
Zn(1)-N(6)	2.0962(18)	Zn(2)-O(1)	2.0879(14)	Zn(3)-N(9)	2.1136(17)
Zn(1)-N(2)	2.1079(18)	Zn(2)-O(4)	2.0967(14)	Zn(3)-N(13)	2.1161(17)
Zn(1)-O(1)	2.1555(14)	Zn(2)-O(7)	2.1009(14)	Zn(3)-O(16)	2.1609(14)
Zn(1)-O(7)	2.1846(14)	Zn(2)-O(10)	2.1087(13)	Zn(3)-O(13)	2.1908(14)
Zn(1)-O(4)	2.1948(14)	Zn(2)-O(13)	2.1171(14)	Zn(3)-O(10)	2.2082(13)
Zn(1)-Zn(2)	2.9885(3)	Zn(2)-Zn(3)	3.0077(3)		
Bond angles(°)					
N(4)-Zn(1)-N(6)	105.07(7)	O(16)-Zn(2)-O(7)	104.54(5)	Zn(1)-Zn(2)-Zn(3)	177.569(11)
N(4)-Zn(1)-N(2)	105.86(7)	O(1)-Zn(2)-O(7)	79.12(5)	N(11)-Zn(3)-N(9)	104.92(7)
N(6)-Zn(1)-N(2)	101.51(7)	O(4)-Zn(2)-O(7)	77.41(5)	N(11)-Zn(3)-N(13)	106.72(6)
N(4)-Zn(1)-O(1)	92.52(6)	O(16)-Zn(2)-O(10)	79.10(5)	N(9)-Zn(3)-N(13)	102.62(7)
N(6)-Zn(1)-O(1)	86.04(6)	O(1)-Zn(2)-O(10)	101.51(6)	N(11)-Zn(3)-O(16)	85.26(6)
N(2)-Zn(1)-O(1)	157.28(6)	O(4)-Zn(2)-O(10)	98.97(5)	N(9)-Zn(3)-O(16)	157.46(6)
N(4)-Zn(1)-O(7)	85.56(6)	O(7)-Zn(2)-O(10)	176.17(5)	N(13)-Zn(3)-O(16)	93.29(6)
N(6)-Zn(1)-O(7)	159.49(6)	O(16)-Zn(2)-O(13)	77.81(5)	N(11)-Zn(3)-O(13)	93.27(6)
N(2)-Zn(1)-O(7)	92.08(6)	O(1)-Zn(2)-O(13)	178.23(5)	N(9)-Zn(3)-O(13)	84.85(6)
O(1)-Zn(1)-O(7)	75.85(5)	O(4)-Zn(2)-O(13)	103.06(5)	N(13)-Zn(3)-O(13)	155.71(6)
N(4)-Zn(1)-O(4)	157.61(6)	O(7)-Zn(2)-O(13)	102.35(5)	O(16)-Zn(3)-O(13)	74.38(5)
N(6)-Zn(1)-O(4)	92.51(6)	O(10)-Zn(2)-O(13)	77.10(5)	N(11)-Zn(3)-O(10)	158.56(6)
N(2)-Zn(1)-O(4)	83.54(6)	O(16)-Zn(2)-Zn(1)	133.38(4)	N(9)-Zn(3)-O(10)	90.93(6)
O(1)-Zn(1)-O(4)	74.68(5)	O(1)-Zn(2)-Zn(1)	46.16(4)	N(13)-Zn(3)-O(10)	83.16(6)
O(7)-Zn(1)-O(4)	73.65(5)	O(4)-Zn(2)-Zn(1)	47.23(4)	O(16)-Zn(3)-O(10)	75.05(5)
N(4)-Zn(1)-Zn(2)	113.92(5)	O(7)-Zn(2)-Zn(1)	46.95(4)	O(13)-Zn(3)-O(10)	73.54(5)
N(6)-Zn(1)-Zn(2)	115.02(5)	O(10)-Zn(2)-Zn(1)	131.14(4)	N(11)-Zn(3)-Zn(2)	114.49(5)
N(2)-Zn(1)-Zn(2)	114.20(5)	O(13)-Zn(2)-Zn(1)	135.61(4)	N(9)-Zn(3)-Zn(2)	114.54(5)
O(1)-Zn(1)-Zn(2)	44.32(4)	O(16)-Zn(2)-Zn(3)	45.92(4)	N(13)-Zn(3)-Zn(2)	112.49(5)
O(7)-Zn(1)-Zn(2)	44.64(4)	O(1)-Zn(2)-Zn(3)	131.50(4)	O(16)-Zn(3)-Zn(2)	43.51(4)
O(4)-Zn(1)-Zn(2)	44.53(4)	O(4)-Zn(2)-Zn(3)	133.34(4)	O(13)-Zn(3)-Zn(2)	44.72(4)
O(16)-Zn(2)-O(1)	100.89(5)	O(7)-Zn(2)-Zn(3)	134.84(4)	O(10)-Zn(3)-Zn(2)	44.49(3)
O(16)-Zn(2)-O(4)	177.69(5)	O(10)-Zn(2)-Zn(3)	47.21(4)		
O(1)-Zn(2)-O(4)	78.19(5)	O(13)-Zn(2)-Zn(3)	46.73(4)		

Table 3. Hydrogen bonding parameters (Å, °) of N17

D-H···A	**D···A/ Å**	**H···A/ Å**	**D-H···A/°**
C9-H9A...O18 [i]	3.613(3)	2.742(2)	149.8(2)
C10-H10B...O17 [ii]	3.253(4)	2.481(2)	136.4(2)
C16-H16A...O9 [iii]	3.369(4)	2.564(3)	145.1(2)
C21-H21A...O11 [iv]	3.285(3)	2.675(2)	123.8(2)
C21-H21A...N17	3.350(10)	2.680(10)	129.6(3)

C25-H25A...N18 [v]	3.299(17)	2.482(16)	146.6(4)
C36-H36A...O3 [vi]	3.335(4)	2.571(3)	135.7(2)
C37-H37B...O3 [vi]	3.582(3)	2.714(2)	149.2(2)
C39-H39A...O5 [vii]	3.468(3)	2.549(2)	169.9(2)
C47-H47A...N15 [vii]	3.436(4)	2.621(4)	141.9(2)
C52-H52A...O11 [iv]	3.523(4)	2.710(3)	146.5(2)
C55-H55B...O3 [iv]	3.398(5)	2.572(2)	144.3(3)
C57-H57C...O6 [viii]	3.435(4)	2.653(2)	138.9(2)
C57-H57A...O8 [ii]	3.358(5)	2.577(3)	138.6(2)

Equivalent positions: (i) x-1,+y,+z, (ii) -x+2,-y+1,-z, (iii) -x+2,-y+2,-z, (iv) -x+1,-y+1,-z+1, (v) -x+2,-y+1,-z+1, (vi) x,+y+1,+z, (vii) x+1,+y,+z, (viii) x+1,+y-1,+z

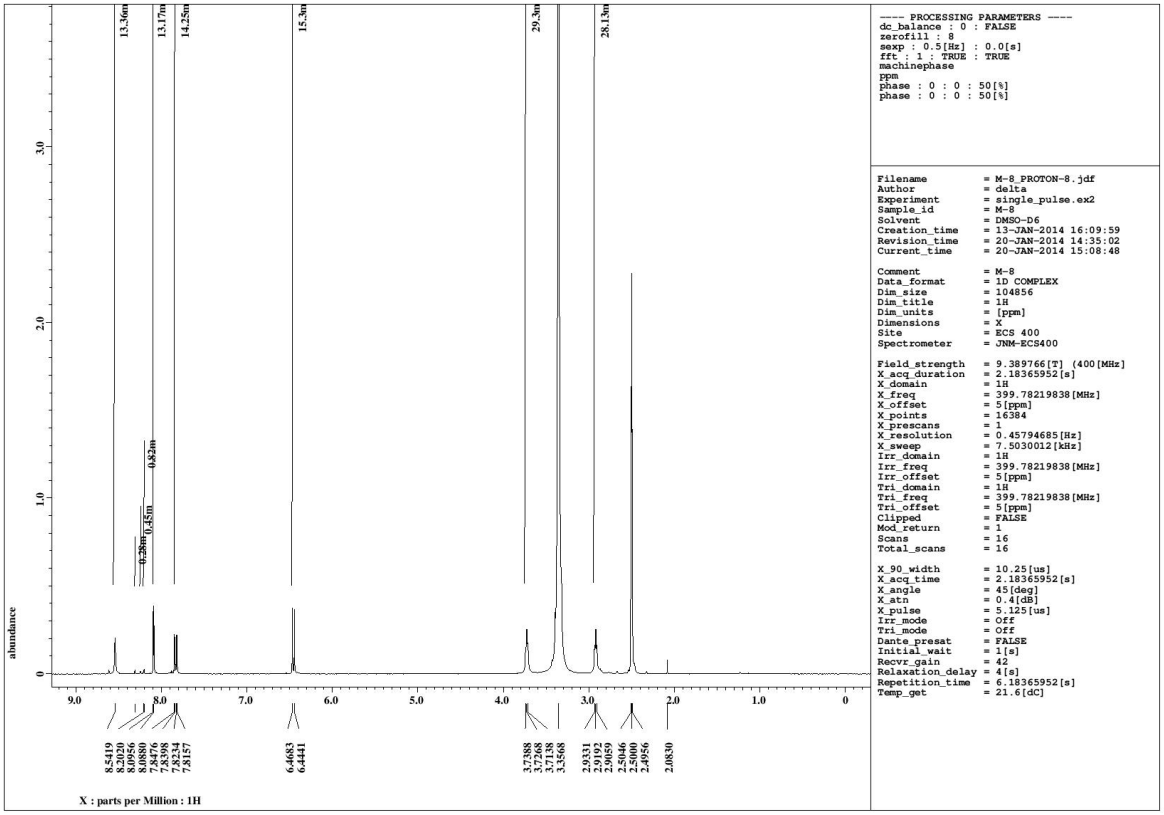

Figure S1. ^{1}H NMR of H_3L_1

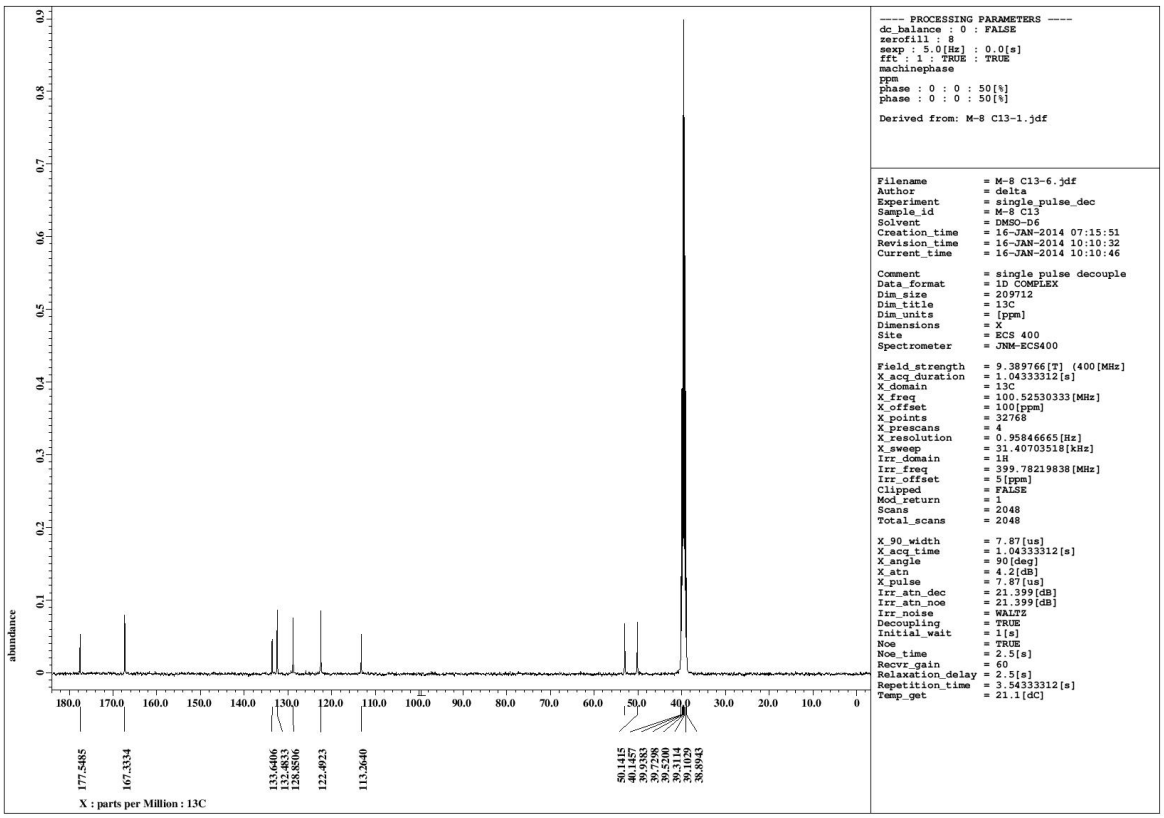

Figure S2. ^{13}C NMR of H_3L_1

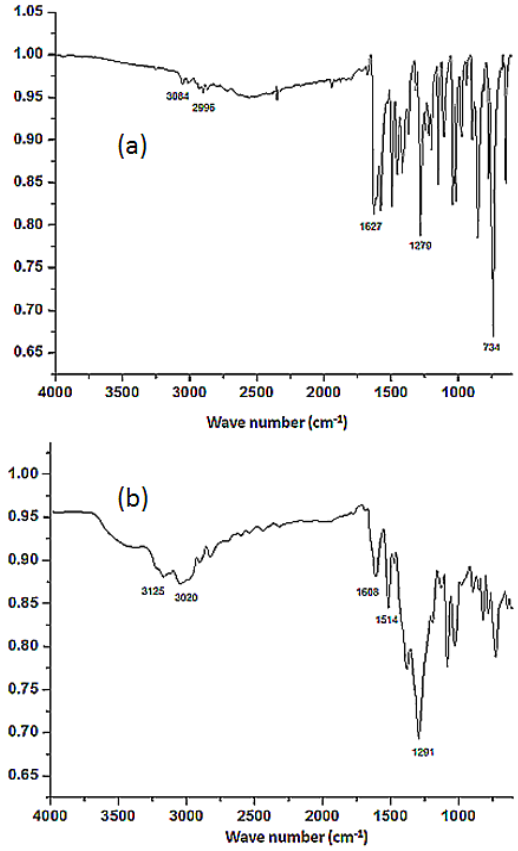

Figure S3: IR spectra of (a) Receptor (H_3L_1) and (b) n17, showing clear shift in Schiff's base peak from 1627 cm^{-1} to 1608 cm^{-1}, marking interaction of –C=N bond with zinc metal ion.

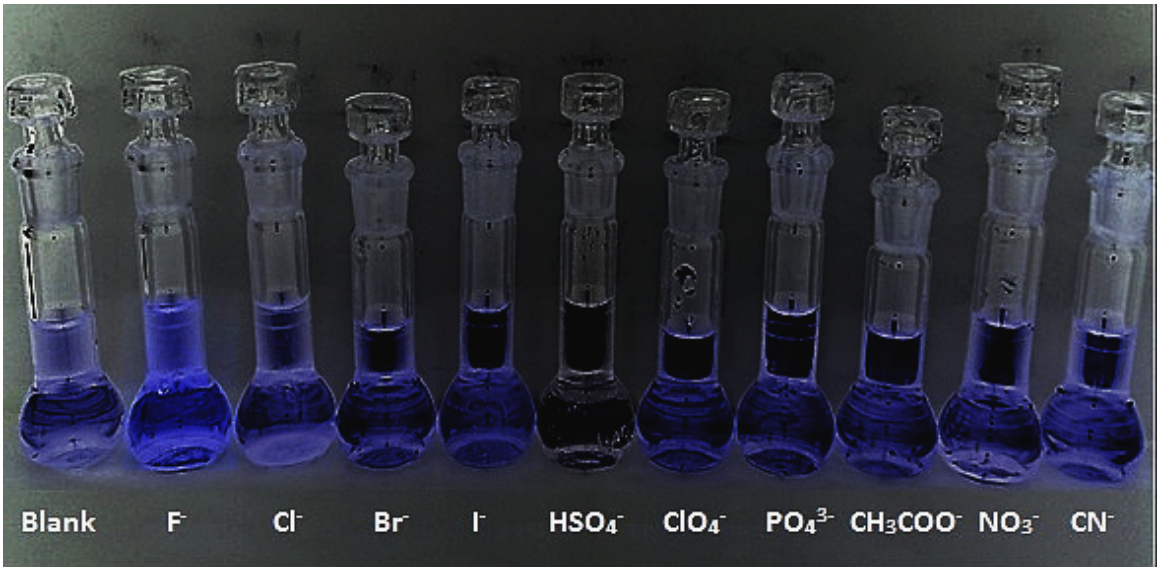

Figure S4. Emission photograph of n17 with different anions

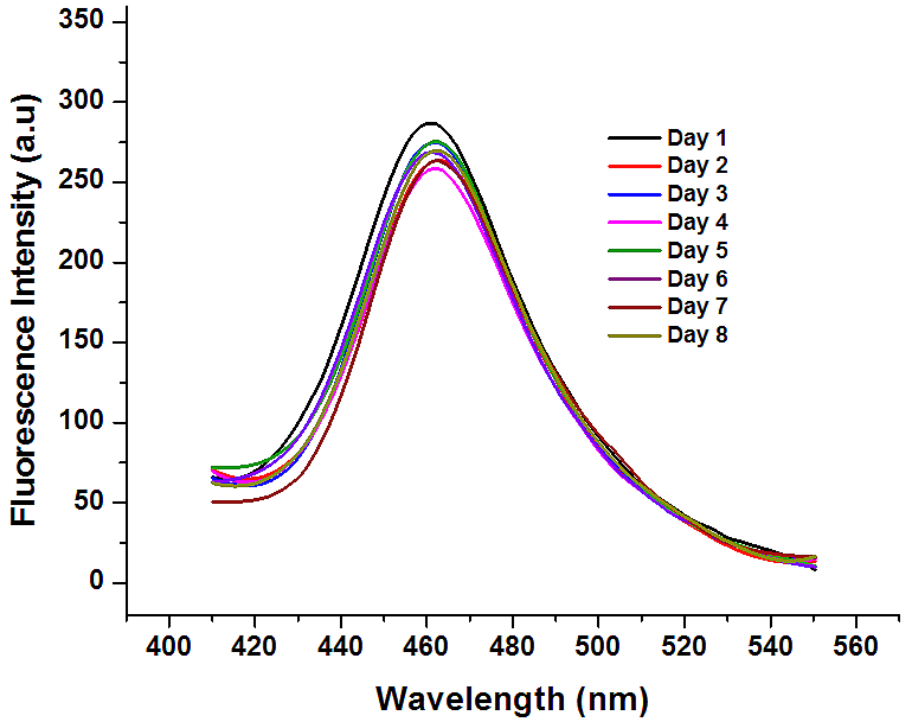

Figure S5. Emission profile of n17 nanoaggregates during various days (1-8

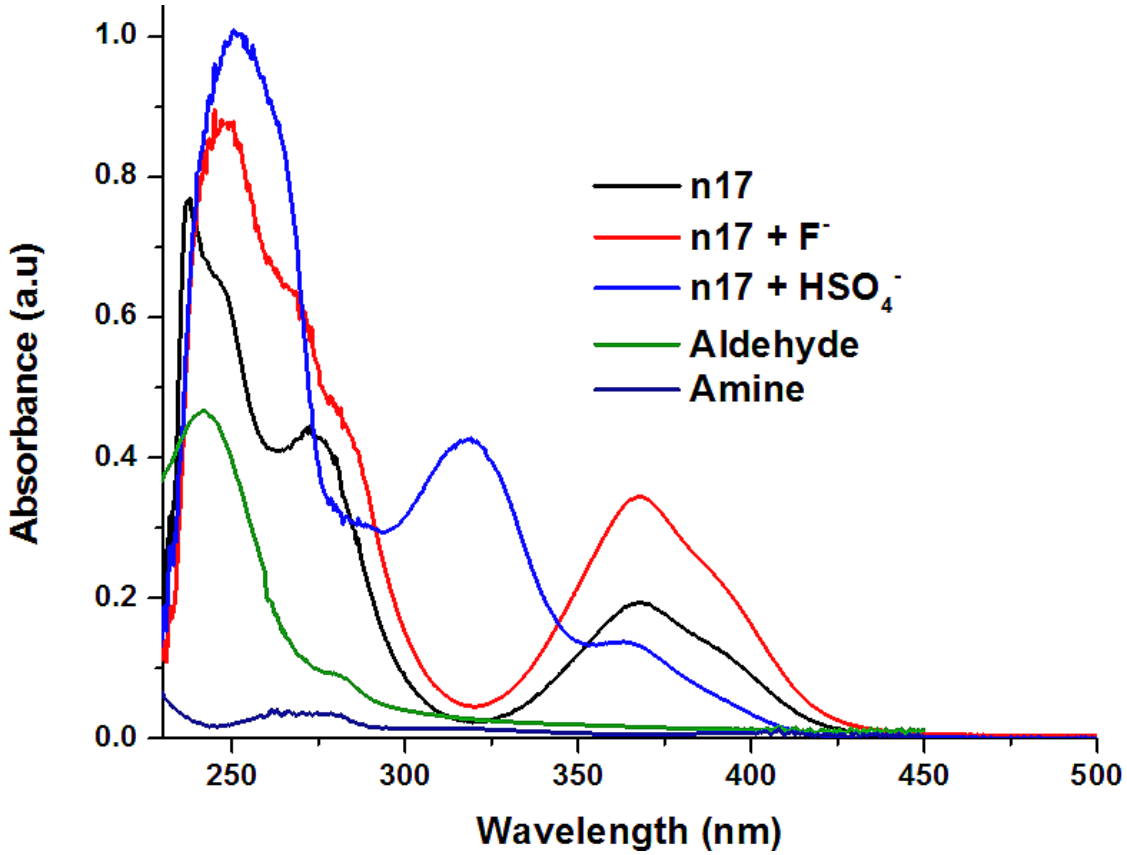

Figure S6. UV-Visible absorbance profile of n17 in presence of F^- and HSO_4^- ions

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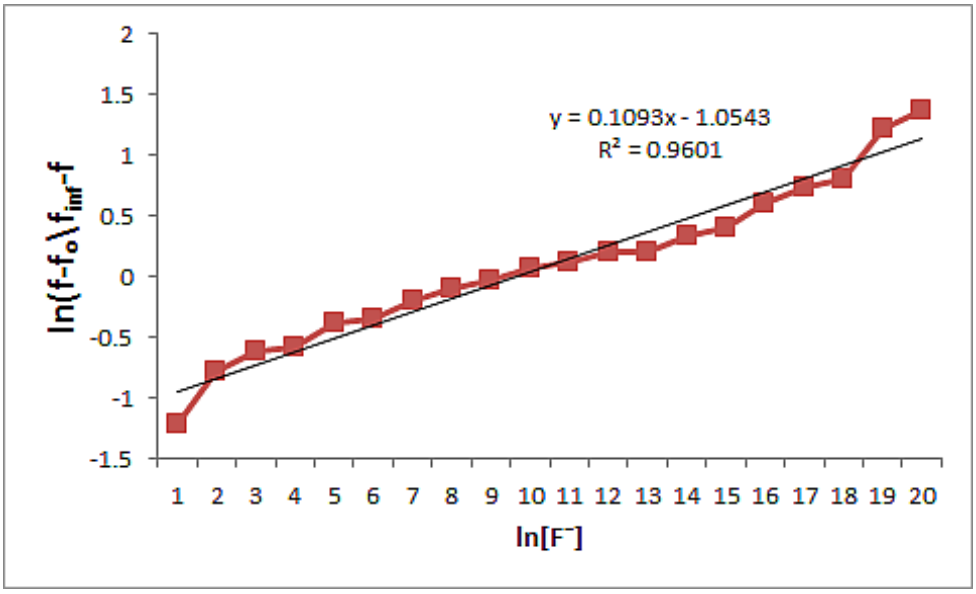

Figure S7: Lehrer Chipman plot for calculation of binding constant and stoichiometry for n17.F^-.

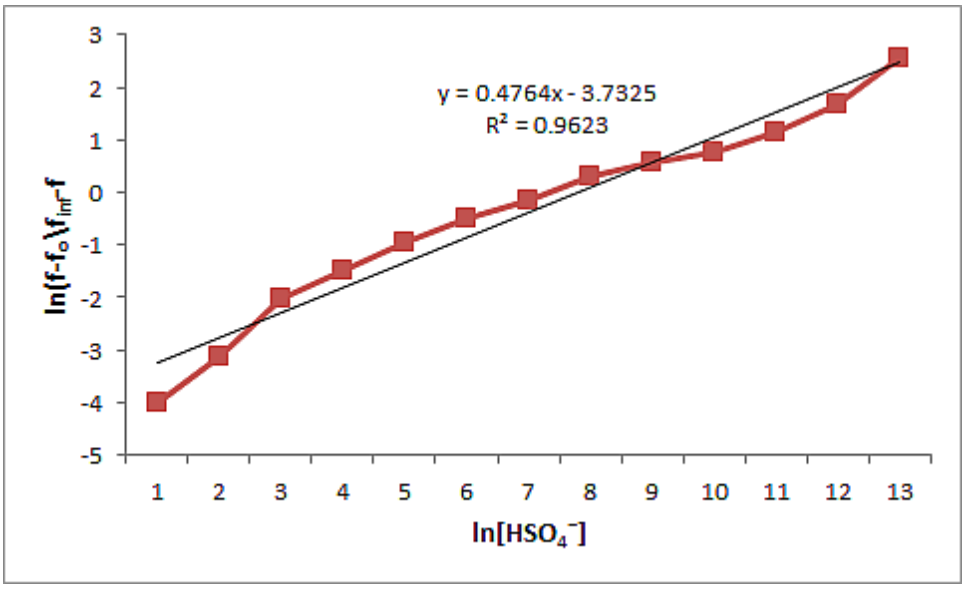

Figure S8: Lehrer Chipman plot for calculation of binding constant and stoichiometry for n17.HSO_4^-