Supporting Information

Optical and Photocatalytic Behaviours of Nanoparticles in the Ti-Zn-O Binary System

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Powder XRD spectra were taken on an X-pert Pro PW3064/60 diffractometer with a high-throughput stage and Cu-Kα radiation (λ = 0.15418 nm). Continuous scans were collected over the 2θ range 20 - 80 ° with a step size of 0.02 ° for a dwell time of 2 s per step.

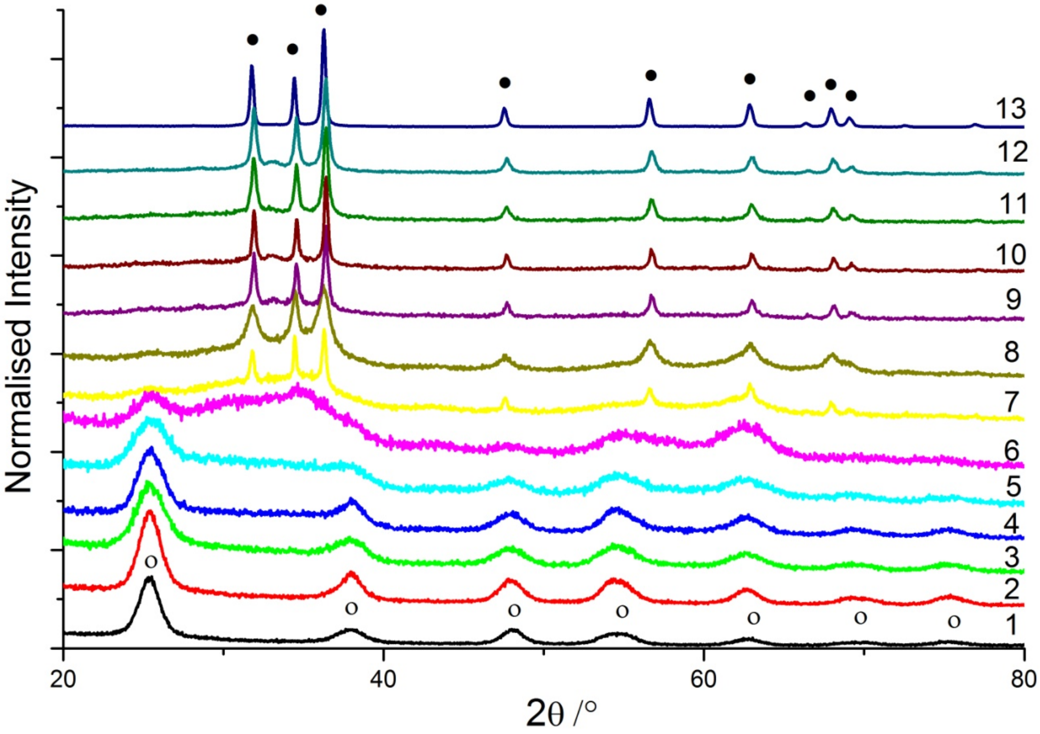


Figure S1: XRD spectra of TiO_2:ZnO nano-coprecipitates (○- anatase peaks, ●- ZnO peaks).

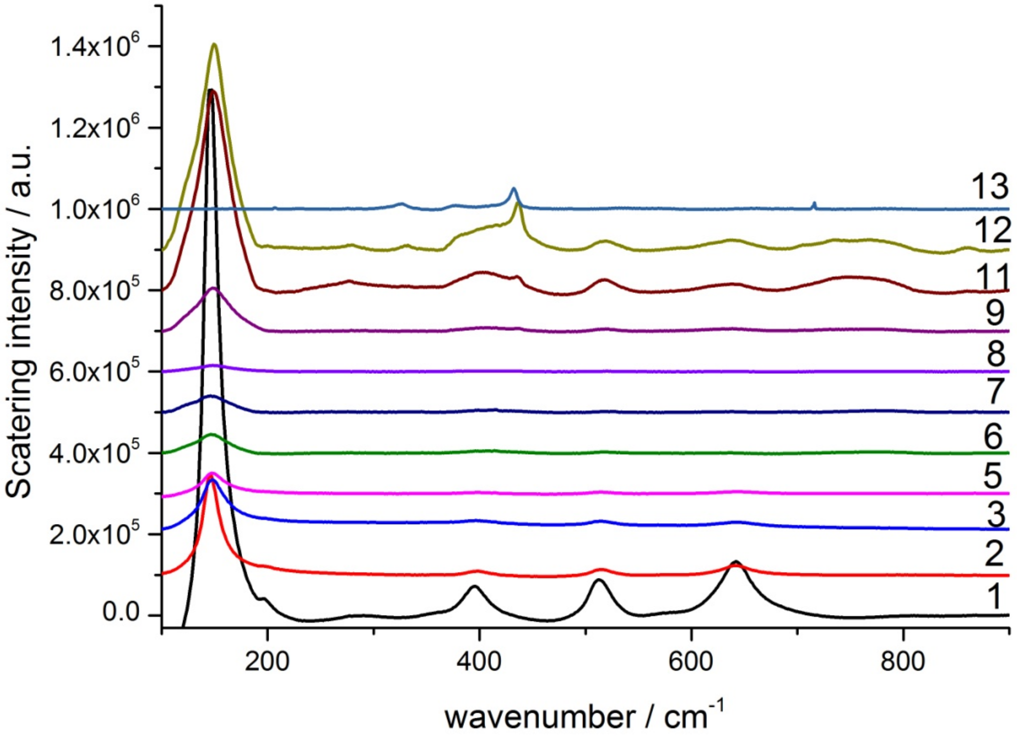


Figure S2: Raman spectra of selected TiO_2: ZnO coprecipitates

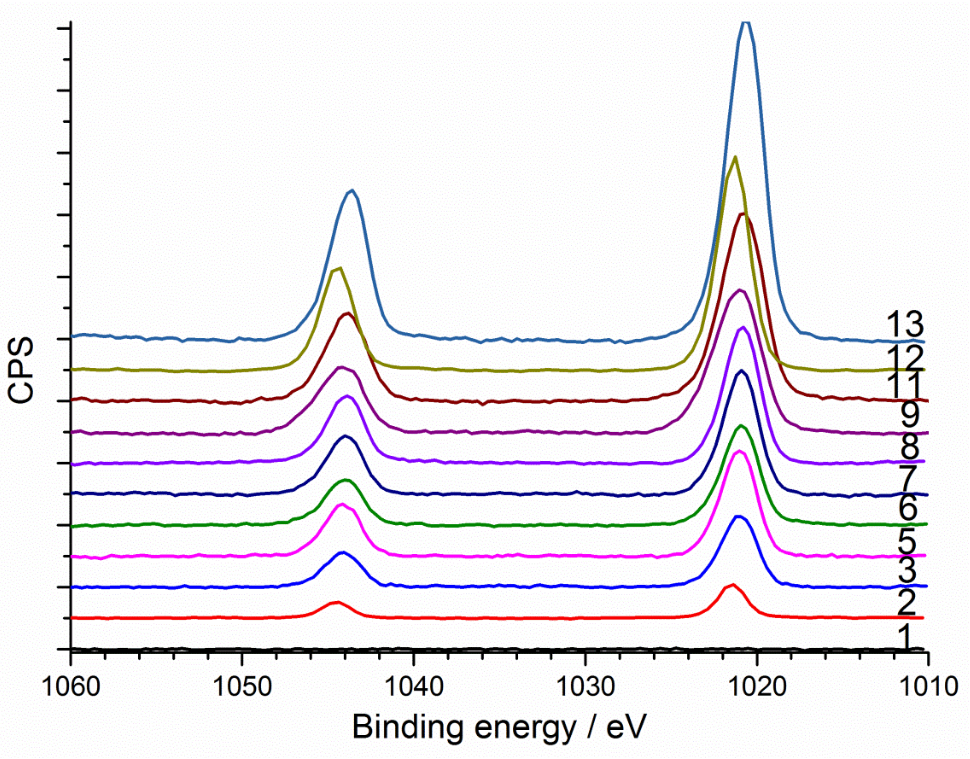


Figure S3: XPS spectra of the Zn 2p region for selected TiO_2:ZnO coprecipitates

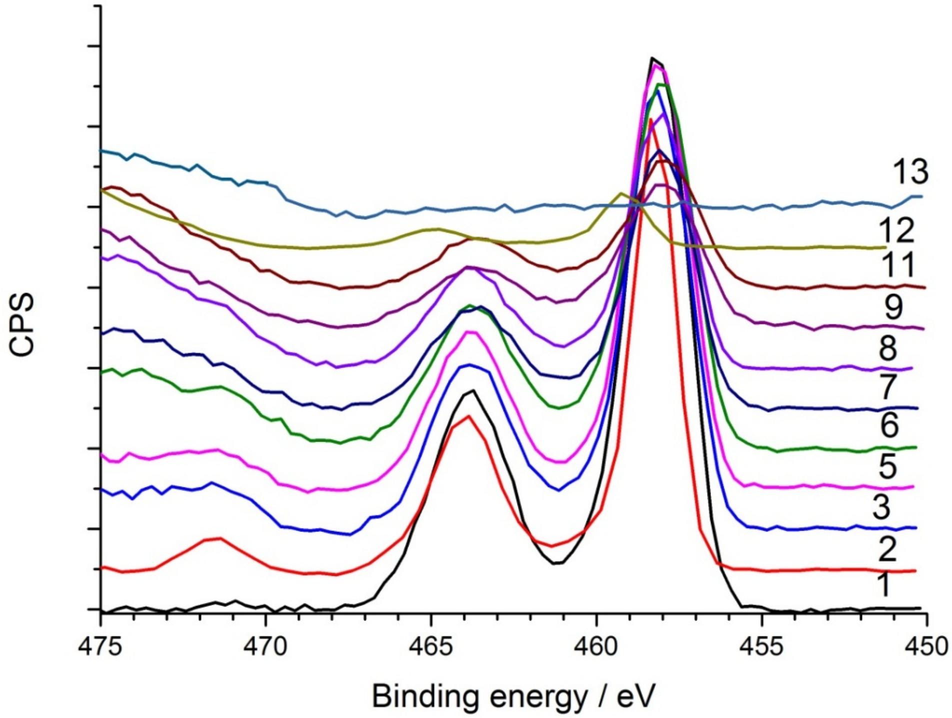


Figure S4: XPS spectra of the Ti 2p region for selected TiO_2:ZnO coprecipitates

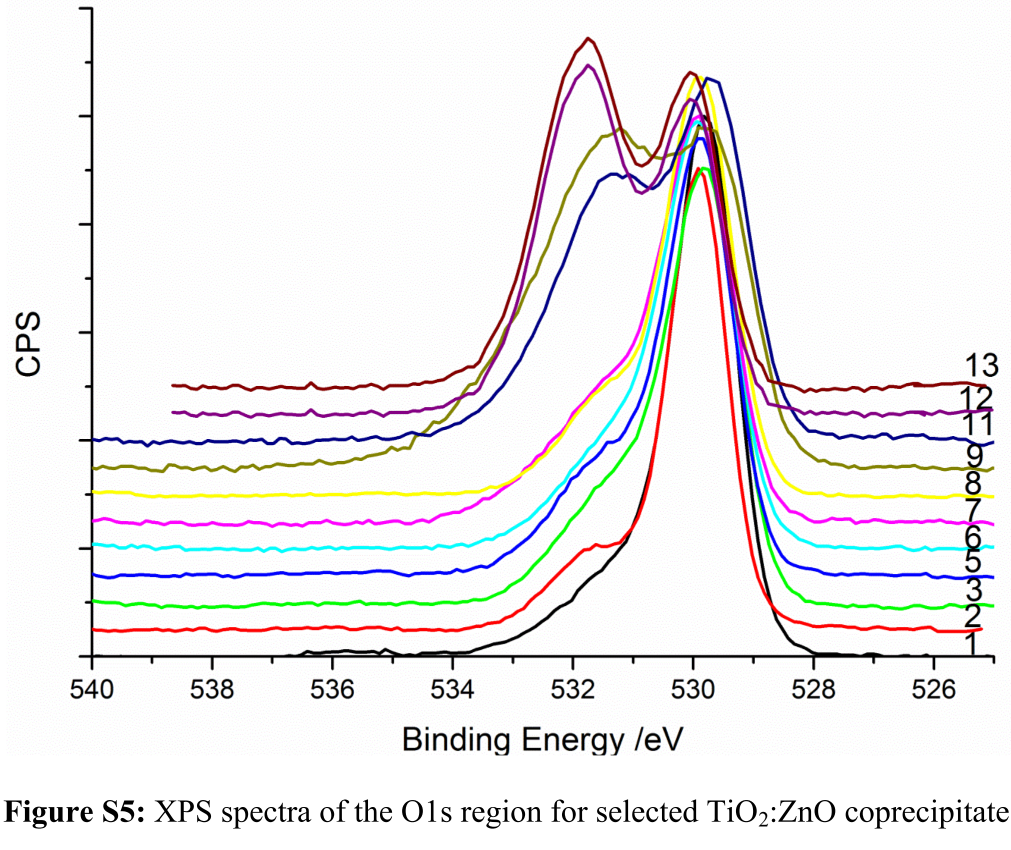


Figure S5: XPS spectra of the O1s region for selected TiO_2:ZnO coprecipitates

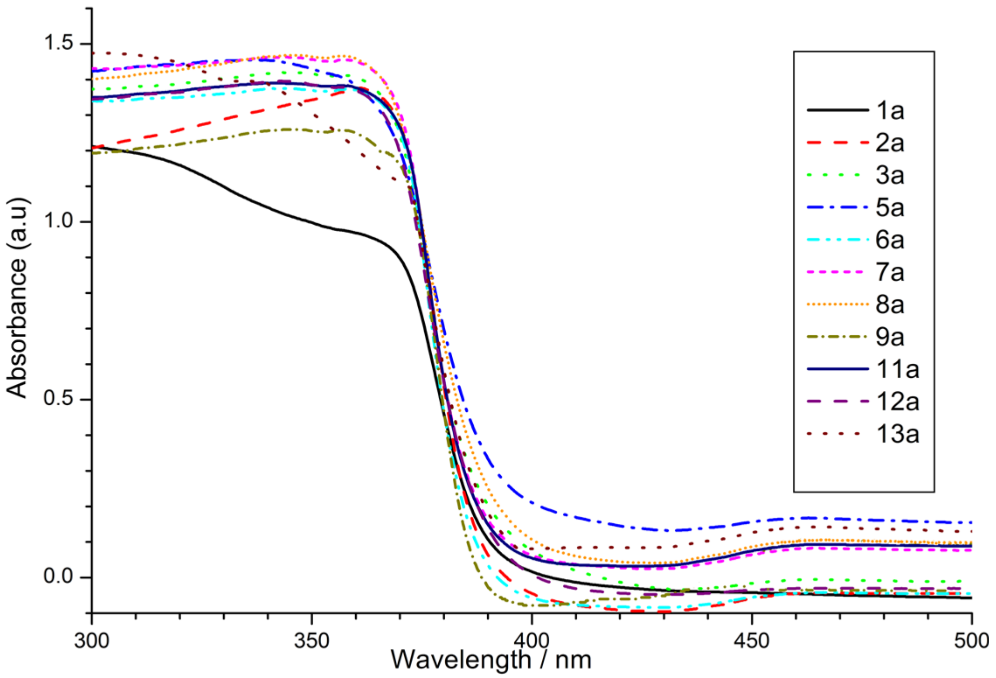
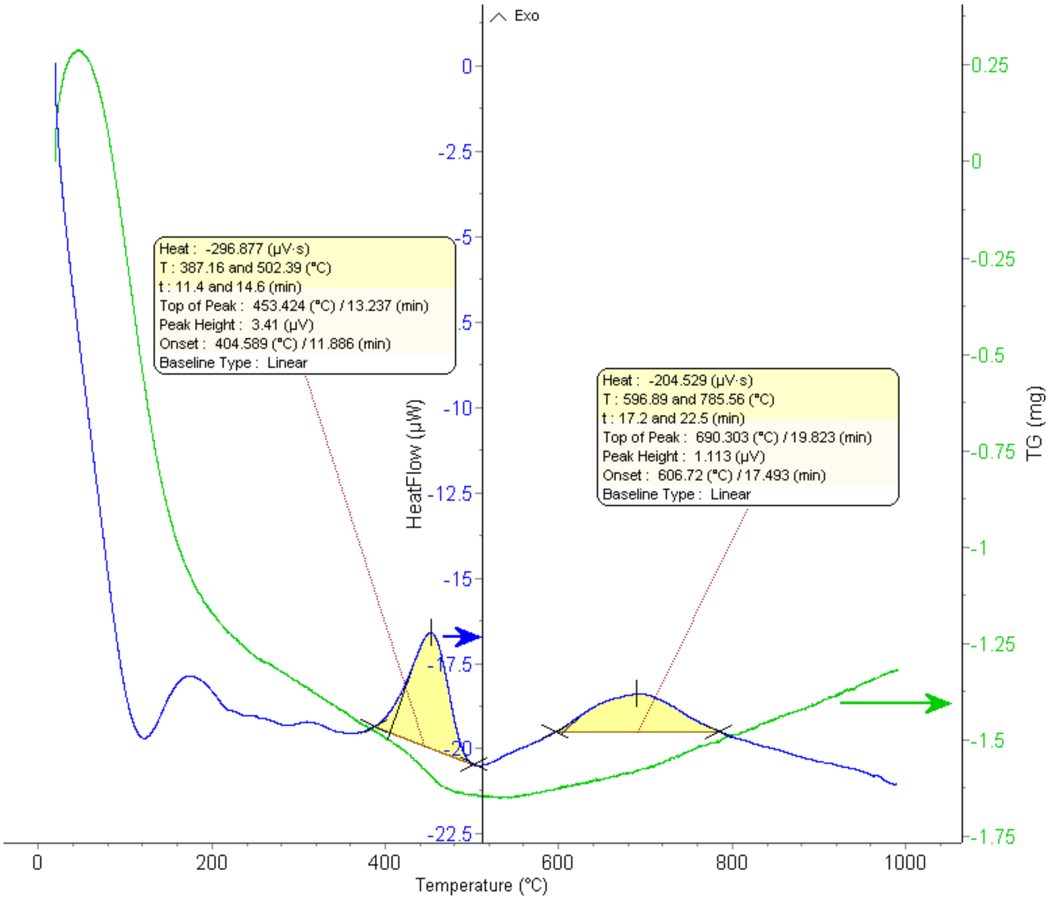


Figure S6: The UV-Vis absorption spectra of the samples after heat treatment to 850 °C for 5 hrs.



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Heat :  -296.877 (μV·s)
T : 387.16 and 502.39 (°C)
t : 11.4 and 14.6 (min)
Top of Peak :  453.424 (°C) / 13.237 (min)
Peak Height :  3.41 (μV)
Onset :  404.589 (°C) / 11.886 (min)
Baseline Type :  Linear
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Heat :  -204.529 (μV·s)
T : 596.89 and 785.56 (°C)
t : 17.2 and 22.5 (min)
Top of Peak :  690.303 (°C) / 19.823 (min)
Peak Height :  1.113 (μV)
Onset :  606.72 (°C) / 17.493 (min)
Baseline Type :  Linear
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Figure S7: STA of sample 8 (60:40 Ti:Zn) heated at 10 °C.min^{-1} in air.

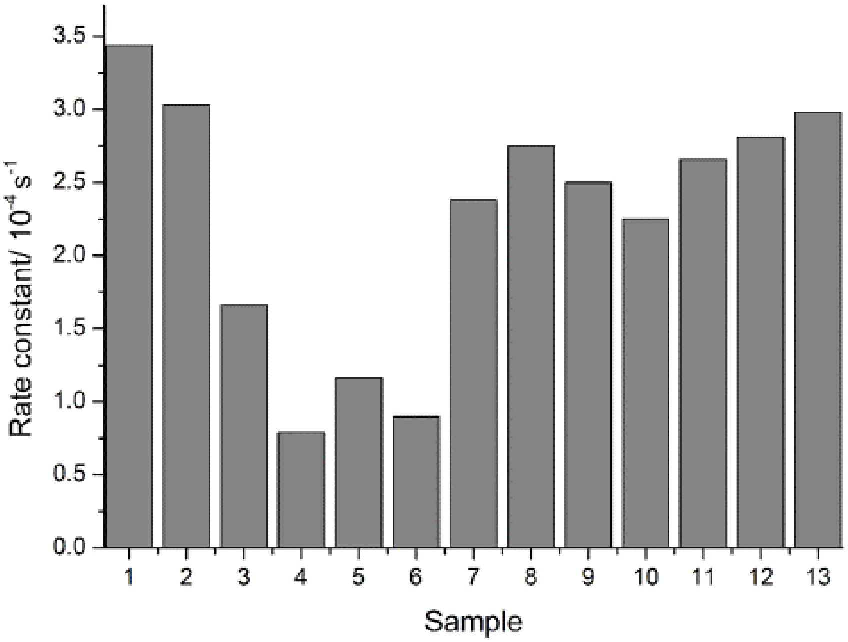

Figure S8: First order rate constant of nanopowders (samples 1-13) for the decolourisation of MB (rate constant of as-prepared samples).

To calculate the bandgap, The Kubelka-Munk (K-M) function and Tauc plots were used. The K-M function, (F(R)) used is shown in equation 1 (R is the reflectance) and the factors for indirect $(F(R).E^{1/2})$ and direct $(F(R).E^{2})$ band gaps used for the Tauc plots were plotted against photon energy. The K-M function defined below for direct and indirect energy transitions was plotted against the photon energy and E_g was determined as the energy coordinate of the point on the low energy side of F(R) curve at which the linear increase starts.

$$F_{KM} = \frac{(1 - R^2)}{2R}$$

Equation (1)

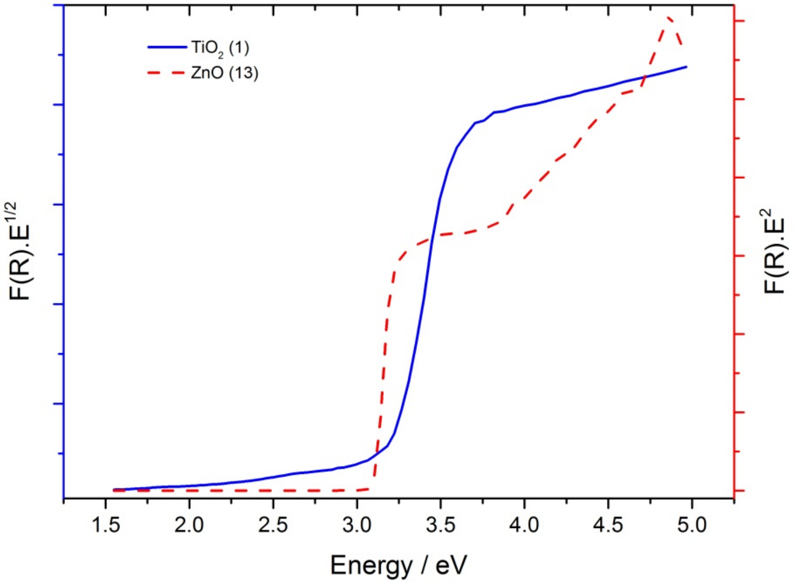

Figure S9: Determination of bandgap values for pure TiO_2 and ZnO samples calculated using Kubelka –Munk function

Table S1: Bandgap values for zinc titanate samples

Sample	Bandgap /eV	
	Direct	**Indirect**
1a	3.25	3.18
2a	3.24	3.23
3a	3.23	3.22
5a	3.20	3.19
6a	3.25	3.24
7a	3.23	3.23
8a	3.32	3.32
9a	3.24	3.23
11a	3.23	3.22
12a	3.24	3.22
13a	3.32	3.31

Adsorption coefficients Q were calculated using the following formula[1]

$$Q = \frac{V\Delta C}{m} \qquad \text{Equation (S1)}$$

Where:
ΔC = the difference between the initial concentration (C_0) and the equilibrium concentration (C),
V= the volume methylene blue solution used (0.05 L)
m = the mass of catalyst (0.1 g).

Table S2: Adsorption coefficient[1] values for Zn-Ti-O samples

Sample	Adsorption Coefficient
100/0	1.10
90/10	0.19
80/20	0.00
70/30	0.15
75/25	0.24
60/40	0.21
50/50	0.06
40/60	0.03
30/70	0.02

Table S3: Adsorption coefficient values for zinc titanate samples (heat- treated)

Sample	**Adsorption Coefficient**
25/75a	0.10
20/80a	0.03
10/90a	0.05
0/100	0.20
20/80	0.06
25/75	0.10
30/70	0.02
Optisol	0.14
P25	0.09

References:

1. S Khezrianjoo, H. D. Revanasiddappa**,** *Chem. Sci. J.,* Vol. 2012: CSJ-85.