catalysts

MDPI

Supplementary Materials

Iron-Zinc Co-doped Titania Nanocomposite: Photocatalytic and Photobiocidal Potential in Combination with Molecular Docking Studies

Nadia Riaz [1, 2, *], Debra Adelina Chia Siew Fen [1], Muhammad Saqib Khan [2], Sadia Naz [3], Rizwana Sarwar [4], Umar Farooq [4], Mohamad Azmi Bustam [1,*] Gaber El-Saber Batiha [5], Islam H. El Azab [6], Jalal Uddin [7,] Ajmal Khan [8,*]

1 Chemical Engineering Department, Universiti Teknologi PETRONAS, 32610 Seri Iskander, Malaysia; nadiariazz@gmail.com (N.R.), debchia991@gmail.com (DACSF), azmibustam@utp.edu.my (MAB)
2 Department of Environmental Sciences, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, 22060, Pakistan; muhammadsaqib@yahoo.com (MSK)
3 Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, 300308, China; Saadia_naaz@hotmail.com (S.N.)
4 Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, 22060, Pakistan; rizwanasarwar@cuiatd.edu.pk (R.S.), umarf@cuiatd.edu.pk (U.F.)
5 Department of Pharmacology and Therapeutics, Faculty of Veterinary Medicine, Damanhour University, Damanhour 22511, AlBeheira, Egypt; gaberbatiha@gmail.com (G.E.B.)
6 Food Science & Nutrition Department, College of Science, Taif University, P.O. box 11099, Taif 21944, Saudi Arabia.; i.helmy@tu.edu.sa (I.H.E.A)
7 Department of Pharmaceutical Chemistry, College of Pharmacy, King Khalid University, Abha 62529, Kingdom of Saudi Arabia. jalaluddinamin@gmail.com (J.U.)
8 Natural and Medical Sciences Research Center, University of Nizwa, P.O. Box 33, Birkat Al Mauz, Nizwa 616, Sultanate of Oman; ajmalkhan@unizwa.edu.om (A.K.)
* Correspondence: nadiariazz@gmail.com (N.R.); ajmalkhan@unizwa.edu.om (A.K.); azmibustam@utp.edu.my (MAB)

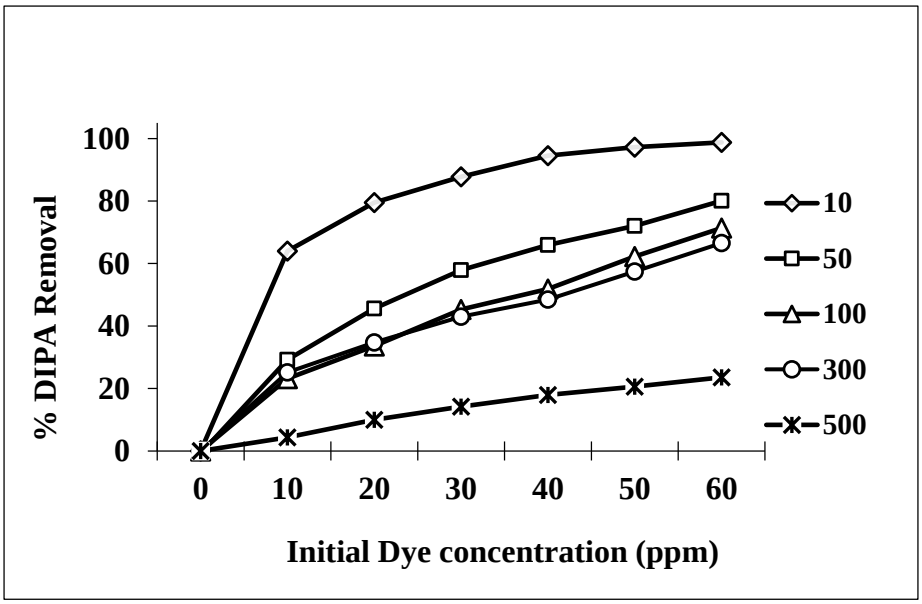


Figure S1. Effect of DIPA concentration versus corresponding irradiation time on % COD removal.

Table S1. Possible assignments of the FTIR peaks.

Peaks (cm^{-1})	Possible Assignment	Related Process Occurring
600-800	Ti-O-Ti vibrations	Different vibration modes of TiO_2
1300-1400, 3400	Stretching vibrations of O-H groups	Physically absorbed moisture
1384	NO_3^-	nitrate (NO_3^-) group

1. Nanocomposite Synthesis

1.1 Coprecipitation (CP) method

A series bimetallic photocatalysts with different Fe:Zn mass composition were prepared using TiO_2 as support via coprecipitation (CP) method. Appropriate amounts of metal salts were dissolved in distilled water, followed by the addition of metals. TiO2 was added into the solution with continuous stirring for 1 h prior to precipitation with 0.25 M NaOH. The preparation temperature was maintained in the range from 8 to 10 °C. The final pH was kept at 14, and the mixture was aged for 1 day. The precipitates were filtered and dried in an oven at 75 °C overnight. The raw photocatalysts were ground into a fine powder, kept in an airtight glass bottle, and stored in a desiccator before calcination.

1.2 Wet impregnation (WI) method

Bimetallic photocatalysts with known total metal loading and Fe:Zn mass composition were prepared using wet impregnation (WI) method with TiO_2 as support. To prepare photocatalysts using WI method, support was added into the metal salt solution. The suspension was stirred for 1 hour before the solvent was evaporated in a water bath at 80°C until a thick paste was obtained. This paste was then dried in an oven at 120°C for 18 hours. The dried photocatalyst was ground with a mortar and pestle, kept in air-tight glass bottle (to avoid moisture) as raw photocatalyst, and stored in a desiccator at room temperature prior to calcination.

1.3. Sol-gel method

Fe-Zn/TiO_2 photocatalysts with different Fe:Zn mass composition were synthesized employing sol-gel method. Fe-ZN/TiO_2 sol solution (with required ratio of Fe:Zn) was prepared using sol-gel method by adding 15ml TTIP in 100ml Ethanol. Iron source was dissolved in ethanol as required. The solution was stirred continuously while adding 1M HCl (2.0ml) at room temperature until a transparent sols were obtained. Dried in oven at 100°C and raw photocatalysts were ground into a fine powder, kept in an airtight glass bottle, and stored in a desiccator before calcination.

2. Schematic representation of the formation mechanism

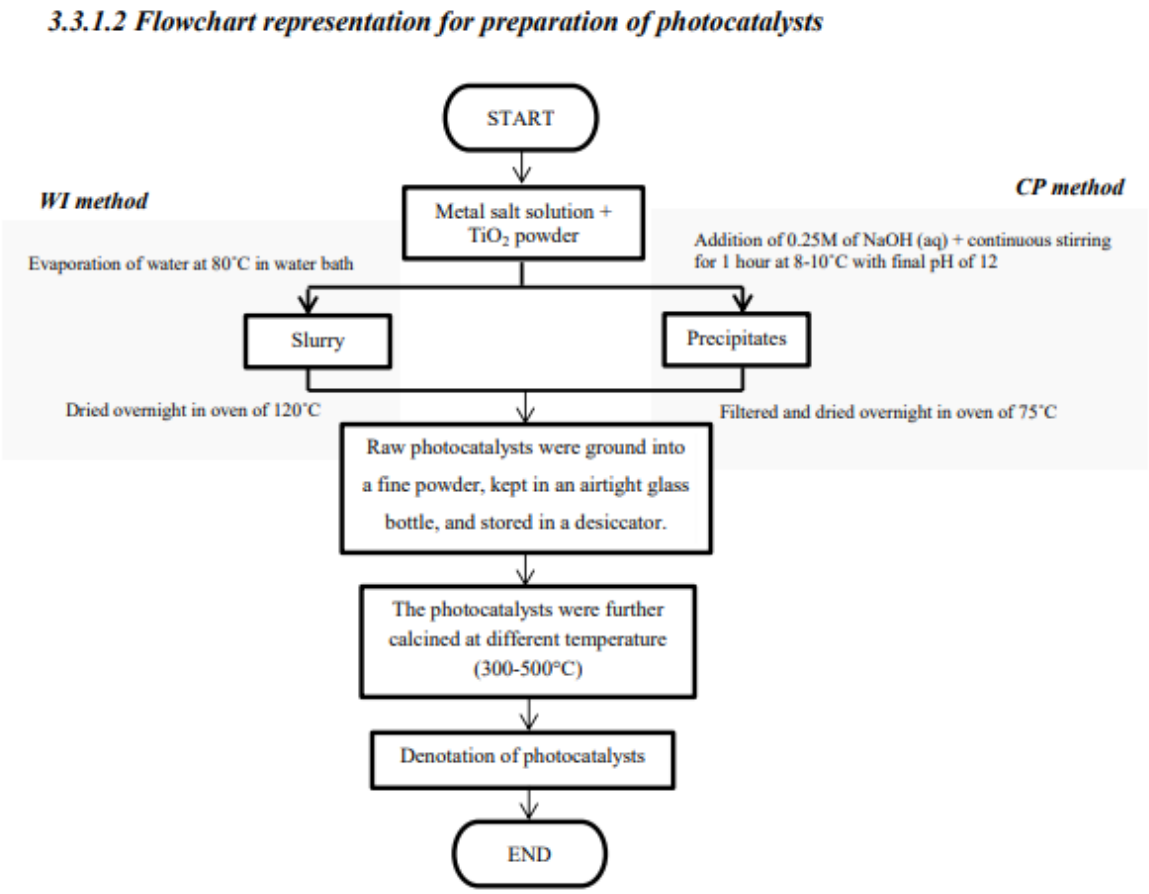
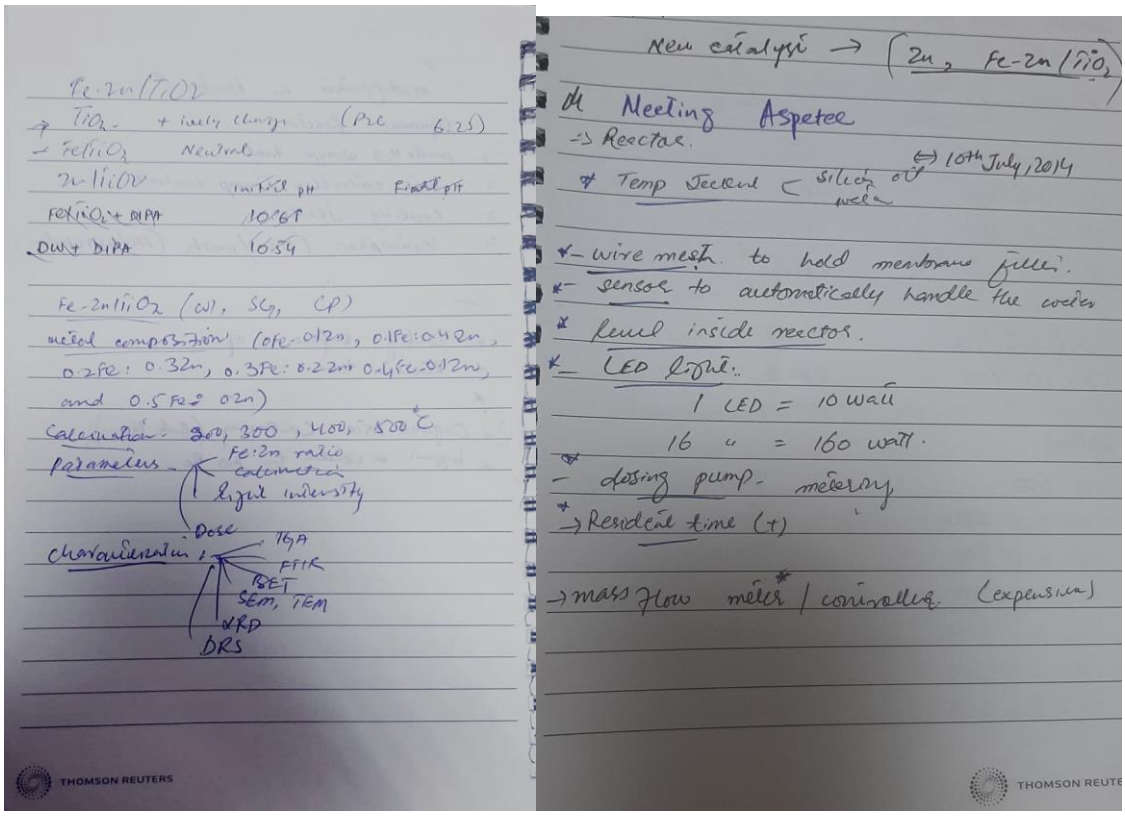


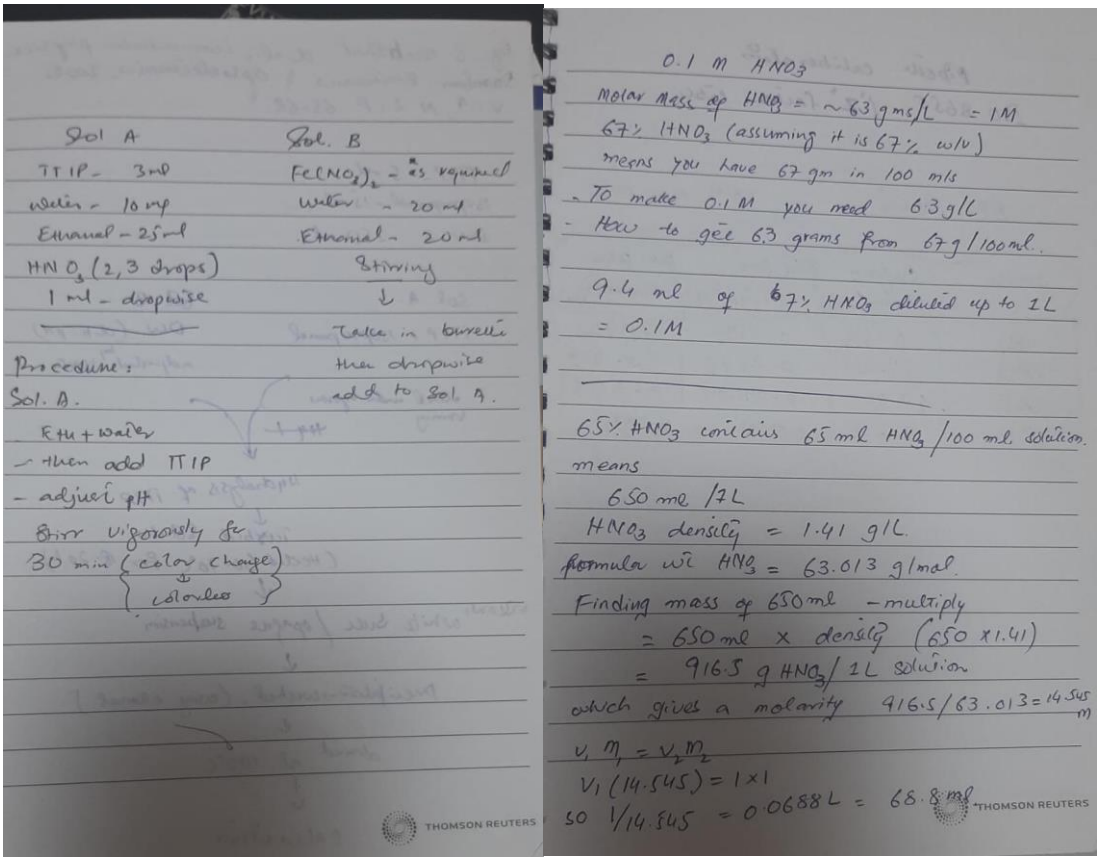
Figure S2. Schematic representation of the formation mechanism.

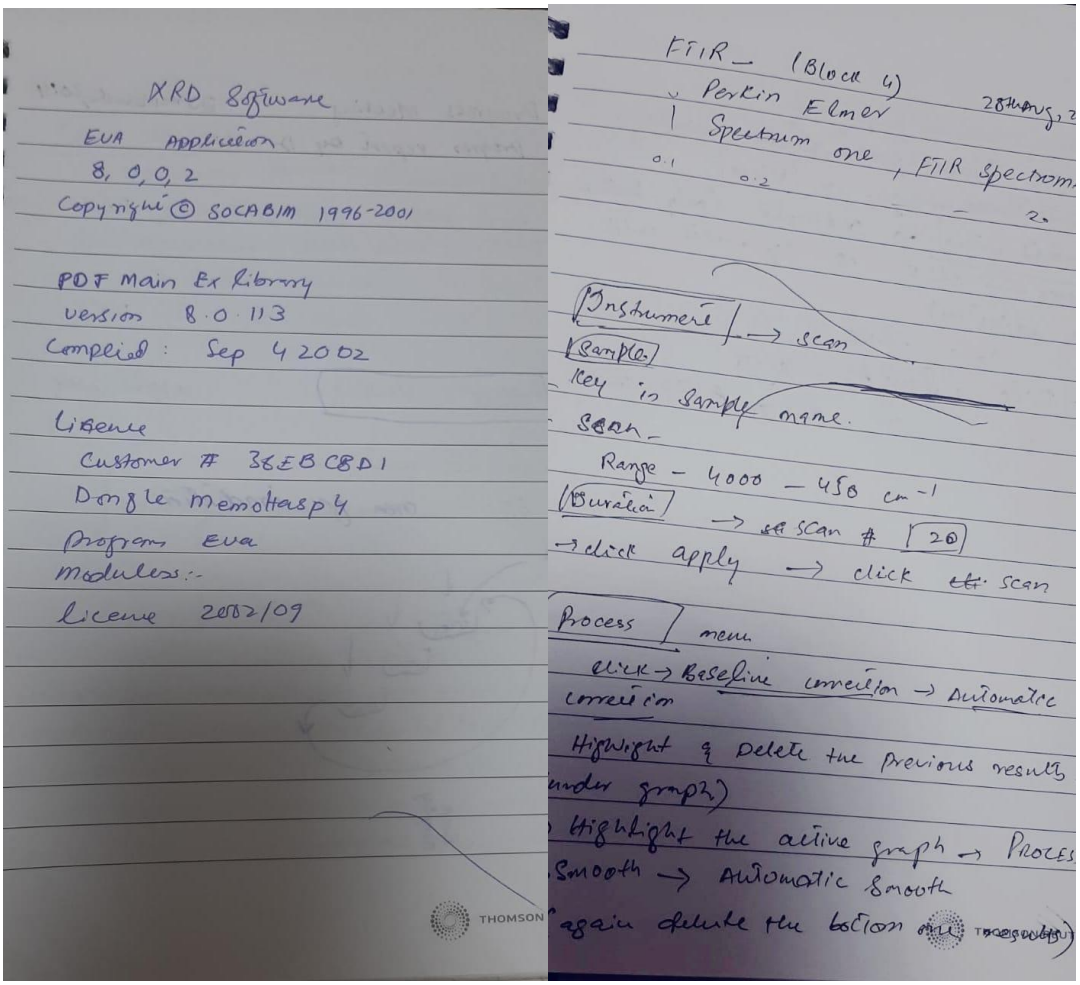
Analysis	Model	Function
Thermogravimetric Analysis (TGA)	Pyris 1	Thermal stability
Fourier-Transformed Infrared Spectroscopy (FTIR)	Perkin Elmer Spectrum one FTIR spectrophotometer	Species (functional group) identification
X-ray Diffraction (XRD)	Bruker D8 Advance Diffractometer	Crystal phases and Crystallite sizes
Field Emission electron microscopy (FESEM)	Supra55VP	Morphology
N_2-physisorption (BET)	BELSORP, Japan	Surface area, pore volume, and average pore diameter

Figure S3. Instruments used for characterization of the photocatalysts.

3. Raw data collected during the experimentation.



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EVA Application
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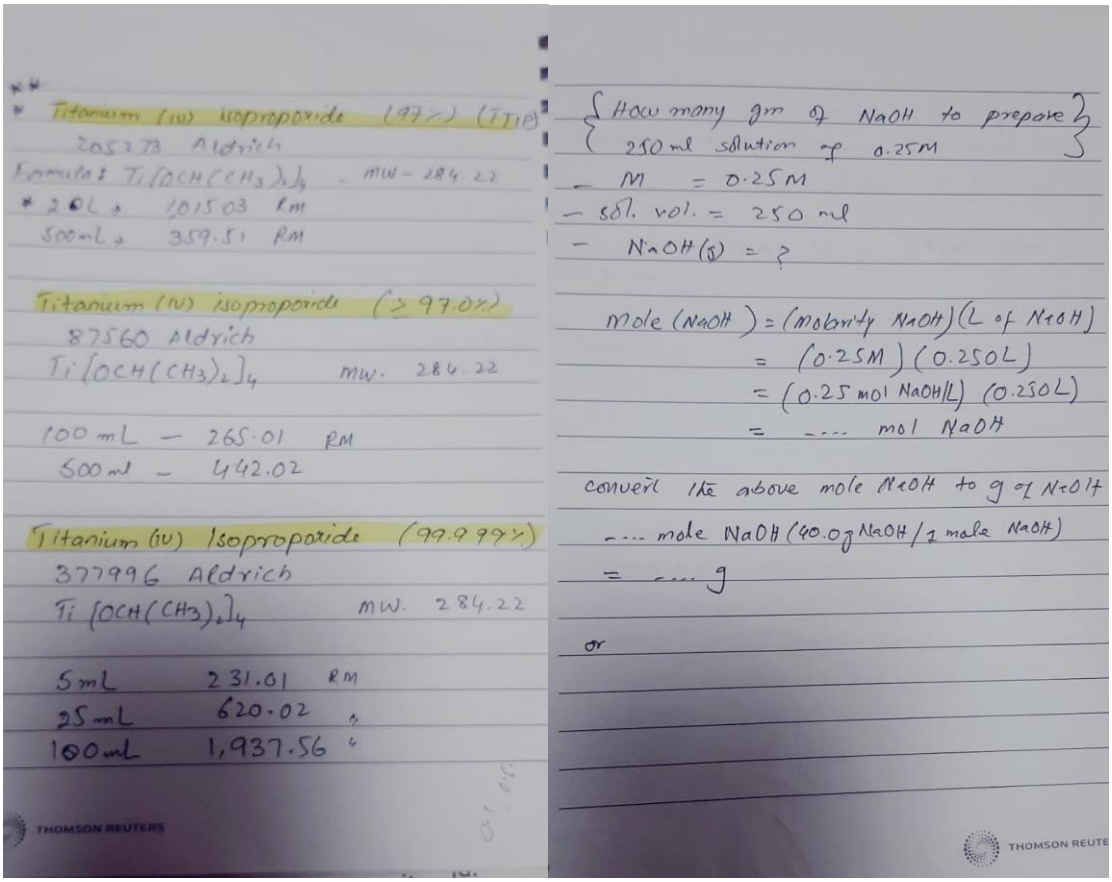

Titanium (IV) isopropoxide (97%) (TTIP)
20573 Aldrich
Formula: $Ti[OCH(CH_3)_2]_4$ - MW - 284.22
* 20L - 1015.03 RM
500mL - 359.51 RM

Titanium (IV) isopropoxide (≥ 97.0%)
87560 Aldrich
$Ti[OCH(CH_3)_2]_4$ MW. 284.22

100 mL - 265.01 RM
500 ml - 442.02

Titanium (IV) Isopropoxide (99.999%)
377996 Aldrich
$Ti[OCH(CH_3)_2]_4$ MW. 284.22

5mL 231.01 RM
25mL 620.02 "
100mL 1,937.56 "

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{How many gm of NaOH to prepare 250 ml solution of 0.25M}

- M = 0.25M
- sol. vol. = 250 ml
- NaOH (g) = ?

mole (NaOH) = (molarity NaOH)(L of NaOH)
= (0.25M)(0.250L)
= (0.25 mol NaOH/L)(0.250L)
= .... mol NaOH

convert the above mole NaOH to g of NaOH
.... mole NaOH (40.0g NaOH / 1 mole NaOH)
= .... g

or

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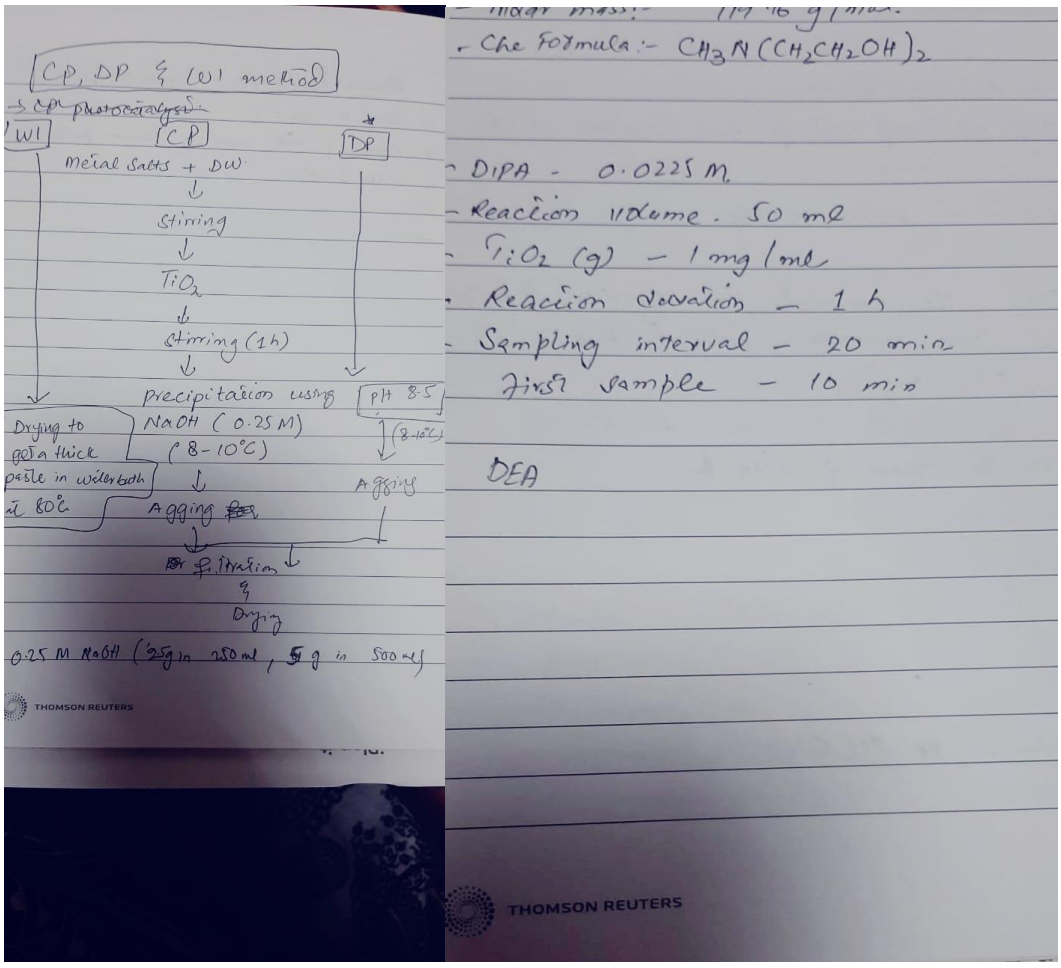
CP, DP & WI method
CP photocatalyst
WI
CP
DP
Metal salts + DW
stirring
TiO_2
stirring (1h)
precipitation using NaOH (0.25 M) (8-10°C)
pH 8.5
(8-10°C)
Drying to get a thick paste in water bath at 80°C
Aging
Aging
filtration & Drying
0.25 M NaOH (25g in 250 ml, 5 g in 500 ml)
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- Che formula :- $CH_3N(CH_2CH_2OH)_2$
- DIPA - 0.0225 M
- Reaction volume - 50 ml
- TiO_2 (g) - 1 mg/ml
- Reaction duration - 1 h
- Sampling interval - 20 min
First sample - 10 min
DEA
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