Wavelength-shift Based Colorimetric Sensing for Peroxide

Number of Edible Oil Using CsPbBr₃ Perovskite Nanocrystals

Yimeng Zhu^{†1}, Feiming Li^{†1}, Yipeng Huang¹, Fangyuan Lin¹, Xi Chen^{*1,2}

 ¹Department of Chemistry and the MOE Key Laboratory of Spectrochemical Analysis & Instrumentation, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China
²State Key Laboratory of Marine Environmental Science, Xiamen University, Xiamen 361005, China
³Shenzhen Research Institute of Xiamen University, Shenzhen 518000, China
E-mail: <u>xichen@xmu.edu.cn</u>. Tel: &Fax: 86-592-2184530

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Materials and Chemicals. Cs₂CO₃, octadecene (ODE), oleic acid (OA), PbBr₂, oleylamine (OAm), I₂, toluene (TOL), sodium oleate (CP), MgSO₄, CaCl₂, FeCl₃, CuCl₂, AgNO₃, PbO, NiCl₂, ethanol. The edible oil samples are bought on the market and collected from the dining room.

Apparatus. UV–vis absorption spectra were recorded using a UV-2550 spectrophotometer (Shimadzu). Fluorescence emission spectra were measured with emission wavelength at 400nm using an FL7100 spectrophotometer. X-ray diffraction (XRD) patterns were acquired using a Rigaku Ultima IV instrument (Kuraray, Japan) with Cu target (40 kV, 20 mA, $\lambda = 1.54051$ A). The TEM images of the samples were acquired through transmission electron microscopy (TEM) with a JEM-1400 microscopy system (JEOL, Japan) at an acceleration voltage of 120 kV.

Preparation of CsPbBr₃ NCs. The CsPbBr₃ NCs was prepared as reported by Maksym V et al¹.with some adaptations. For the preparation of Cs-oleate, 0.814 g of Cs₂CO₃ (2.5 mmol), 40 mL of octadecene and 2.5 mL of oleic acid were loaded into 3-neck flask, dried under vacuum at 120 °C for Cs₂CO₃ dissolving, and then heated under N₂ to 150 °C. For the synthesis of CsPbBr₃ NCs, 0.069g PbBr₂, 5 mL of octadecene, 0.5 mL of oleylamine and 0.5 mL of oleic acid were loaded into 3-neck flask, and dried under vacuum at 120 °C for PbBr₂ dissolving. Then the mixed precursors were heated under N₂ to 150°C and 0.4 mL of prepared Cs-oleate solution was quickly injected. Immediately following, the reaction mixtures were cooled by the ice water bath with shaking. Finally, the CsPbBr₃ NCs were purified via high speed centrifugation (at 10000 rpm for 10 minutes), followed by redispersion in toluene.



Figure S1. a) XRD patterns of CsPbBr₃ NCs powder sealed in a glass tube before and after storage for one month (blue color line: one month storage; black color line: newly prepared). b) Fluorescence emission wavelength shift of CsPbBr₃ NCs with different storage time for the same edible oil sample

Preparation of OLAM-I (oleylammonium Iodide). The OLAM-I was prepared by mixed iodine with oleylamine for high temperature reaction². 0.75 g of I_2 (3 mmol) and 4 ml of oleylamine were loaded into flask, and heated up to 120 °C with the appearance of light brown. The temperature was raised to 200 °C and the OLAM-I (6 mmol) solution was cooled, followed by dilution in toluene.

Determination of peroxide number of edible oil. The edible oil did not require complex pretreatment. 0.22 mL of edible oil was added into OLAM-I solution (1ml, 2.5 mmol in TOL, prepared as described above), and then reacted for 10 minutes with the solution turning pale yellow. Then CsPbBr₃ NCs solution (0.5 mL of the saturated solution was diluted to 1ml) was added into above redox reaction mixtures. The halogen exchange quickly reacted about 5 minutes. Finally, the fluorescence color of the reaction solution under UV lamp was compared with the color chart, indicating whether the peroxide number of edible oil exceeds the standard. If the edible oil is high peroxide number, it will undergo redox reaction with more iodide ions, making less iodide ions exchange halogen with CsPbBr₃ NCs added later, so the fluorescence display tends to be green. Otherwise, the fluorescence display tends to be red.

Preparation of edible oil with different peroxide number. The oil with high peroxide number that had been fried were mixed with toluene solution by volume ratios of 0:10, 1:9, 2:8, 3:7, 4:6, 5:5, 6:4, and 7:3. The mixed standard oil samples were measured and labeled according to the national test standard GB/T 5009.227-2016³. The peroxide number were detected as shown in Table S1.

Standard oil	1	2	3	4	5	6	7	8
samples	(0:10)	(1:9)	(2:8)	(3:7)	(4:6)	(5:5)	(6:4)	(7:3)
peroxide number g/100g	0.0091	0.0711	0.1299	0.2057	0.3094	0.3899	0.4845	0.5596

Table S1. The peroxide number of the mixed standard oil samples

Table S2. Reproducible experimental data

		Same batch repeatability (n=6)						Batch repeatability (n=3)		
Samples		1	2	3	4	5	6	1	2	3
peroxide	EM WL /nm	638.4	637.8	638	637.6	637.4	637.6	637.2	638.6	638
number=0	RSD	0.0561%					0.1101%			
peroxide	EM WL /nm	549	550.2	549.2	549.2	550.2	549.4	549	550.8	550.2
number =0.4	RSD	0.0967%					0.1666%			
peroxide	EM WL /nm	538.6	537.2	537.8	538.2	538.2	538.6	538.8	537.8	537
number =0.5	RSD	0.0990%					0.1677%			

Preparation of metallic oleates. Different metallic cationic oleates were synthesized according to the report of Xu et al⁴. with some adaptations. Take the Ca²⁺ solution for an example. 0.01 mmol of inorganic salts (CaCl₂) dissolved in 0.5 mL of H₂O. Then sodium oleate dissolved in H₂O-ethanol solution (v:v = 1:1). 0.5

mL of sodium oleate solution was added into inorganic salts (CaCl₂) solution (Na:Cu mole ratio about 2:1).

Then, the mixture was centrifugally separated and dried at 80 °C overnight. Finally, the calcium oleate dissolved in TOL, diluting to a concentration of 2 mol/L. Other metallic cationic oleates used in experiment were synthesized by the same way. 5 μ L of metallic cationic oleate solutions were taken in the experiment.



Figure S2. Oil test results with different interferences added (0.00001 mmol of oleate, 5 μ L of H₂O, 5 μ L of oleic acid separately added in 0.22 mL of oil)



Table S3: Determination of peroxide number for edible oil samples

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