Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Formation dynamics of mesocrystals composed of organically modified CeO_2 nanoparticles: Analogy to particle formation model

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Supporting Information

X-ray diffraction patterns of cerium oxide are shown here. The crystallite size was calculated from XRD data by Halder-Wagner method. Halder-Wagner equation can be written as follows:

$$\left(\frac{\beta}{\tan\theta}\right)^2 = \frac{K\lambda}{D} \times \frac{\beta}{\tan\theta\sin\theta} + 16\varepsilon^2$$

Here, β is integral breadth (in radians), θ is Bragg angle, K is a constant (= 4/3 for the mean volume-weighted size of spherical crystallites), λ (= 0.15418 nm) is the wavelength of the Cu Kα X-ray, D is the crystallite size, and ε is micro strain of the crystal.

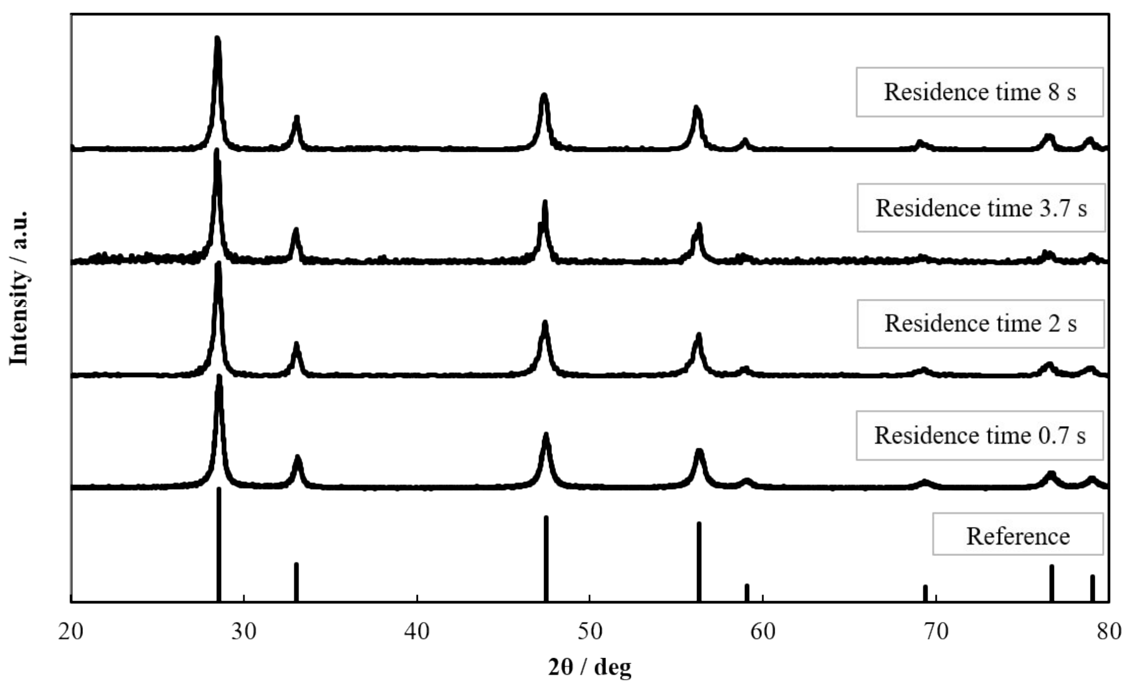
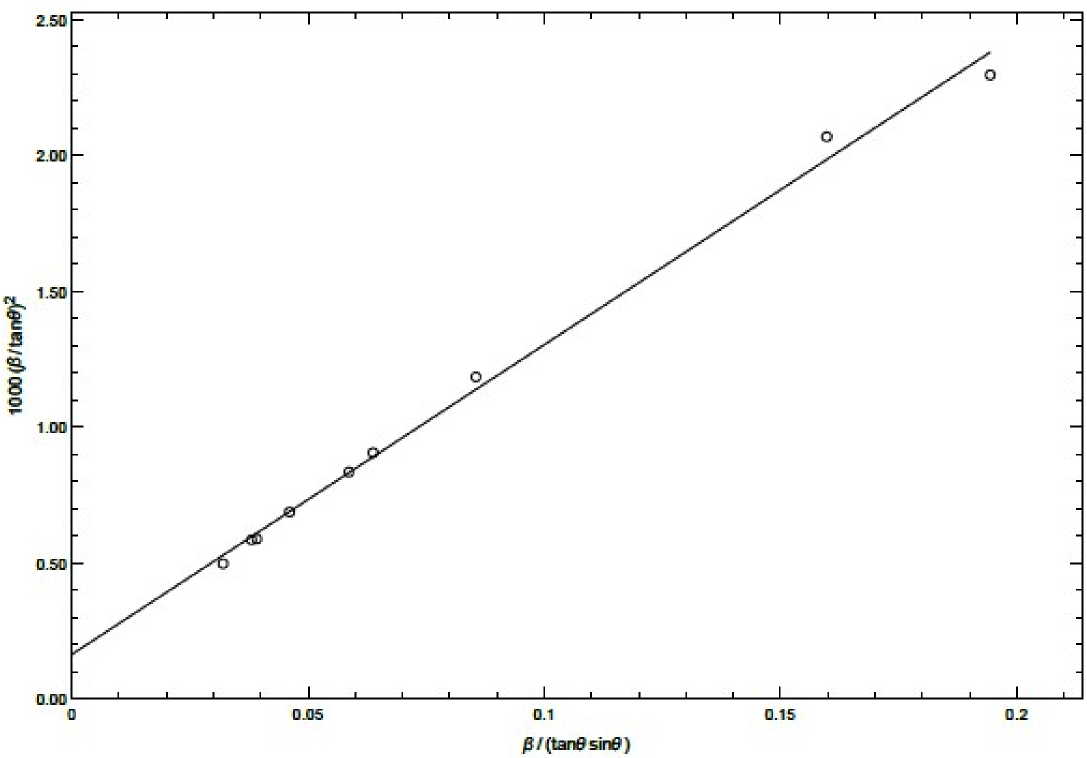


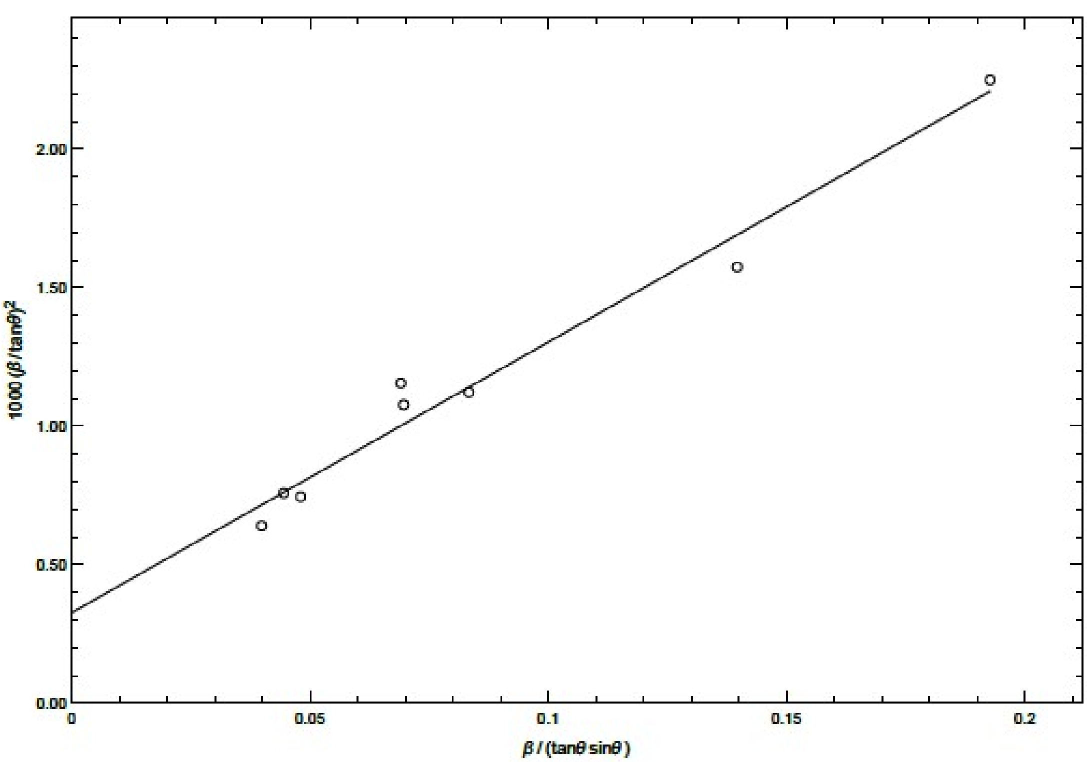
Figure S1. XRD pattern of cerium oxide synthesized in the presence of L-glutamic acid at 548 K, 25 MPa, [Ce][Glu] 1:3

(A)



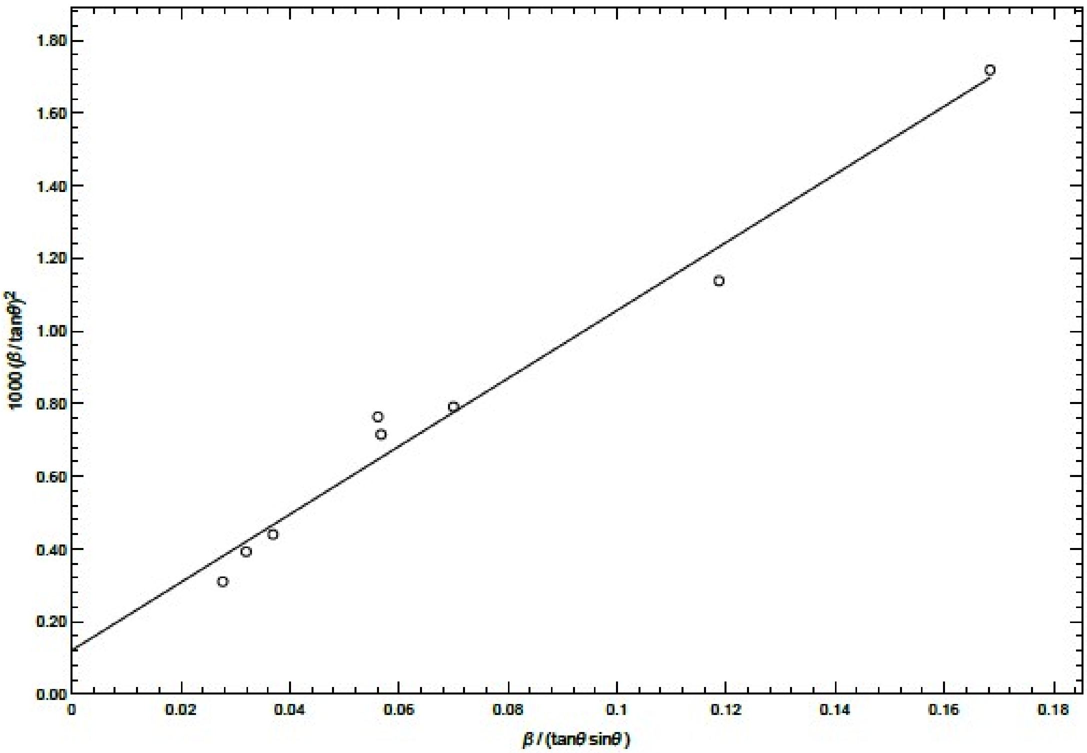
2.50
2.00
1.50
1.00
0.50
0.00
1000 $(\beta / \tan\theta)^2$
0
0.05
0.1
0.15
0.2
$\beta / (\tan\theta \sin\theta)$

(B)



2.00
1.50
1.00
0.50
0.00
1000 $(\beta / \tan\theta)^2$
0
0.05
0.1
0.15
0.2
$\beta / (\tan\theta \sin\theta)$

(C)


1000 (β / tanθ)²
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
β / (tanθ sinθ)

(D)

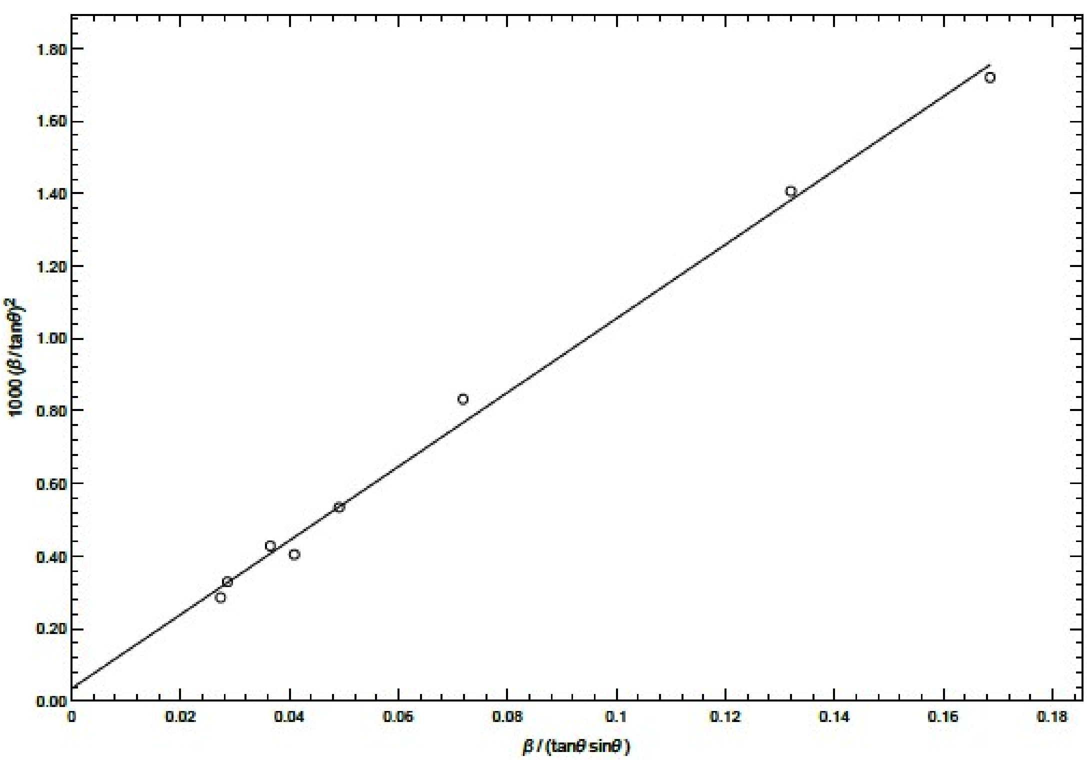

1000 (β / tanθ)²
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
β / (tanθ sinθ)

Figure S2. Halder-Wagner plots obtained from XRD patterns of cerium oxide synthesized in the presence of L-glutamic acid at 548 K, 25 MPa, [Ce][Glu] 1:3 (A) 0.7 s, (B) 2.0 s, (C) 3.7 s (D) 8.0 s

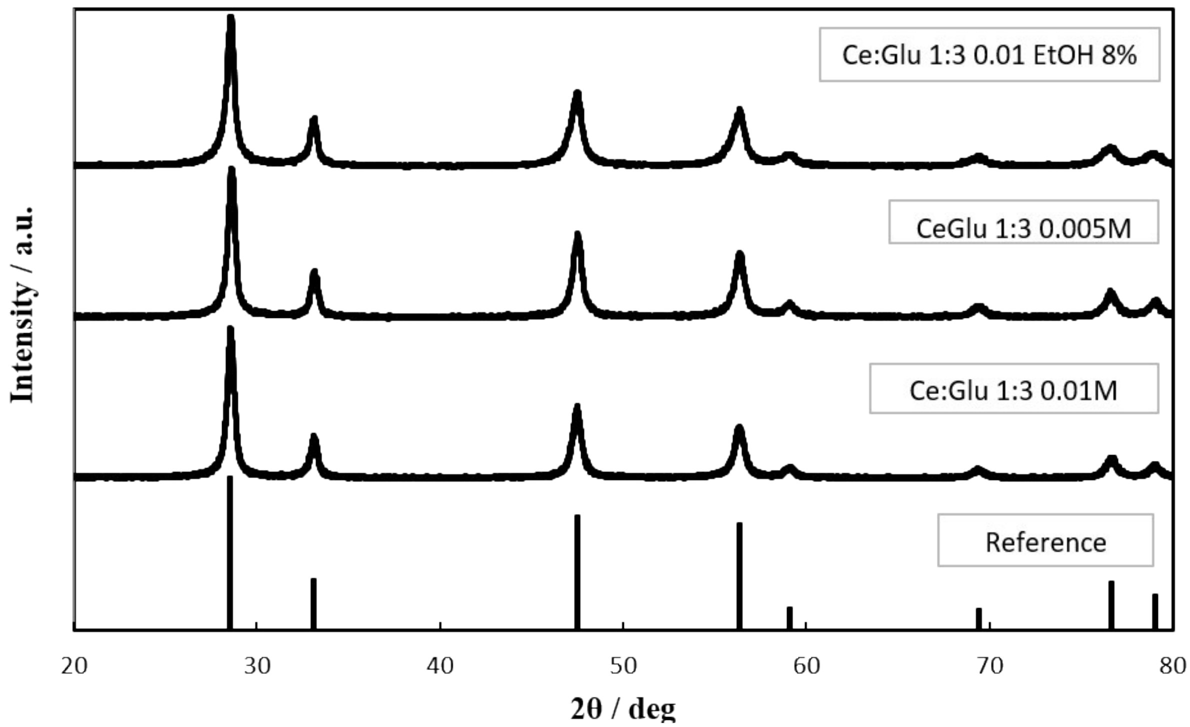
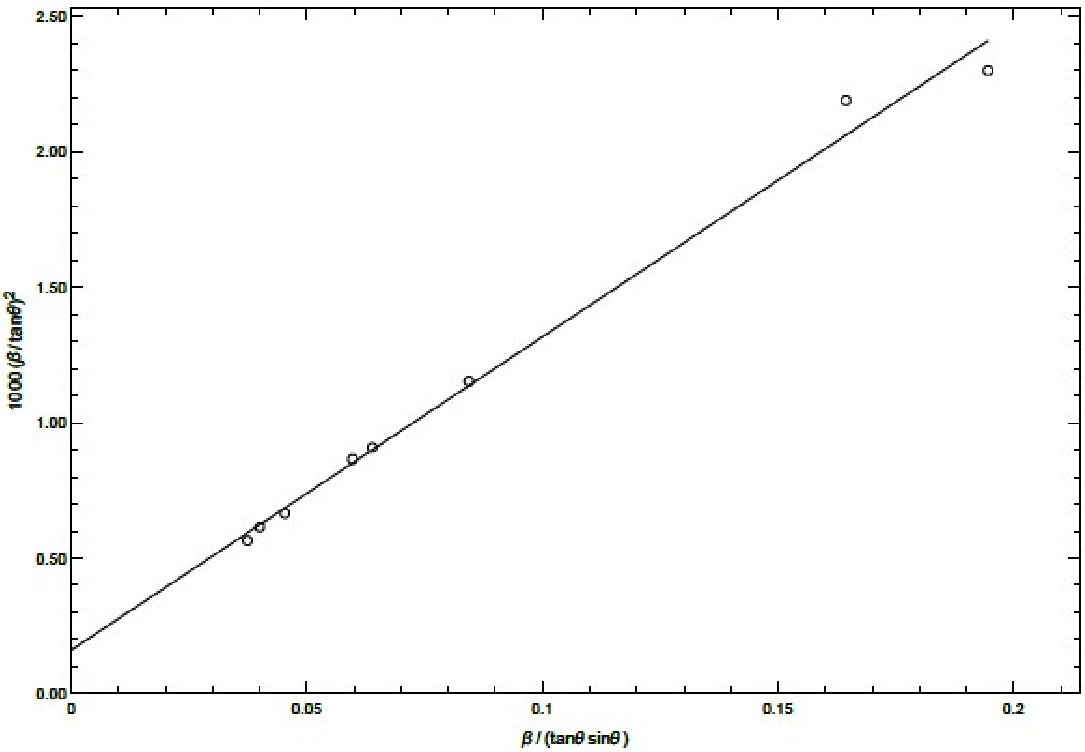


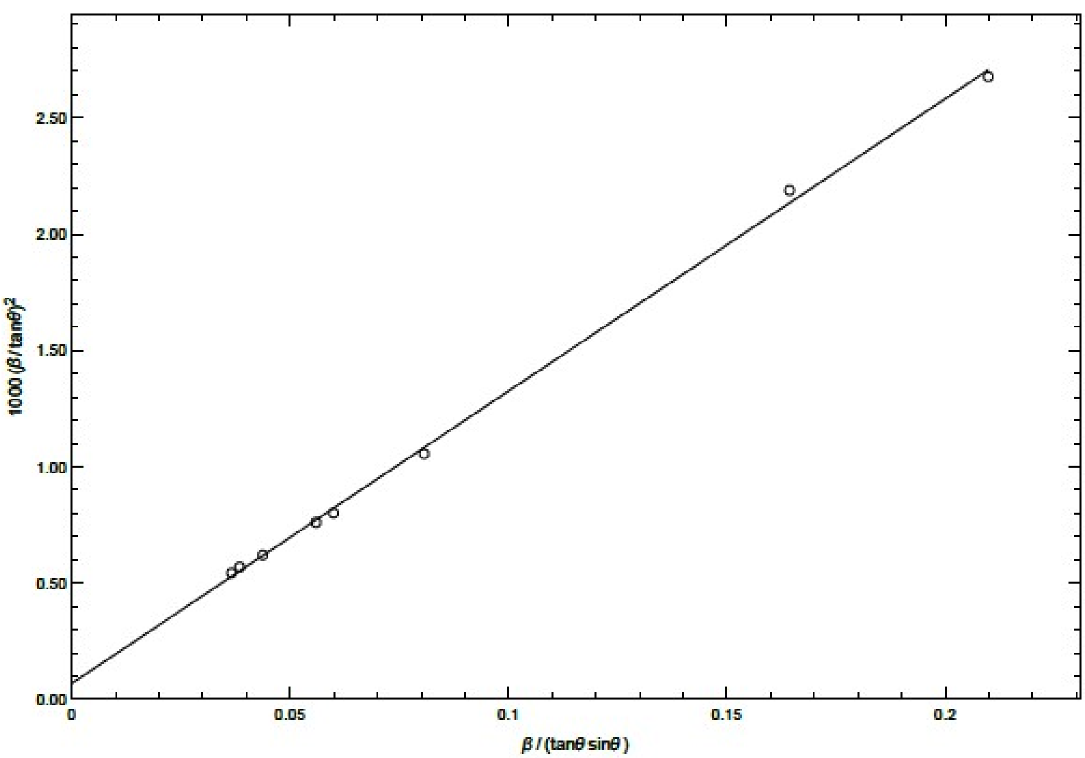
Figure S3. XRD pattern of cerium oxide synthesized in the presence of glutamic acid with different concentration or adding of ethanol with a molar fraction of x_{EtOH} = 8% at 548 K, 25 MPa, [Ce][Glu] 1:3, 0.7s

(A)



2.50
2.00
1.50
1.00
0.50
0.00
1000 (β / tanθ)²
0
0.05
0.1
0.15
0.2
β / (tanθ sinθ)

(B)



2.50
2.00
1.50
1.00
0.50
0.00
1000 (β / tanθ)²
0
0.05
0.1
0.15
0.2
β / (tanθ sinθ)

(C)

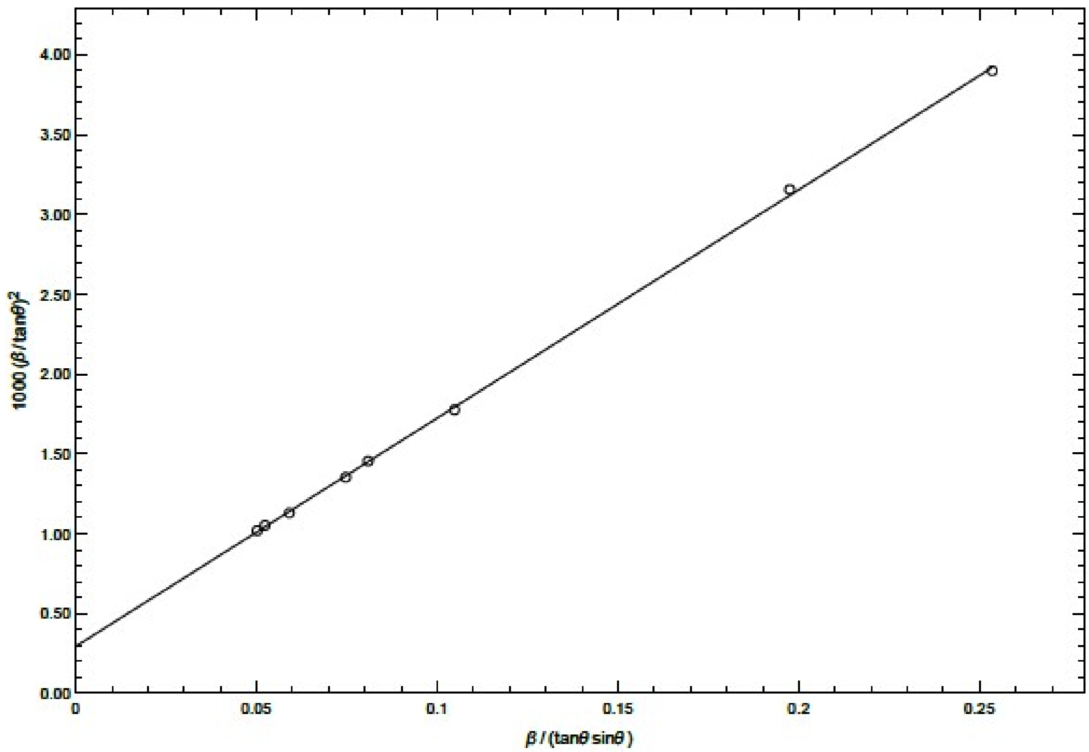


Figure S4. Halder-Wagner plots obtained from XRD patterns of cerium oxide synthesized in the presence of glutamic acid with different concentration (A) 0.01 M, (B) 0.005 M, or (C) adding of ethanol with a molar fraction of x_{EtOH} = 8% at 548 K, 25 MPa, [Ce][Glu] 1:3, 0.7s

Table S1 Summary of the results of Halder-Wagner analysis for XRD data

HW plot	Fig. S2 (A)	Fig. S2 (B)	Fig. S2 (C)	Fig. S2 (D)	Fig. S4 (A)	Fig. S4 (B)	Fig. S4 (C)
Conditions	0.7 s	2.0 s	3.7 s	8.0 s	0.01 M	0.005 M	Ethanol
D [nm]	18.0	21.1	22.0	20.2	17.8	16.4	14.4
ε [-]	0.0032	0.0045	0.0027	0.0015	0.0032	0.0021	0.0043