Electronic Supporting Information

Hydroxypropyl-β-cyclodextrin as a versatile additive for the formation of metastable tetragonal zirconia exhibiting high thermal stability

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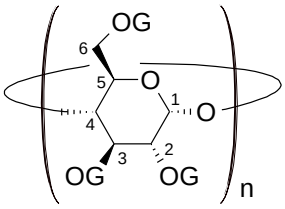
Table S1. Chemical structure and characteristics of the cyclodextrin derivatives



G : H or R

Abbreviation	n	Substituent R	Carbons bearing the OR group	Number of R groups per CD	Molecular weight (g mol^{-1})
α-CD	6	(-)	(-)	0	972
γ-CD	8	(-)	(-)	0	1297
HP-β-CD	7	CH_2-CHOH-CH_3	2, 3 and 6	4.2	1380
CrysMe-α-CD	7	CH_3	2, 3 and 6	4.9	1204
RaMe-β-CD	7	CH_3	2, 3 and 6	12.6	1314

Table S2. Structural parameters by Rietveld refinement of the calcined zirconia samples

Sample	Method	Additive	Weight ratio (%)	Lattice constants			
				a, b, c (Å)	**α, β, γ (deg)**	**Crystallite size (Å)**	**Strain (%)**
Zr-Ref	1	/	m-ZrO_2: 84.8	a=5.142; b=5.194; c =5.306	α, γ=90; β=98.909	82.8	0.0029
			t-ZrO_2: 15.2	a, b=3.590; c =5.1571	α, β, γ=90	94.0	0.0045
Zr-HP1	1	HP-β-CD	t-ZrO_2: 100	a, b=3.598; c =5.173	α, β, γ=90	392	0.0044
Zr_HP3	3	HP-β-CD	m-ZrO_2: 31.4	a=5.145; b=5.184; c =5.312	α, γ=90; β=98.60	69.0	0.0028
			t-ZrO_2: 68.6	a, b=3.620; c =5.081	α, β, γ=90	272	0.0055
Zr_CD3	3	α-CD	t-ZrO_2: 100	a, b=3.594; c =5.156	α, β, γ=90	327	0.0052
Zr_CrysMe3	3	CrysMe-β-CD	m-ZrO_2: 18.2	a=5.145; b=5.184; c =5.312	α, γ=90; β=98.60	26.8	0.0152
			t-ZrO_2: 81.8	a, b=3.5963; c =5.156	α, β, γ=90	403	0.0056
Zr_RaMe3	3	RaMe-β-CD	m-ZrO_2: 51.8	a=5.171; b=5.185; c =5.325	α, γ=90; β=98.47	57.6	0.0052
			t-ZrO_2: 48.2	a, b=3.607; c =5.161	α, β, γ=90	58.1	0.0030

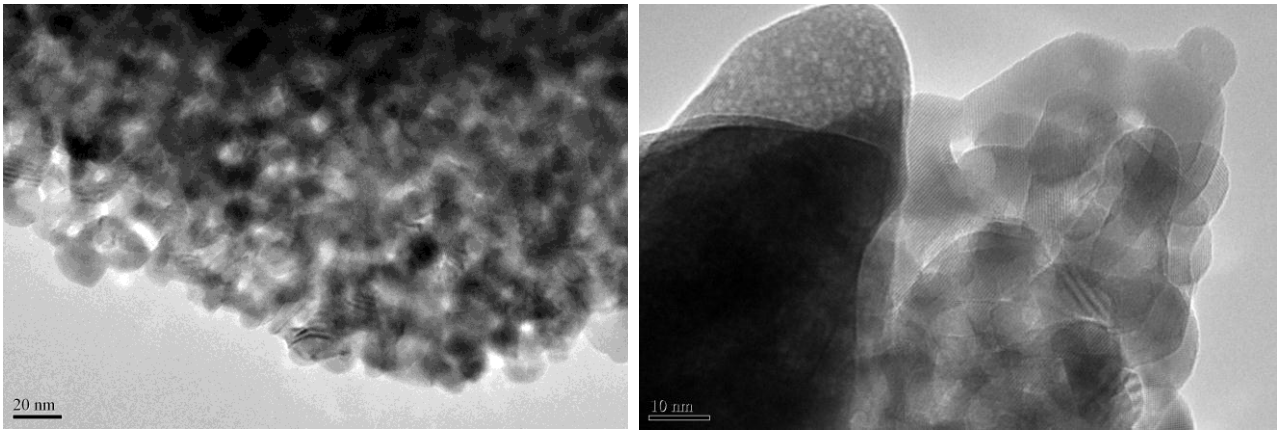


Fig. S1. TEM pictures of the controlled ZrO_2 (Zr-Ref) with different magnifications : (a) 20 nm and (b) 10 nm

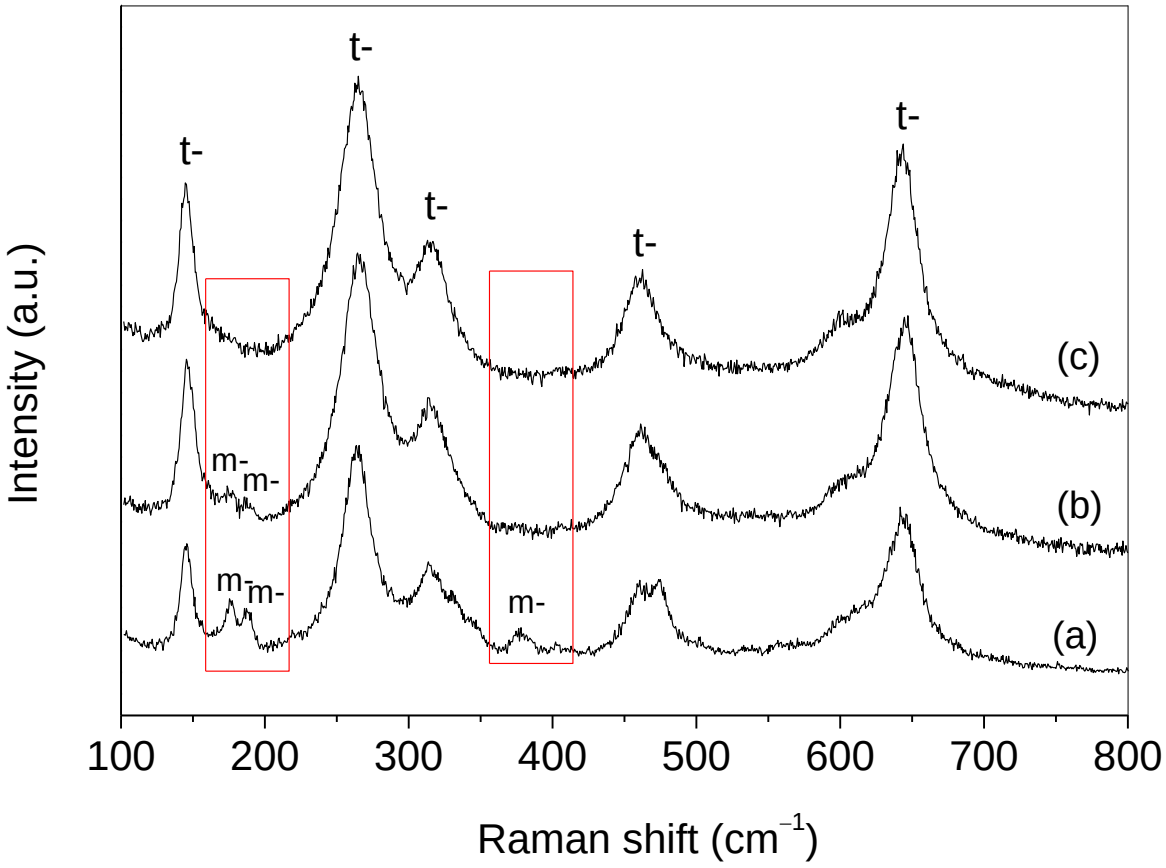


Fig. S2. Raman spectra of ZrO_2 materials after calcination at 600°C for 4 hours obtained from the different methods of precipitation: (a) addition of HP-β-CD in the $ZrOCl_2$ solution as described in the method 2, (b) addition of HP-β-CD in the $NH_3 \cdot H_2O$ solution as described in the method 3 and (c) addition of HP-β-CD both in the $ZrOCl_2$ and $NH_3 \cdot H_2O$ solutions as described in the method 1. m- and t- indicate the monoclinic and tetragonal phase, respectively.

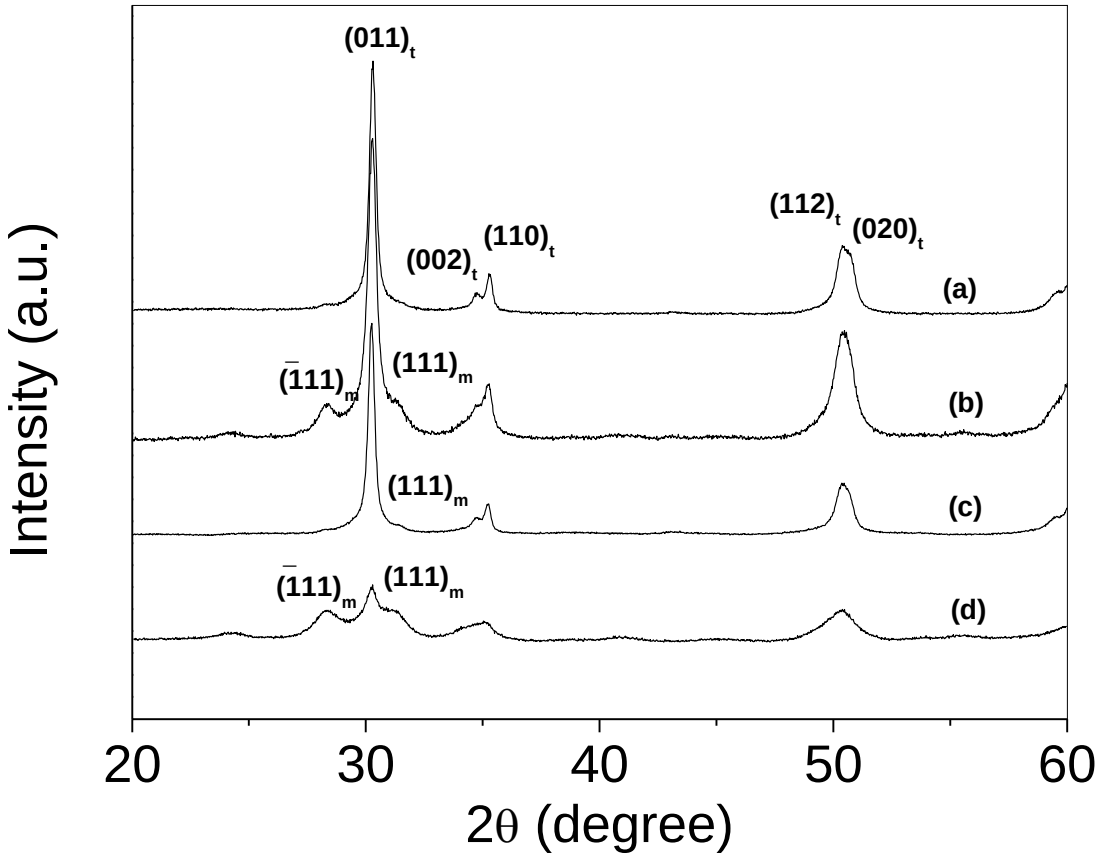


Fig. S3. XRD patterns of ZrO_2 materials after calcination at 600°C for 4 hours obtained from the method 3 by using the following organic additive: (a) of α-CD, (b) HP-β-CD, (c) CrysMe-β-CD and (d) RaMe-β-CD.