ARTICLE

Supporting Information

Octadecene-free Colloidal Synthesis of $CsPbI_3$ Nanocrystals with Improved Size, Shape and Phase Control

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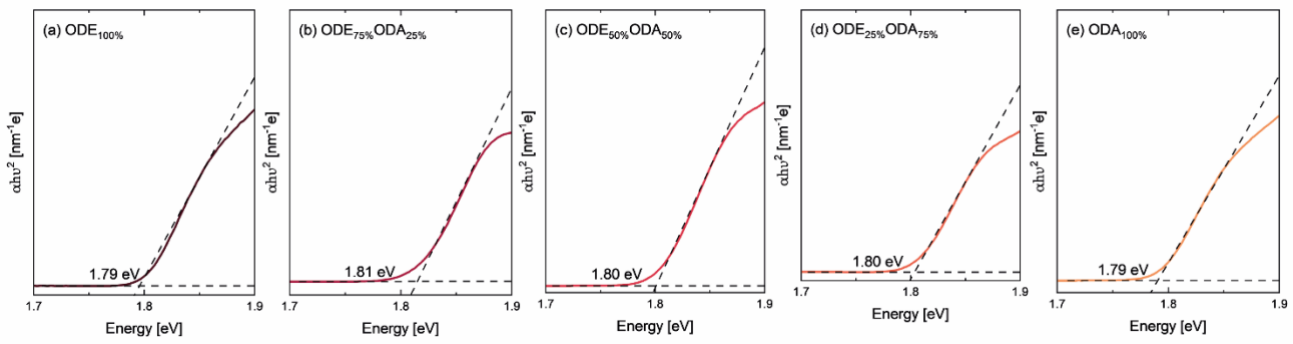

Figure S1: Tauc-plot for samples with estimated band-gap (a) $ODE_{100\%}$ 1.79 eV, (b) $ODE_{75\%}ODA_{25\%}$ 1.81 eV, (c) $ODE_{50\%}ODA_{50\%}$ 1.80 eV, (d) $ODE_{25\%}ODA_{75\%}$ 1.80 eV, and (e) $ODA_{100\%}$ 1.79 eV.

Table S1: XPS results for a range of samples of $CsPbI_3$ showing the expected ratio of elements.

XPS	$ODE_{100\%}$	$ODE_{75\%}ODA_{25\%}$	$ODE_{50\%}ODA_{50\%}$	$ODE_{25\%}ODA7_{5\%}$	$ODA_{100\%}$
Pb (%)	16,52	16,94	16,66	16,87	16,57
Cs (%)	20,61	20,24	21,07	20,11	20,49
I (%)	62,87	62,82	62,27	63,02	62,94

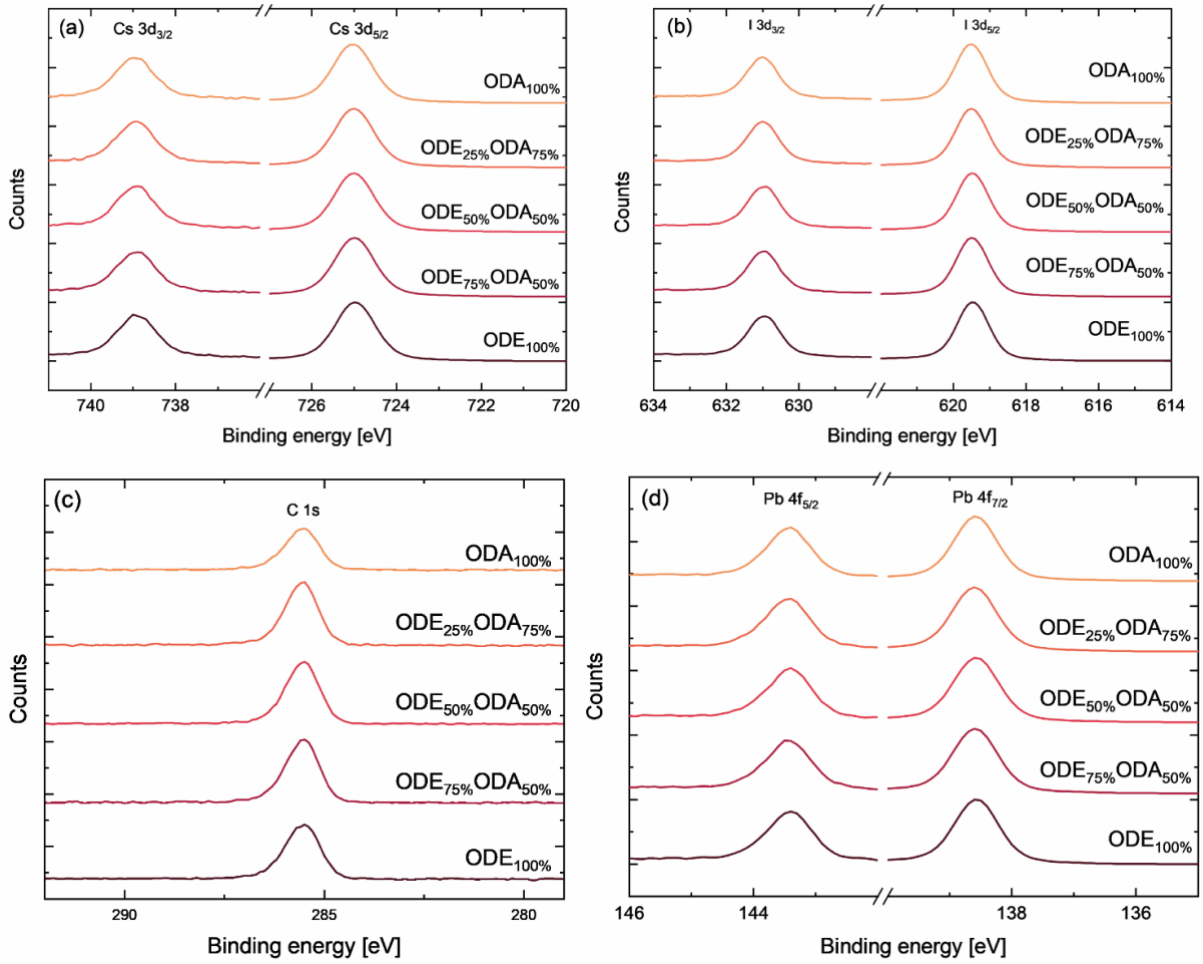

Figure S2: XPS data shows no shift of the (a) Cs, (b) I, and (d) Pb peaks. No metallic lead was observed in the sample.

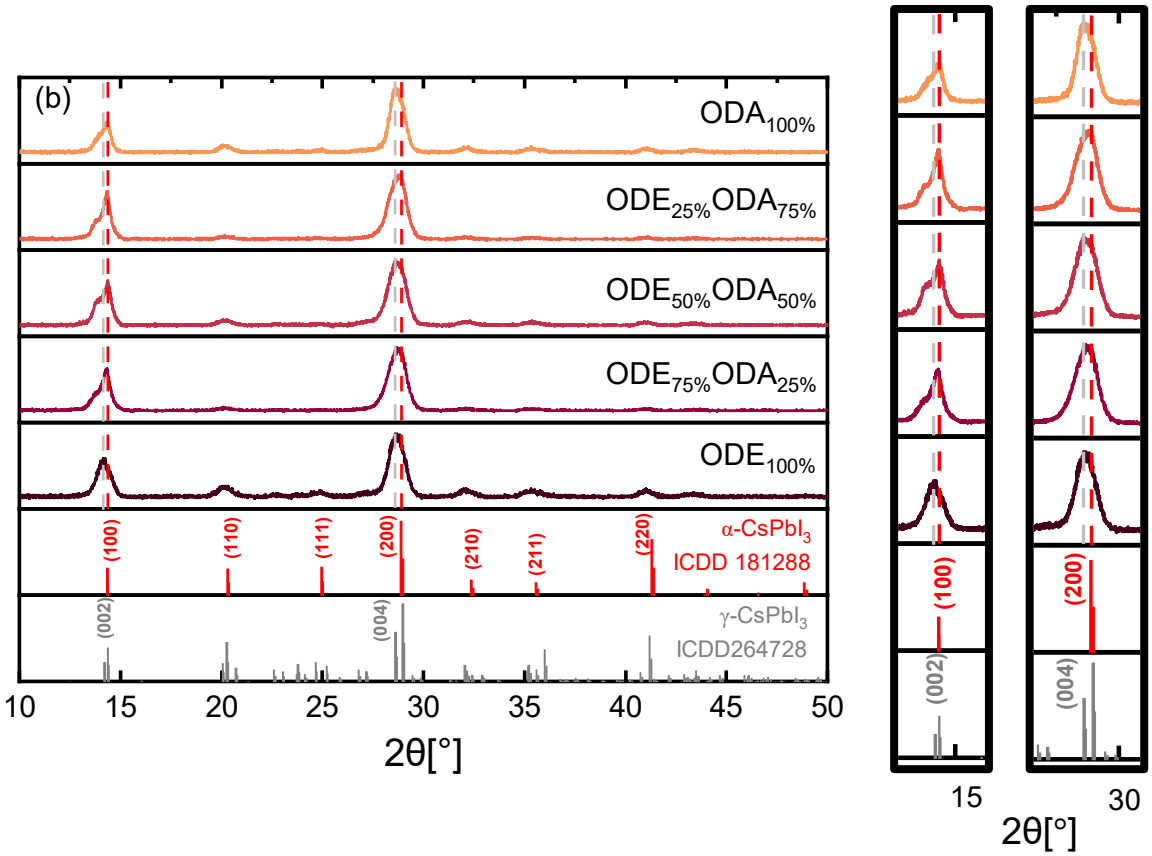

Figure S3: Zoom-in of the reflection peaks at 13-16° and 28-31° showing the shift on the central peak at 14° and 28°.

Experimental measurement of the reciprocal lattice vectors and best fitting parameters

For the assessment of the fitting between the structural model and the experimental data, we define the χ^2 function by:

$$\chi^2 = \sum_i^N \frac{\left(q_{mod,i} - q_{meas,i}\right)^2}{\Delta q_i^2} + \sum_i^{N-1} \frac{\left(\alpha_{mod,i} - \alpha_{meas,i}\right)^2}{\Delta \alpha_i^2}$$

comparing the measured lengths of the reciprocal lattice vectors $q_{meas,i}$ with the values derived from the corresponding structure models $q_{meas,i}$ as well as the corresponding angles $\alpha_{meas,i}$ between the vectors with the values $\alpha_{mod,i}$ expected from the models. The weighting factors are determined by experimental limitations, including calibration and distortion uncertainties, as well as the finite pixel size. For each image, $N = 4$ reflections were measured, leading to 4 length values and 3 angles. The experimental data and the best fitting model values are summarized in **Table S2.**

Table S2: Experimental data for the reciprocal lattice vectors measured in Fig. 4 b) and e) in comparison with the best fitting zone-axis of the structure model for the orthorhombic and cubic phase.

Image 260211_CsPbI3_ODA_380kX_ap18_0179_sub_000

measurement				orthorhombic [-110]					
ODA cubic	q*nm	angle/°	angle_n/°	h	k	l	d/Angstr.	q*nm	angle/°
1	6,38	120,5	0	4	4	0	1,544	6,477	0,0
2	4,56	75,8	44,7	2	2	-4	2,197	4,553	44,7
3	6,34	30,8	89,7	0	0	-8	1,563	6,399	90,0
4	4,49	-14,4	134,9	-2	-2	-4	2,197	4,553	135,3
				cubic [010]					
				h	k	l	d/Angstr.	q*nm	angle/°
				-4	0	0	1,574	6,353	0,0
				-2	0	-2	2,226	4,492	45,0
				0	0	4	1,574	6,353	90,0
				2	0	-2	2,226	4,492	135,0

Image 260211_CsPbI3_ODE_380kX_ap18_0219_sub_000

measurement				orthorhombic [-110]					
ODE cubic	q*nm	angle/°	angle_n/°	h	k	l	d/Angstr.	q*nm	angle/°
1	6,39	152,2	0	0	0	-8	1,563	6,399	0
2	3,56	88,8	63,4	2	2	-2	2,768	3,612	63,7
3	3,56	-0,6	152,8	1	1	4	2,789	3,586	153,2
4	3,56	36,3	115,9	2	2	2	2,768	3,612	116,3
				cubic [001]					
				h	k	l	d/Angstr.	q*nm	angle/°
				-4	0	0	1,574	6,353	0
				-1	2	0	2,816	3,551	63,4
				2	-1	0	2,816	3,551	153,4
				1	2	0	2,816	3,551	116,6

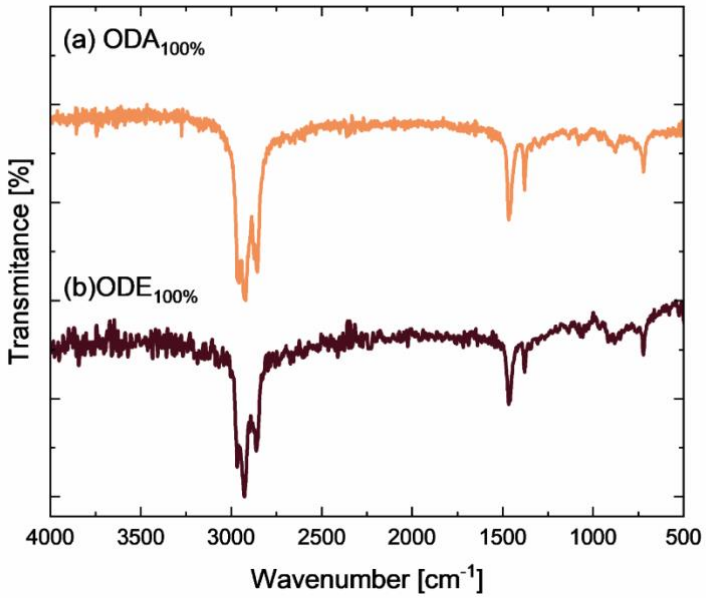

Figure S4: FTIR spectra measured on drop-cast (a) ODA and (b) ODE NCs.

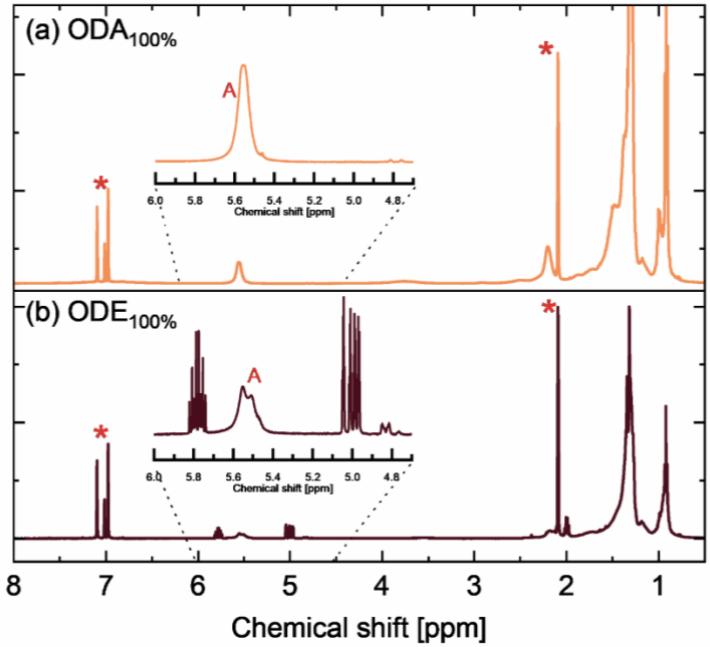

Figure S5: ^{1}H-NMR spectra in toluene-d_8: marked with A are resonances attributed olefinic protons of OA and OLA bound to NCs surface, marked with * are residual proton signals of toluene-d_8.

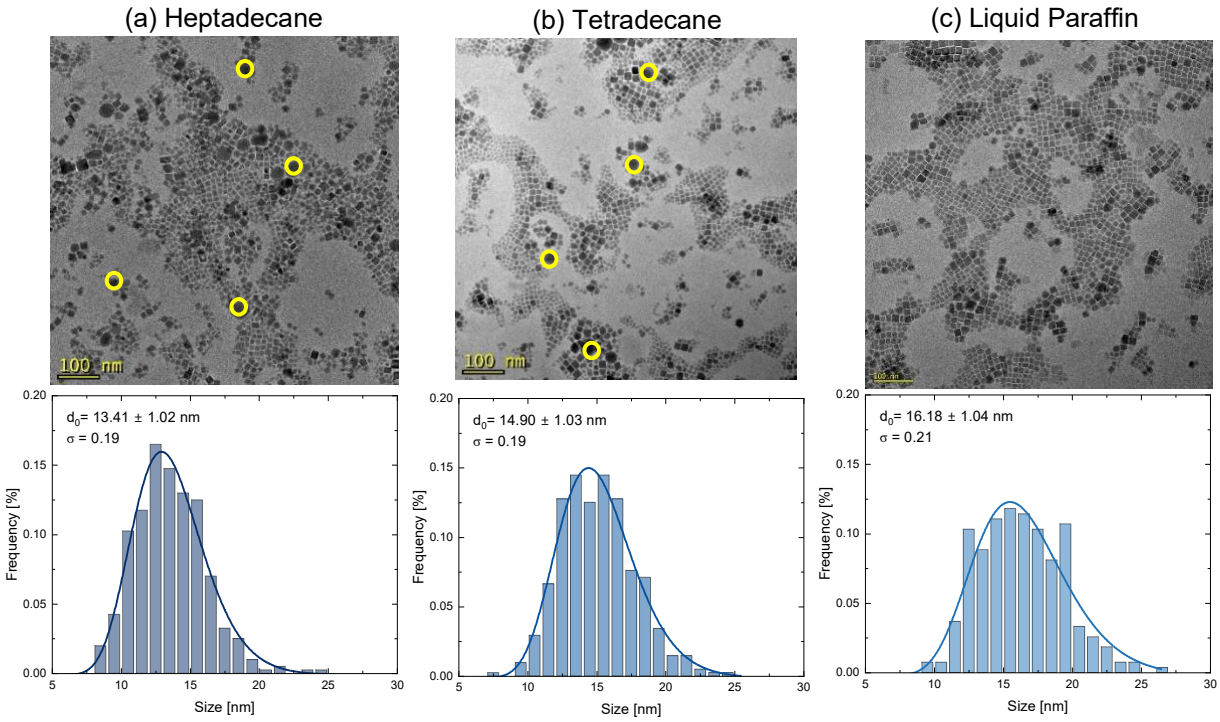

Figure S6: TEM images and size distribution analysis using different inert solvents (a) Heptadecane, (b) Tetradecane and (c) Liquid Paraffin.

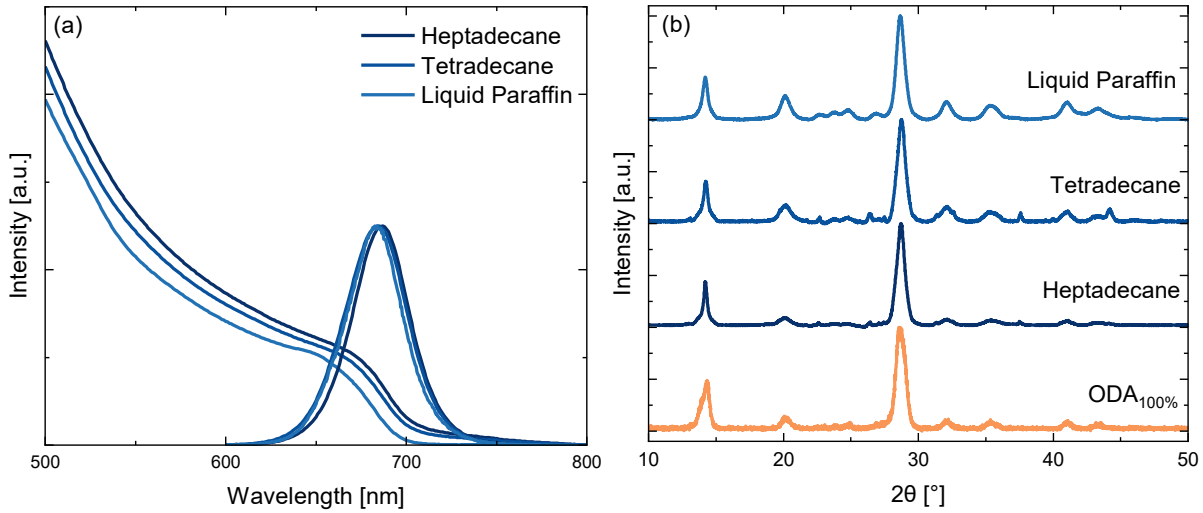

Figure S7: Normalized measurements of (a) steady-state PL and UV-vis, and (b) XRD diffractions using inert solvents. In (b) we have $ODA_{100\%}$ as a comparison across those solvents.