Characterization of a double metal cyanide (DMC) type catalyst in the polyoxypropylation process. Effects of the catalyst concentration.

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Table S1. Analytical characteristics of the DMC catalysts: DMC1, DMC2 – zinc hexacyanocobaltate(III) with different water contents; DMC 3-5 – DMC catalysts obtained according to the procedure (samples of independent product lots).

Sample	w_{Zn}**, % wt.**	w_{Co}**, % wt.**	w_{Zn}/w_{Co}	w_{C}**, % wt.**	w_{N}**, % wt.**	w_{C}/w_{N}	w_{Cl}**, % wt.**	w_{tBuOH} **calc., % wt.**
1	2	3	4	5	6	7	8	9
DMC 1	18.87	11.79	1.64	14.55	16.945	0.859	0.695	0.00(0.04)*
DMC 2	24.49	15.23	1.67	17.14	20.025	0.856	0.535	0.00(-0.04)*
DMC 3	26.35	11.67	2.40	24.92	17.825	1.398	9.625	14.86
DMC 4	28.42	12.43	2.09	24.99	17.04	1.467	8.65	16.01
DMC 5	27.80	12.10	2.80	23.80	17.46	1.364	9.90	13.63
* the calculated values are parenthesized								

Table S2. Average conversion rates for PO during the synthesis of PPG 2700 and PPG 10000, in the presence of KOH and DMC catalysts.

Product molecular weight, as calculated from the synthesis mass balance, *g/mol*	2700		10000	
Type of catalyst	KOH	DMC	KOH	DMC
Catalyst concentration as calculated per product wt, *ppm*	3000	30	3000	30
Type of starter	Polyoxypropylene glycol, M_n=450		Polyoxypropylene glycol, M_n=2700	
Amount of starter, *g*	100	100	162	162
Addition of PO monomer, *g*	500	500	438	438
Rp', $\frac{g_{PO}}{g_{PPG} \cdot h}$	135	590	95	333

$Rp'_{(DMC)}/Rp'_{(KOH)}$	4.4		3.5	
$Rp, \frac{g_{PO}}{g_{cat} \cdot g_{PPG} \cdot h}$	75	32 787	53	18 518
$Rp_{(DMC)}/Rp_{(KOH)}$	437		349	

Table S3. Coefficients $p_{PO}^{DMC}(0)$and*k'*, vs. concentration of DMC catalyst.

[DMC] ***ppm***	$\boldsymbol{p_{PO}^{DMC}(0)}$ ***kPa***	***k'*** ***min^{-1}***	$\boldsymbol{R^2}$
30	1608	0.0667	0.99
40	2027	0.1154	0.99
50	1724	0.1641	0.97
75	2241	0.2650	0.98
100	1500	0.3691	0.86

Table S4. Results of an assessment of unsaturation number for various types and concentrations of catalyst for the propoxylation products PPG 2700; PPG 10000 and PPG 50000.

Unsaturation number [meq/g]			
Catalyst concentration	PPG 2 700	PPG 10 000	PPG 50 000
DMC 30 *ppm*	0.00618	0.008365	
DMC 50 *ppm*	0.00695	0.01189	
DMC 100 *ppm*	0.00905	0.01306	0.018255
KOH 3000 *ppm*	0.02378	0.09352	

Table S5. Dependence of dispersity (*MWD*) of the tested polyoxypropylenediols with the molecular weights 2700 and 10000, depending on the catalyst concentration.

Catalyst concentration, *ppm*	*MWD*	
	PPG 2700	PPG 10000

30	1.48	1.07
50	1.14	1.06
100	1.06	1.05