Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information

High-throughput ultrasonic synthesis and in situ crystallisation investigation of metal phosphonocarboxylates

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Table S1 Metal 4-(phosphonomethyl)benzoates reported in the literature.

Compound	**Space group**	**Cell parameters**	**Structure motive**	**Lit.**
$[Cd_2(H_2O)_2(H\mathbf{PMBC})_2]$	*Pca*2$_1$	a = 10.0229(2) Å b = 5.9580(1) Å c = 34.9009(6) Å $\alpha = \beta = \gamma = 90°$	layers of corner-shared MnO_6-polyhedra; H-bonds between –COOH groups; isotypic with $[Mn_2(H_2O)_2(H\mathbf{PMBC})_2]$	[1]
$[Cu(H_2O)_2(H_2\mathbf{PMBC})_2]$	*P*-1	a = 4.5914(6) Å b = 5.9810(8) Å c = 17.811(3) Å α = 81.513(16)° β = 86.272(16)° γ = 82.251(15)°	isolated CuO_6-polyhedra; two O-atoms from phosphonates, two from water molecules; H-bonds between –COOH groups; isotypic with $[Mn(H_2O)_2(H_2\mathbf{PMBC})_2]$	[1]
$[Mn(H_2O)_2(H_2\mathbf{PMBC})_2]$	*P*-1	a = 4.6198(1) Å b = 5.9379(2) Å c = 18.0676(2) Å α = 83.119(2)° β = 88.307(2)° γ = 84.461(2)°	isolated MnO_6-polyhedra; two O-atoms from phosphonates, two from water molecules; H-bonds between –COOH groups; isotypic with $[Cu(H_2O)_2(H_2\mathbf{PMBC})_2]$	[1]
$[Mn_2(H_2O)_2(H\mathbf{PMBC})_2]$	*Pca*2$_1$	a = 9.8261(1) Å b = 5.8393(1) Å c = 35.2520(4) Å $\alpha = \beta = \gamma = 90°$	layers of corner-shared MnO_6-polyhedra; H-bonds between –COOH groups; isotypic with $[Cd_2(H_2O)_2(H\mathbf{PMBC})_2]$	[1]
$[Pb_3(\mathbf{PMBC})_2]$	*C*2/*c*	a = 4.7167(9) Å b = 18.753(4) Å c = 22.781(5) Å β = 91.07(3)°	two PbO_5-polyhedra and one PbO_4-polyhedra alternating in a corner-shared chain	[2]
$[Zn(H_2\mathbf{PMBC})_2]$	*P*-1	a = 5.3512(2) Å b = 11.3828(4) Å c = 15.8307(5) Å α = 99.338(2)° β = 92.850(2)° γ = 95.350(2)°	isolated ZnO_4-polyhedra; all four O-atoms from phosphonate groups; H-bonds between –COOH groups	[3]
$[Zn(H_2O)_4(H_2\mathbf{PMBC})_2]$	*P*-1	a = 4.7633(2) Å b = 6.9325(4) Å c = 16.5314(9) Å α = 83.236(3)° β = 89.669(3)° γ = 83.006(2)°	isolated ZnO_6-polyhedra; four O-atoms from water molecules, two from phosphonates; H-bonds between –COOH groups	[3]
$[Zn(H\mathbf{PMBC})]$	*P*-1	a = 5.1888(2) Å b = 10.5838(5) Å c = 17.3514(1) Å α = 81.139(2)° β = 88.525(2)° γ = 89.389(3)°	structure not determined	[3]
$[Zn_3(H_2O)_2(\mathbf{PMBC})_2] \cdot H_2O$	*P*2$_1$/*a*	a = 10.7950(2) Å b = 9.3322(2) Å	isolated units of ZnO_6-polyhedra corner-shared with two ZnO_4-polyhedra each	[3]

$c = 21.6181(4)$ Å
$\beta = 91.584(1)°$

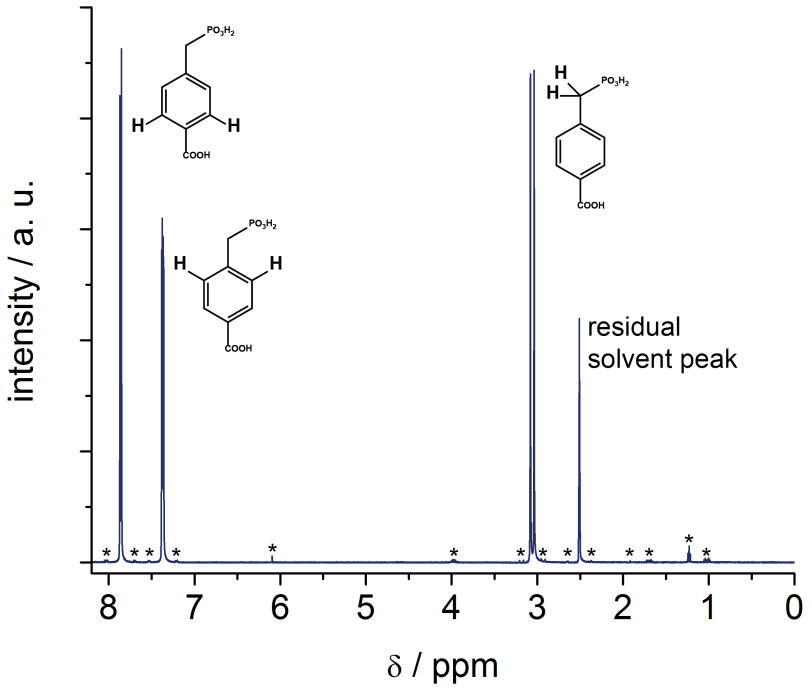


Fig. S1 ^{1}H-NMR spectrum of H_3**PMBC**. Minor signals labelled by asterisks are either ^{13}C satellite peaks or residual solvent and reactant peaks.

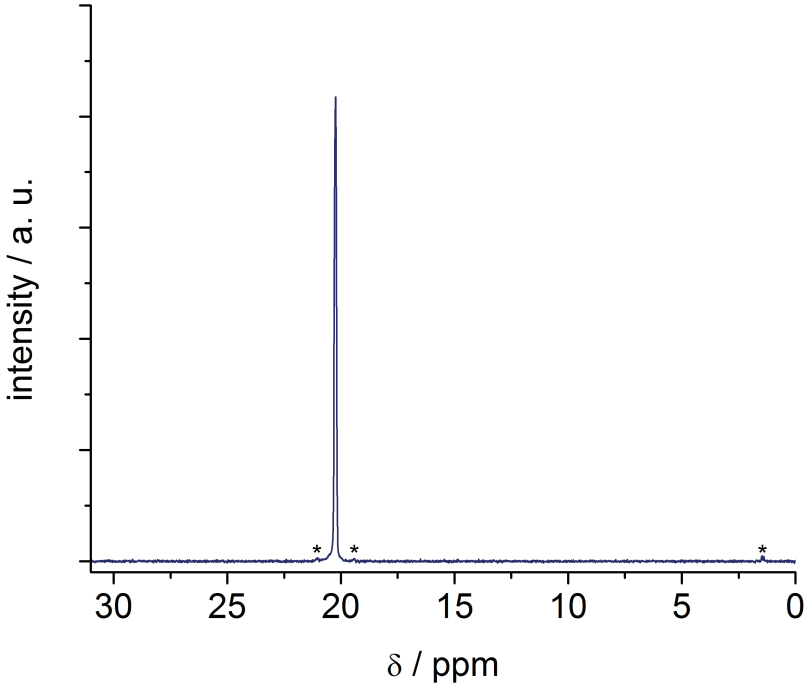


Fig. S2 ^{31}P-NMR spectrum of H_3**PMBC**. Minor signals labelled by asterisks are ^{13}C satellite peaks and a minor triethylphosphite impurity.

Table S2 Parameters for the high-throughput investigation under **ultrasonic** conditions. The abbreviation M, L and B stand for metal salt, H_3**PMBC** and KOH respectively. The values [M], [L] and [B] given without units represent the molar ratios of the reactants.

No.	metal salt	[M]	[L]	[B]	[M] / mmol L^{-1}	[L] / mmol L^{-1}	[B] / mmol L^{-1}	Product
1	$MgCl_2 \cdot 6\ H_2O$	1	1	0	50.0	50.0	0.0	■
2	$Ca(NO_3)_2 \cdot 4\ H_2O$	1	1	0	50.0	50.0	0.0	■
3	$SrCl_2 \cdot 6\ H_2O$	1	1	0	50.0	50.0	0.0	■
4	$Ba(NO_3)_2$	1	1	0	50.0	50.0	0.0	■
5	$Cu(NO_3)_2 \cdot 3\ H_2O$	1	1	0	50.0	50.0	0.0	■
6	$MnCl_2 \cdot 2\ H_2O$	1	1	0	50.0	50.0	0.0	■
7	$NiCl_2 \cdot 6\ H_2O$	1	1	0	50.0	50.0	0.0	■
8	$CoCl_2 \cdot 6\ H_2O$	1	1	0	50.0	50.0	0.0	■
9	$Zn(NO_3)_2 \cdot 6\ H_2O$	1	1	0	50.0	50.0	0.0	■
10	$FeCl_2 \cdot 4\ H_2O$	1	1	0	50.0	50.0	0.0	■
11	$Pb(O_2C_2H_3)_2 \cdot 3\ H_2O$	1	1	0	50.0	50.0	0.0	■
12	$SnCl_2 \cdot 2\ H_2O$	1	1	0	50.0	50.0	0.0	■
13	$MgCl_2 \cdot 6\ H_2O$	1	1	3	20.0	20.0	60.0	□
14	$Ca(NO_3)_2 \cdot 4\ H_2O$	1	1	3	20.0	20.0	60.0	□
15	$SrCl_2 \cdot 6\ H_2O$	1	1	3	20.0	20.0	60.0	□
16	$Ba(NO_3)_2$	1	1	3	20.0	20.0	60.0	□
17	$Cu(NO_3)_2 \cdot 3\ H_2O$	1	1	3	20.0	20.0	60.0	■
18	$MnCl_2 \cdot 2\ H_2O$	1	1	3	20.0	20.0	60.0	□
19	$NiCl_2 \cdot 6\ H_2O$	1	1	3	20.0	20.0	60.0	□
20	$CoCl_2 \cdot 6\ H_2O$	1	1	3	20.0	20.0	60.0	□
21	$Zn(NO_3)_2 \cdot 6\ H_2O$	1	1	3	20.0	20.0	60.0	■
22	$FeCl_2 \cdot 4\ H_2O$	1	1	3	20.0	20.0	60.0	■
23	$Pb(O_2C_2H_3)_2 \cdot 3\ H_2O$	1	1	3	20.0	20.0	60.0	■
24	$SnCl_2 \cdot 2\ H_2O$	1	1	3	20.0	20.0	60.0	□

■ $[Ca(H_2O)_2(H_2$**PMBC**$)_2]$, ■ $[Mn(H_2O)_2(H_2$**PMBC**$)_2]$, ■ $[Ni(H_2O)_4(H_2$**PMBC**$)_2]$, ■ $[Zn(H_2O)_4(H_2$**PMBC**$)_2]$, ■ unknown crystalline product, ■ X-ray amorphous, □ no precipitate

Table S3 Parameters for the high-throughput investigation under **ultrasonic** conditions. The abbreviation M, L and B stand for $Ca(NO_3)_2 \cdot 4\ H_2O$, H_3**PMBC** and KOH respectively. The values [M], [L] and [B] given without units, represent the molar ratios of the reactants.

No.	[M]	[L]	[B]	[M] / mmol L^{-1}	[L] / mmol L^{-1}	[B] / mmol L^{-1}	Product
1	1	1	0	50.0	50.0	0.0	■
2	1	1	1	33.3	33.3	33.3	■
3	1	1	2	25.0	25.0	50.0	□
4	1	1	3	20.0	20.0	60.0	■
5	1	1	4	16.7	16.7	66.7	□
6	1	1	5	14.3	14.3	71.4	□
7	1	1	6	12.5	12.5	75.0	□
8	1	1	7	11.1	11.1	77.8	□
9	2	1	0	66.7	33.3	0.0	■
10	2	1	1	50.0	25.0	25.0	■
11	2	1	2	40.0	20.0	40.0	□
12	2	1	3	33.3	16.7	50.0	□
13	2	1	4	28.6	14.3	57.1	■
14	2	1	5	25.0	12.5	62.5	■
15	2	1	6	22.2	11.1	66.7	■
16	2	1	7	20.0	10.0	70.0	■
17	1	2	0	33.3	66.7	0.0	■
18	1	2	1	25.0	50.0	25.0	■
19	1	2	2	20.0	40.0	40.0	■
20	1	2	3	16.7	33.3	50.0	■
21	1	2	4	14.3	28.6	57.1	□
22	1	2	5	12.5	25.0	62.5	□
23	1	2	6	11.1	22.2	66.7	■
24	1	2	7	10.0	20.0	70.0	■

■ $[Ca(H_2O)_2(H_2$**PMBC**$)_2]$, ■ unknown crystalline product, □ no precipitate

Table S4 Parameters for the high-throughput investigation under **conventional** heating. The abbreviation M, L and B stand for $Ca(NO_3)_2 \cdot 4\ H_2O$, H_3**PMBC** and KOH respectively. The values [M], [L] and [B] given without units, represent the molar ratios of the reactants.

No.	[M]	[L]	[B]	[M] / mmol L^{-1}	[L] / mmol L^{-1}	[B] / mmol L^{-1}	Product
1	1	1	0	50.0	50.0	0.0	■
2	1	1	1	33.3	33.3	33.3	■
3	1	1	2	25.0	25.0	50.0	□
4	1	1	3	20.0	20.0	60.0	■
5	1	1	4	16.7	16.7	66.7	■
6	1	1	5	14.3	14.3	71.4	■
7	1	1	6	12.5	12.5	75.0	■
8	1	1	7	11.1	11.1	77.8	■
9	2	1	0	66.7	33.3	0.0	■
10	2	1	1	50.0	25.0	25.0	■
11	2	1	2	40.0	20.0	40.0	□
12	2	1	3	33.3	16.7	50.0	■
13	2	1	4	28.6	14.3	57.1	■
14	2	1	5	25.0	12.5	62.5	■
15	2	1	6	22.2	11.1	66.7	■
16	2	1	7	20.0	10.0	70.0	■
17	1	2	0	33.3	66.7	0.0	■
18	1	2	1	25.0	50.0	25.0	■
19	1	2	2	20.0	40.0	40.0	■
20	1	2	3	16.7	33.3	50.0	■
21	1	2	4	14.3	28.6	57.1	■
22	1	2	5	12.5	25.0	62.5	□
23	1	2	6	11.1	22.2	66.7	□
24	1	2	7	10.0	20.0	70.0	■

■ $[Ca(H_2O)_2(H_2$**PMBC**$)_2]$, ■ unknown crystalline product, □ no precipitate

Table S5 Parameters for the high-throughput investigation under **ultrasonic** conditions. The abbreviation M, L and B stand for $NiCl_2 \cdot 6\ H_2O$, H_3**PMBC** and KOH respectively. The values [M], [L] and [B] given without units represent the molar ratios of the reactants.

No.	[M]	[L]	[B]	[M] / mmol L^{-1}	[L] / mmol L^{-1}	[B] / mmol L^{-1}	Product
1	1	1	0	50.0	50.0	0.0	■
2	1	1	1	33.3	33.3	33.3	■
3	1	1	2	25.0	25.0	50.0	■
4	1	1	3	20.0	20.0	60.0	□
5	1	1	4	16.7	16.7	66.7	■
6	1	1	5	14.3	14.3	71.4	■
7	1	1	6	12.5	12.5	75.0	■
8	1	1	7	11.1	11.1	77.8	□
9	2	1	0	66.7	33.3	0.0	□
10	2	1	1	50.0	25.0	25.0	■
11	2	1	2	40.0	20.0	40.0	■
12	2	1	3	33.3	16.7	50.0	■
13	2	1	4	28.6	14.3	57.1	■
14	2	1	5	25.0	12.5	62.5	■
15	2	1	6	22.2	11.1	66.7	□
16	2	1	7	20.0	10.0	70.0	□
17	1	2	0	33.3	66.7	0.0	■
18	1	2	1	25.0	50.0	25.0	■
19	1	2	2	20.0	40.0	40.0	■
20	1	2	3	16.7	33.3	50.0	■
21	1	2	4	14.3	28.6	57.1	□
22	1	2	5	12.5	25.0	62.5	□
23	1	2	6	11.1	22.2	66.7	□
24	1	2	7	10.0	20.0	70.0	□

■ $[Ni(H_2O)_4(H_2$**PMBC**$)_2]$, ■ X-ray amorphous, □ no precipitate

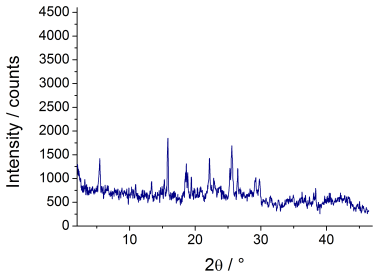
Table S6 Parameters for the high-throughput investigation under **conventional** heating. The abbreviation M, L and B stand for $NiCl_2 \cdot 6\ H_2O$, H_3**PMBC** and KOH respectively. The values [M], [L] and [B] given without units represent the molar ratios of the reactants.

No.	[M]	[L]	[B]	[M] / mmol L^{-1}	[L] / mmol L^{-1}	[B] / mmol L^{-1}	Product
1	1	1	0	50.0	50.0	0.0	■
2	1	1	0.5	40.0	40.0	20.0	■
3	1	1	1	33.3	33.3	33.3	□
4	1	1	1.5	28.6	28.6	42.9	□
5	1	1	2	25.0	25.0	50.0	■
6	1	1	2.5	22.2	22.2	55.6	■
7	1	1	3	20.0	20.0	60.0	■
8	1	1	3.5	18.2	18.2	63.6	■
9	1	2	0	33.3	66.7	0.0	■
10	1	2	0.5	28.6	57.1	14.3	■
11	1	2	1	25.0	50.0	25.0	■
12	1	2	1.5	22.2	44.4	33.3	■
13	1	2	2	20.0	40.0	40.0	■
14	1	2	2.5	18.2	36.4	45.5	□
15	1	2	3	16.7	33.3	50.0	■
16	1	2	3.5	15.4	30.8	53.8	■
17	2	1	0	66.7	33.3	0.0	■
18	2	1	0.5	57.1	28.6	14.3	■
19	2	1	1	50.0	25.0	25.0	□
20	2	1	1.5	44.4	22.2	33.3	■
21	2	1	2	40.0	20.0	40.0	■
22	2	1	2.5	36.4	18.2	45.5	■
23	2	1	3	33.3	16.7	50.0	■
24	2	1	3.5	30.8	15.4	53.8	■

■ $[Ni(H_2O)_4(H_2$**PMBC**$)_2]$, ■ unknown crystalline product (PXRD pattern Fig. S4), □ no precipitate

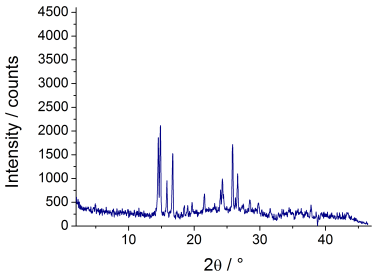
PXRD patterns found in the metal screening experiment via HT ultrasonic synthesis

Mg^{2+}; 1:1:0

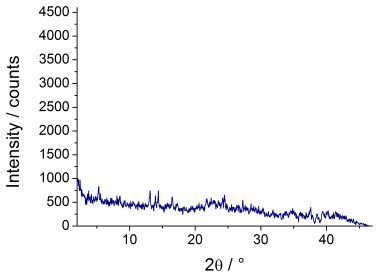


Ca^{2+}; 1:1:0

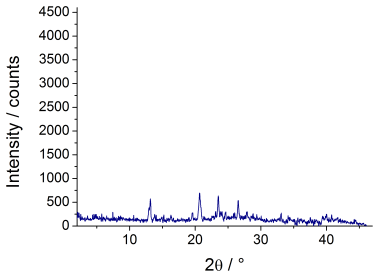
($[Ca(H_2O)_2(H_2$**PMBC**$)_2]$)



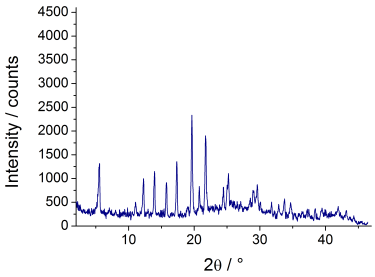
Sr^{2+}; 1:1:0



Ba^{2+}; 1:1:0

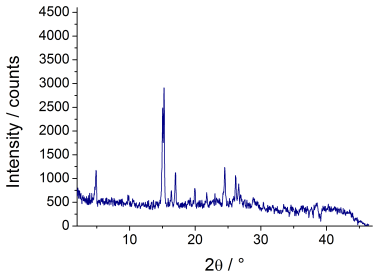


Cu^{2+}; 1:1:0



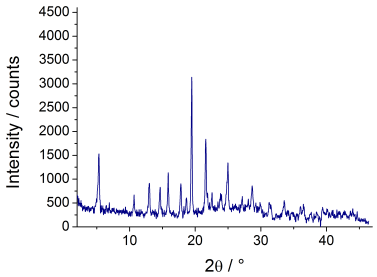
Mn^{2+}; 1:1:0

($[Mn(H_2O)_2(H_2$**PMBC**$)_2]$)

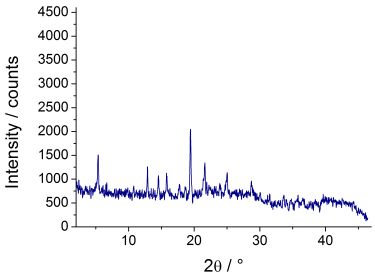


Ni^{2+}; 1:1:0

($[Ni(H_2O)_4(H_2$**PMBC**$)_2]$)

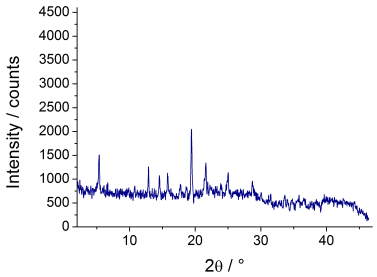


Co^{2+}; 1:1:0

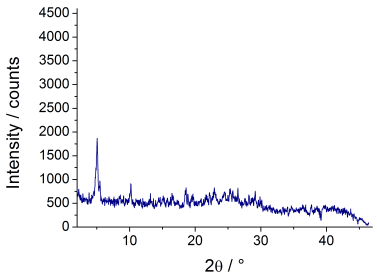


Zn^{2+}; 1:1:0

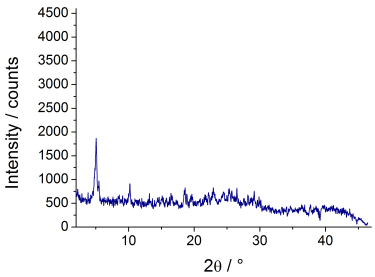
($[Zn(H_2O)_4(H_2$**PMBC**$)_2]$)



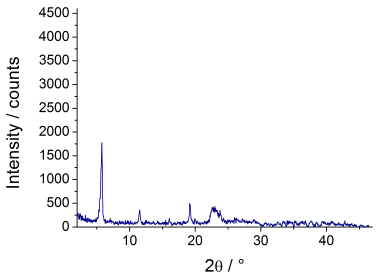
Fe^{2+}; 1:1:0



Pb^{2+}; 1:1:0



Sn^{2+}; 1:1:0



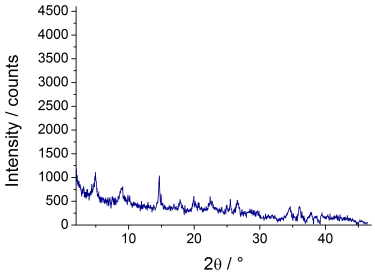
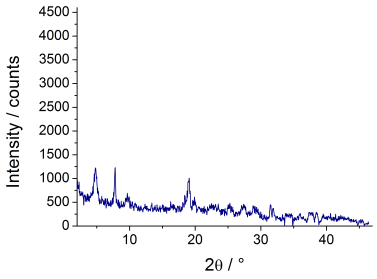
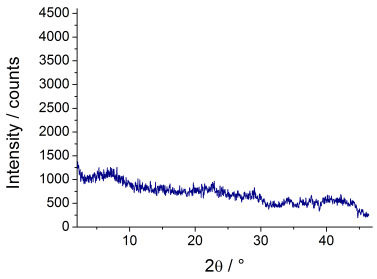
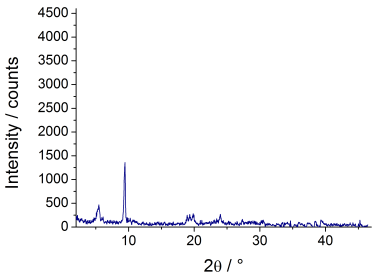
Mg^{2+}; 1:1:3	**Ca^{2+}; 1:1:3**	**Sr^{2+}; 1:1:3**
no precipitate	*no precipitate*	*no precipitate*
Ba^{2+}; 1:1:3	**Cu^{2+}; 1:1:3**	**Mn^{2+}; 1:1:3**
		
Ni^{2+}; 1:1:3	**Co^{2+}; 1:1:3**	**Zn^{2+}; 1:1:3**
no precipitate	*no precipitate*	
Fe^{2+}; 1:1:3	**Pb^{2+}; 1:1:3**	**Sn^{2+}; 1:1:3**
		*no precipitate*

Fig. S3 PXRD patterns found in the HT ultrasonic metal screening. The cation and the molar ratios metal:ligand:base is given above each depiction.

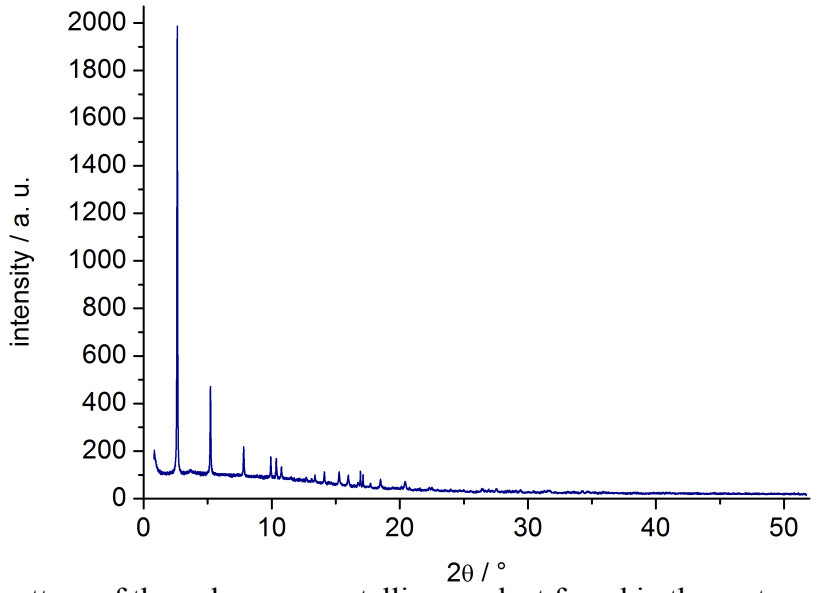


Fig. S4 PXRD pattern of the unknown crystalline product found in the system $NiCl_2 \cdot 6H_2O/H_3$**PMBC**/KOH/H_2O under conventional heating at higher KOH concentrations.

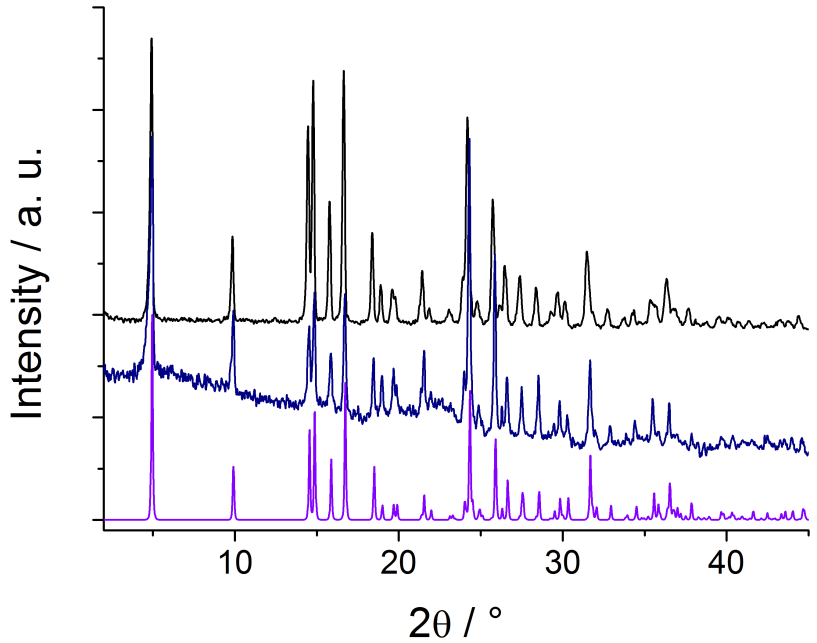


Fig. S5 PXRD patterns of $[Ca(H_2O)_2(H_2$**PMBC**$)_2]$ obtained by conventional (black) and ultrasonic (blue) HT synthesis compared to the theoretical pattern (violet) predicted based on the crystal structure determined by single-crystal diffraction.

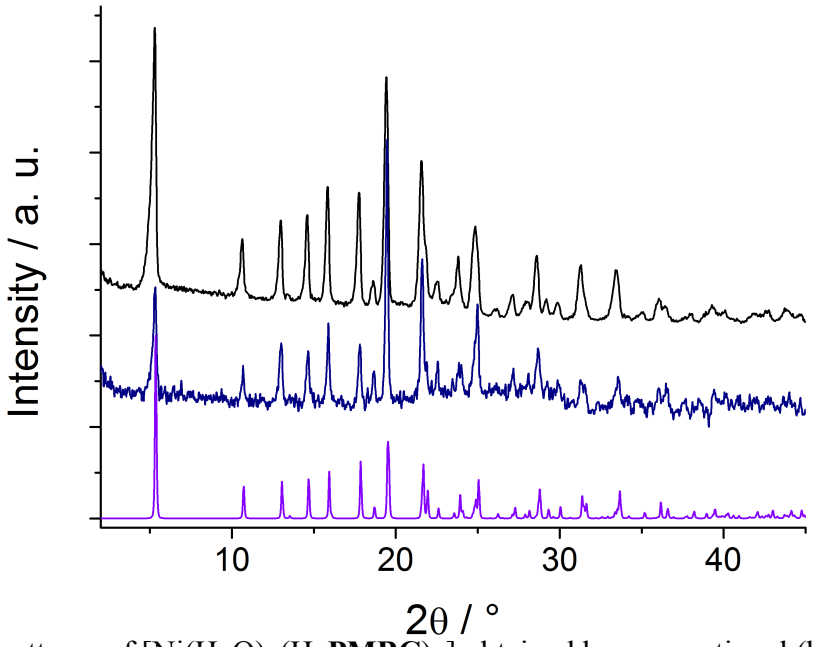


Fig. S6 PXRD patterns of $[Ni(H_2O)_4(H_2\mathbf{PMBC})_2]$ obtained by conventional (black) and ultrasonic (blue) HT synthesis compared to the theoretical pattern (violet) predicted based on the crystal structure determined by single-crystal diffraction.

PXRD patterns found in the screening experiments via HT ultrasonic and conventional synthesis

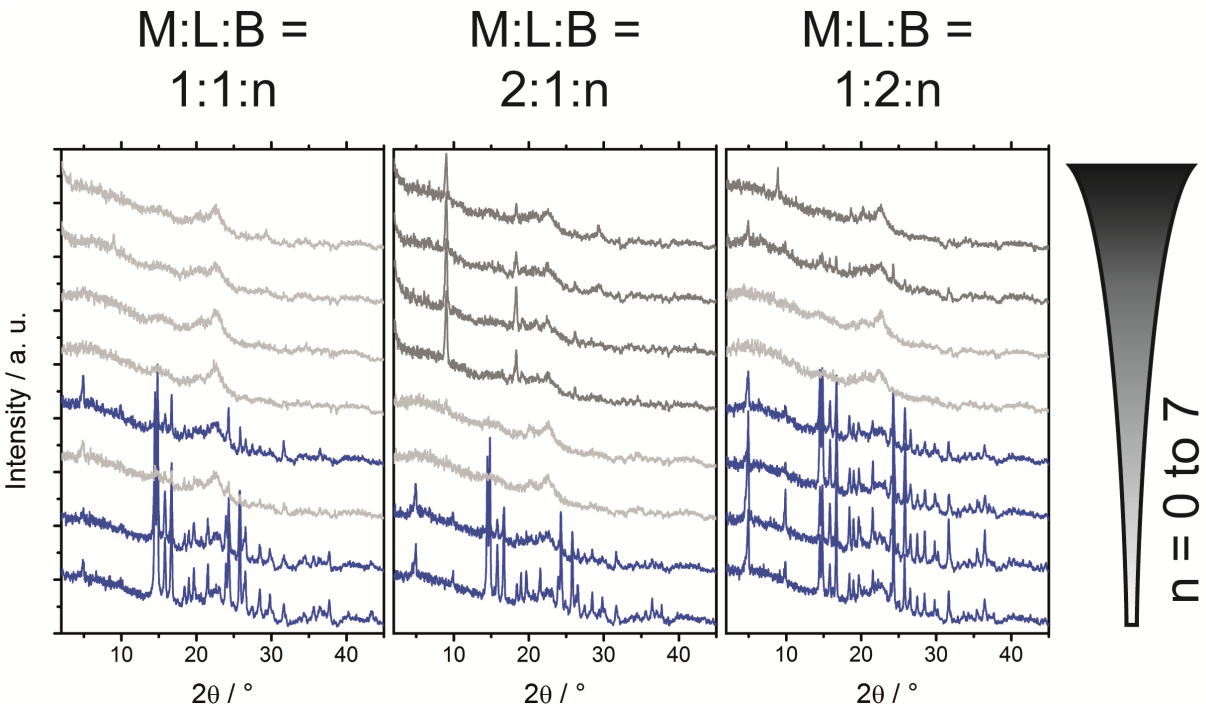


Fig. S7. PXRD patterns in the system $Ca(NO_3)_2 \cdot 4\ H_2O/H_3\mathbf{PMBC}$/KOH in HT ultrasonic synthesis. The abbreviation M, L and B stand for $Ca(NO_3)_2 \cdot 4\ H_2O$, $H_3\mathbf{PMBC}$ and KOH respectively. The phase $[Ca(H_2O)_2(H_2\mathbf{PMBC})_2]$ is coloured in blue, phase mixtures are depicted in dark grey, samples without precipitate are depicted in light grey.

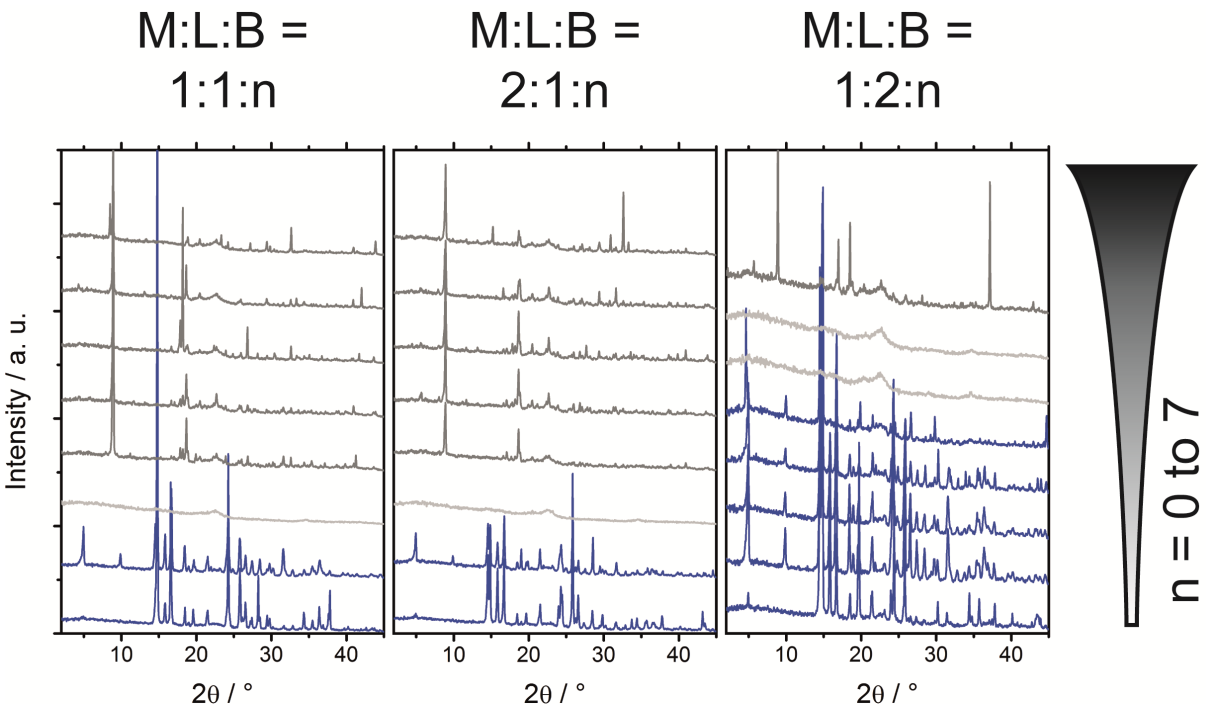


Fig. S8. PXRD patterns in the system $Ca(NO_3)_2 \cdot 4\ H_2O/H_3$**PMBC**/KOH in HT conventional synthesis. The abbreviation M, L and B stand for $Ca(NO_3)_2 \cdot 4\ H_2O$, H_3**PMBC** and KOH respectively. The phase $[Ca(H_2O)_2(H_2$**PMBC**$)_2]$ is coloured in blue, phase mixtures are depicted in dark grey, samples without precipitate are depicted in light grey.

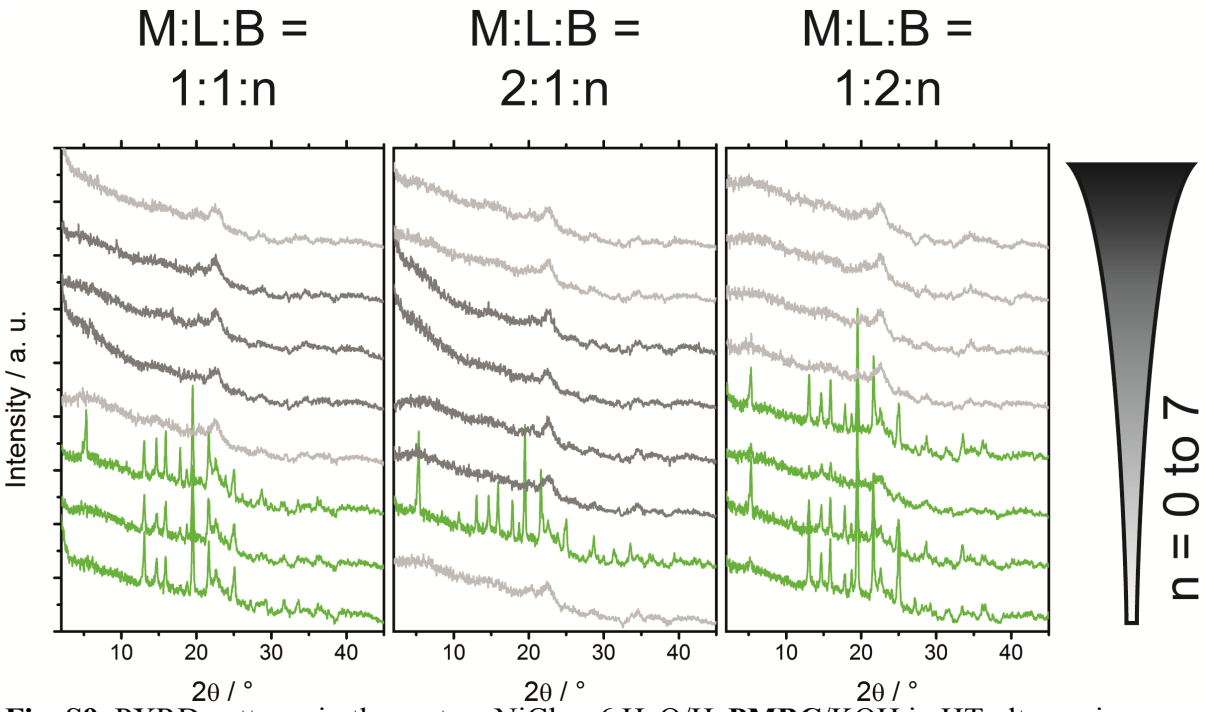


Fig. S9. PXRD patterns in the system $NiCl_2 \cdot 6\ H_2O/H_3$**PMBC**/KOH in HT ultrasonic synthesis. The abbreviation M, L and B stand for $NiCl_2 \cdot 6\ H_2O$, H_3**PMBC** and KOH respectively. The phase $[Ni(H_2O)_4(H_2$**PMBC**$)_2]$ is coloured in blue, X-ray amorphous products are depicted in dark grey, samples without precipitate are depicted in light grey.

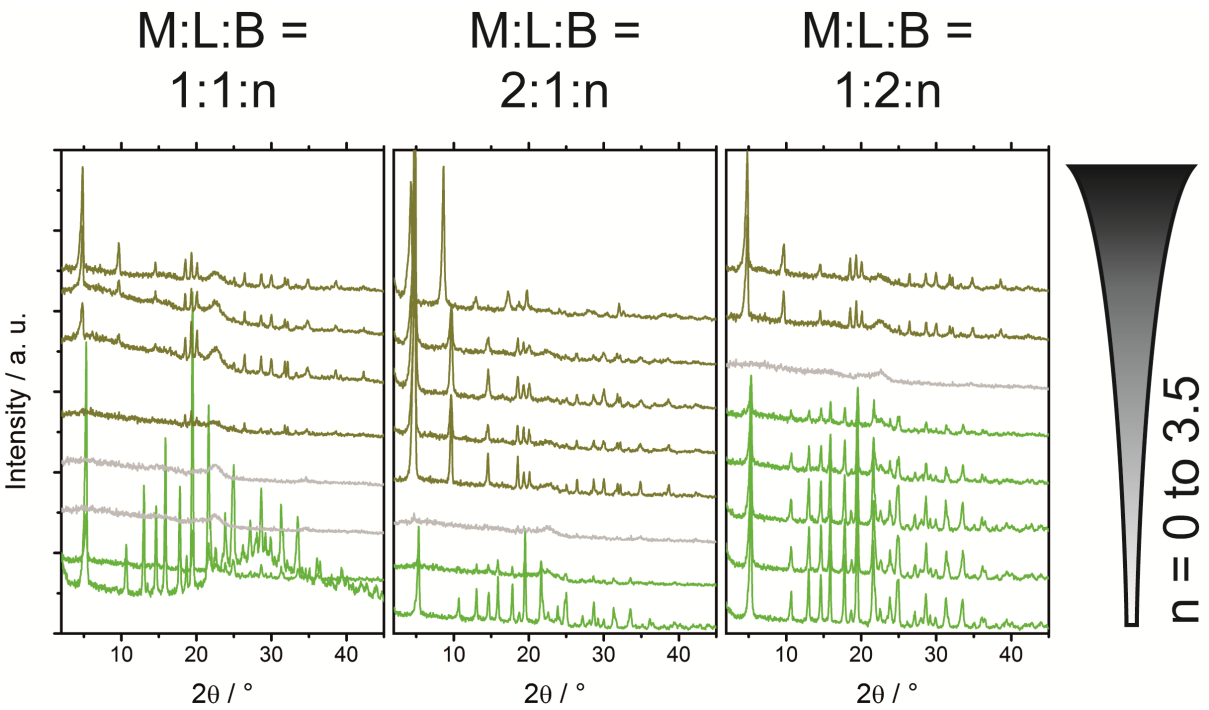


Fig. S10. PXRD patterns in the system $NiCl_2 \cdot 6\ H_2O$/H_3**PMBC**/KOH in HT ultrasonic synthesis. The abbreviation M, L and B stand for $NiCl_2 \cdot 6\ H_2O$, H_3**PMBC** and KOH respectively. The phase $[Ni(H_2O)_4(H_2$**PMBC**$)_2]$ is coloured in blue, unknown phase mixtures are depicted in dark yellow, samples without precipitate are depicted in light grey.

Description of the high-throughput (HT) ultrasonic device UIO250MTP

The Hielscher UIO250MTP (Fig. S7) is equipped with a water bath placed on top of the ultrasonic sonotrode. The sonotrode generates a vibration field uniform over the entire area of the water bath in order to subject the entire high-throughput reactor to the same ultrasound intensity. The maximal power of the sonotrode is 200 W. Cellstar 24 well cell culture plates were used as HT reactors and these were sealed with viewseal transparent foil (Fig. S8) both available from Greiner bio-one.

Fig. S11 Utilised HT ultrasonic device UIO250MTP by Hielscher. Picture provided by the company.

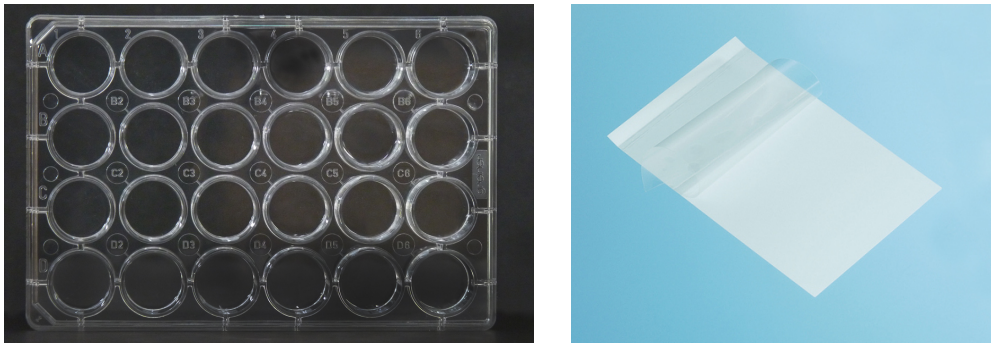


Fig. S12 Utilised Cellstar 24 well cell culture plates (left) und the viewseal foil (right) available from Greiner bio-one. Pictures provided by the company.

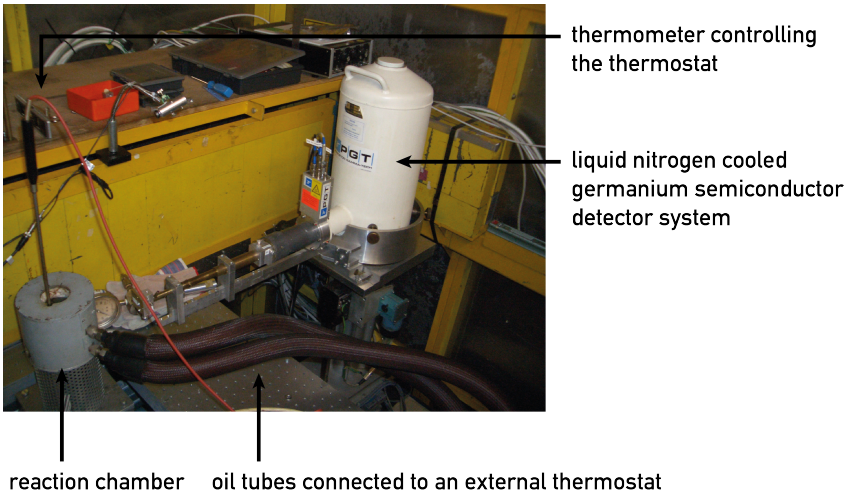


Fig. S13 Depiction of the reactor system used for in situ EDXRD measurements at HASYLAB, beamline F3 at DESY.

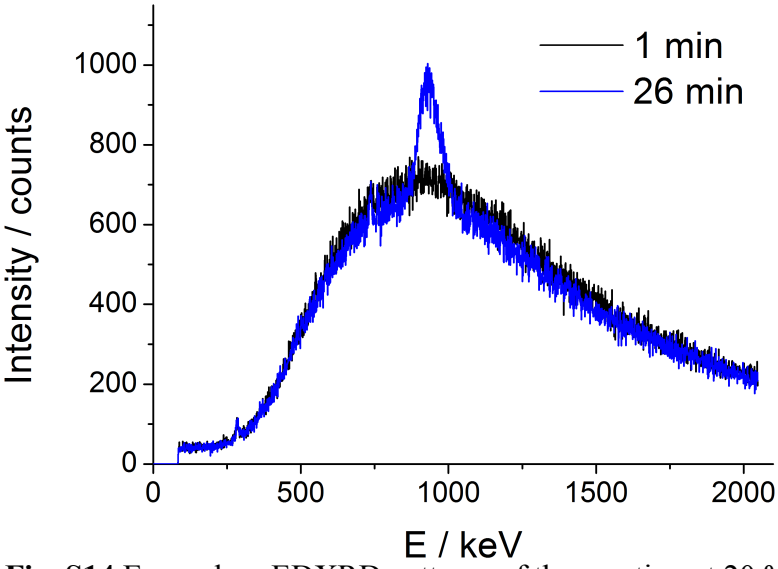


Fig. S14 Exemplary EDXRD patterns of the reaction at 20 % amplitude after 1 min (beginning) and 26 min (after the reaction is completed). The observed peak corresponds to the 001 reflex at 2θ = 5.36° in the PXRD measured with Cu-$K_{\alpha 1}$-radiation.

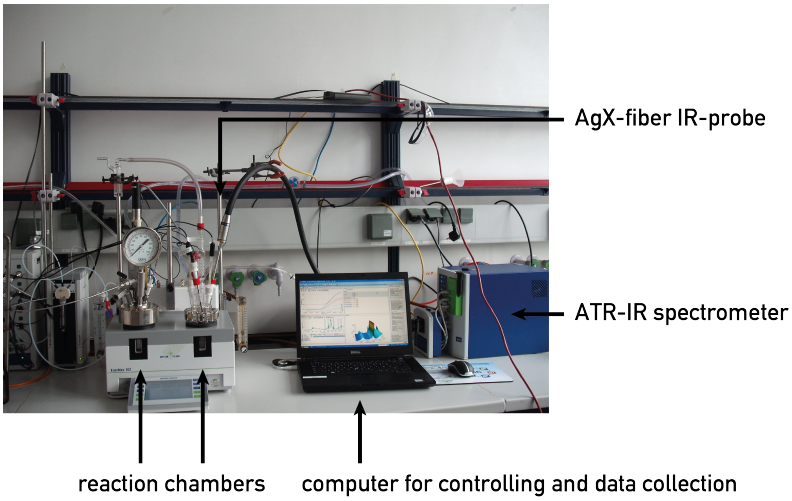


Fig. S15 Depiction of the Mettler Toledo EasyMax™ automated reactor system.

Table S7 Selected bond lengths for $[Ca(H_2O)_2(H_2\mathbf{PMBC})_2]$ and $[Ni(H_2O)_4(H_2\mathbf{PMBC})_2]$.

Bond	Bond lengths /Å	Bond	Bond lengths /Å
Ca1-O1	2.3271(14)	C2-C7	1.385(3)
Ca1-O2	2.4056(14)	C3-C4	1.378(3)
Ca1-O4	2.3322(14)	C4-C5	1.386(3)
P1-O1	1.4945(14)	C5-C6	1.380(3)
P1-O2	1.5184(12)	C5-C8	1.481(3)
P1-O3	1.5764(15)	C6-C7	1.382(3)
P1-C1	1.7881(19)	C8-O5	1.249(3)
C1-C2	1.507(3)	C8-O6	1.272(3)
C2-C3	1.380(3)		
Ni1-O1	2.0982(13)	C2-C7	1.390(3)
Ni1-O6	2.0860(14)	C3-C4	1.384(3)
Ni1-O7	2.0506(15)	C4-C5	1.385(3)
P1-O1	1.506(2)	C5-C6	1.390(3)
P1-O2	1.561(2)	C5-C8	1.480(3)
P1-O3	1.518(2)	C6-C7	1.384(3)
P1-C1	1.790(3)	C8-O4	1.254(3)
C1-C2	1.514(3)	C8-O5	1.277(3)
C2-C3	1.391(3)		

Table S8 Selected angles for $[Ca(H_2O)_2(H_2\mathbf{PMBC})_2]$ and $[Ni(H_2O)_4(H_2\mathbf{PMBC})_2]$.

Atoms	Angles /°	Atoms	Angles /°
O1-Ca1-O2	95.55(5)	C2-C7-C6	120.99(19)
O1-Ca1-O4	89.25(5)	C3-C2-C7	118.64(17)
O2-Ca1-O4	94.80(5)	C3-C4-C5	120.39(19)
O1-P1-C1	111.95(9)	C4-C5-C6	119.27(17)
O1-P1-O2	114.16(7)	C4-C5-C8	119.95(18)
O1-P1-O3	109.96(7)	C5-C6-C7	119.98(19)
O2-P1-C1	106.27(8)	C6-C5-C8	120.78(18)
O2-P1-O3	108.30(7)	O5-C8-C5	119.19(19)
O3-P1-C1	105.77(9)	O5-C8-O6	123.32(18)
P1-C1-C2	116.54(13)	O6-C8-C5	117.49(19)
C1-C2-C3	121.09(17)		
C1-C2-C7	120.27(17)		
C2-C3-C4	120.72(19)		
O1-Ni1-O6	90.5(1)	C2-C3-C4	120.3(2)
O1-Ni1-O7	90.3(1)	C2-C7-C6	120.6(2)
O6-Ni1-O7	90.1(1)	C3-C2-C7	119.0(2)
O1-P1-C1	112.3(1)	C3-C4-C5	120.5(2)
O1-P1-O2	109.9(1)	C4-C5-C6	119.4(2)
O1-P1-O3	113.8(1)	C4-C5-C8	121.2(2)
O2-P1-C1	106.0(1)	C5-C6-C7	120.2(2)
O2-P1-O3	107.9(1)	C6-C5-C8	119.4(2)
O3-P1-C1	106.4(1)	O4-C8-C5	119.4(2)
P1-C1-C2	115.9(2)	O4-C8-O5	123.0(2)
C1-C2-C3	120.9(2)	O5-C8-C5	117.6(2)
C1-C2-C7	120.1(2)		

References

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2. H.-H. Z. Jin Hu, Yan-Ning Cao, Chun-Gang Zhang, Shuai Zhang, Yi-Ping Chen, Rui-Qing Sun, *Chin.J.Struct.Chem.*, 2009, **28**, 939-946.
3. N. Stock and T. Bein, *Angewandte Chemie International Edition*, 2004, **43**, 749-752.