Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

First examples of aliphatic zirconium MOFs and the influence of inorganic anions on their crystal structures

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Figures S1-S4: Additional PXRD data

Figures S5-S7, Tab. S1: TG-experiments

Crystallographic Information

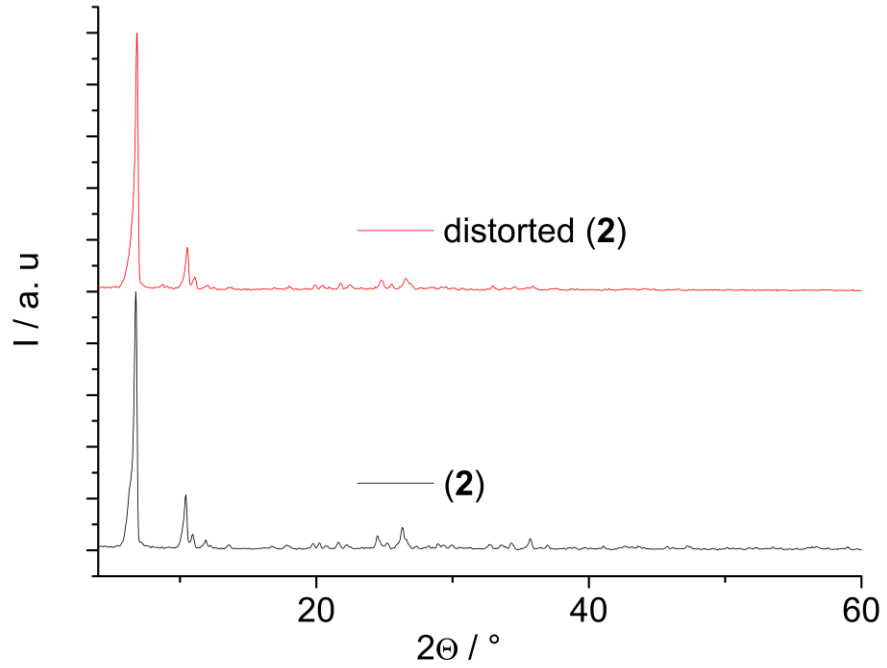

Figure S1: PXRD patterns of **2** (black line) and the slightly distorted polymorph of **2** (red line), the latter showing two weak additional peaks at an angle of ≈ 8 °.

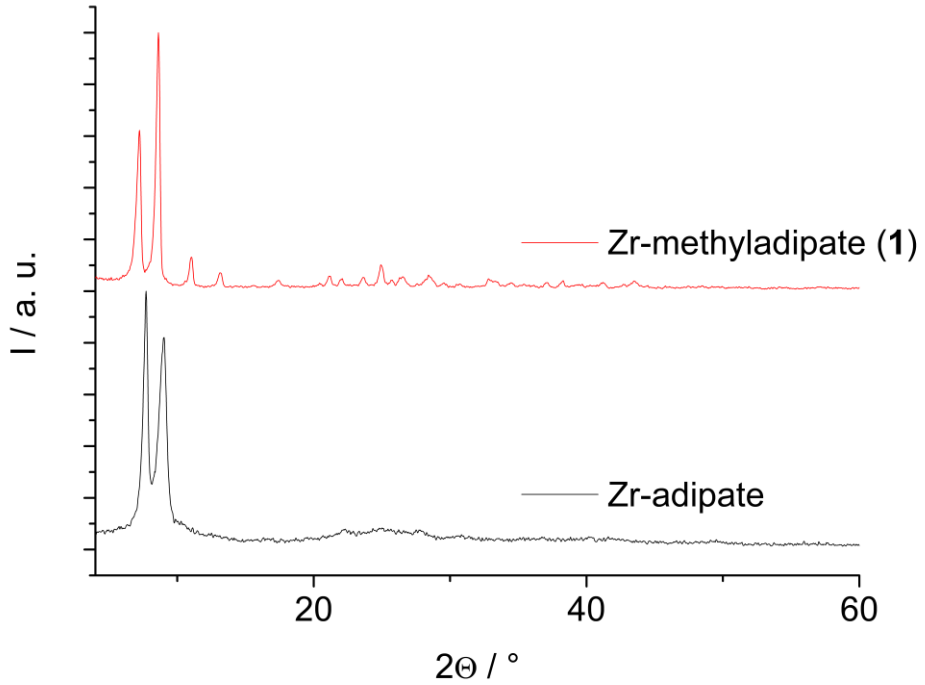

Figure S2: PXRD patterns of **1** (red line) and the product obtained under nearly identical conditions, replacing 3-methyladipic acid with adipic acid (black line).

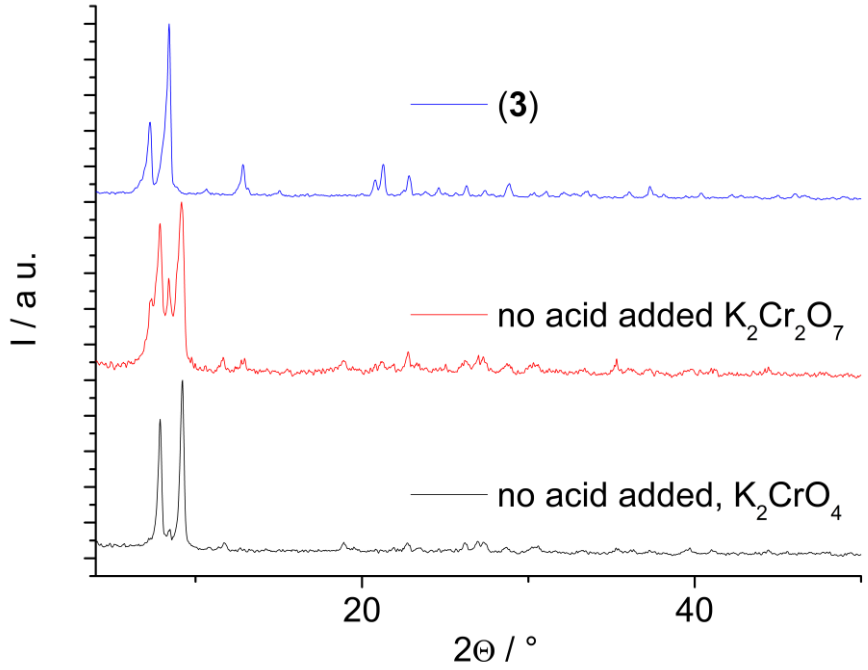

Figure S3: PXRD patterns of **3** (blue line) and the products which were obtained using different amounts of precursors without adding any nitric acid to the synthesis mixture.

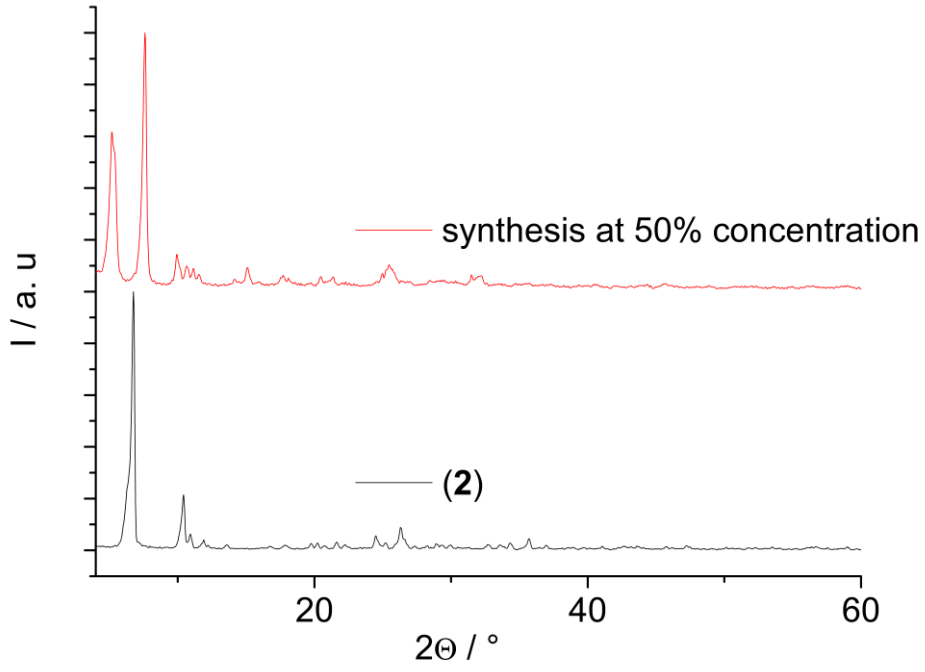

Figure S4: PXRD patterns of **2** (black line) and the product which was obtained using only half the amount of reactant given in the synthesis procedure of **2** (red line).

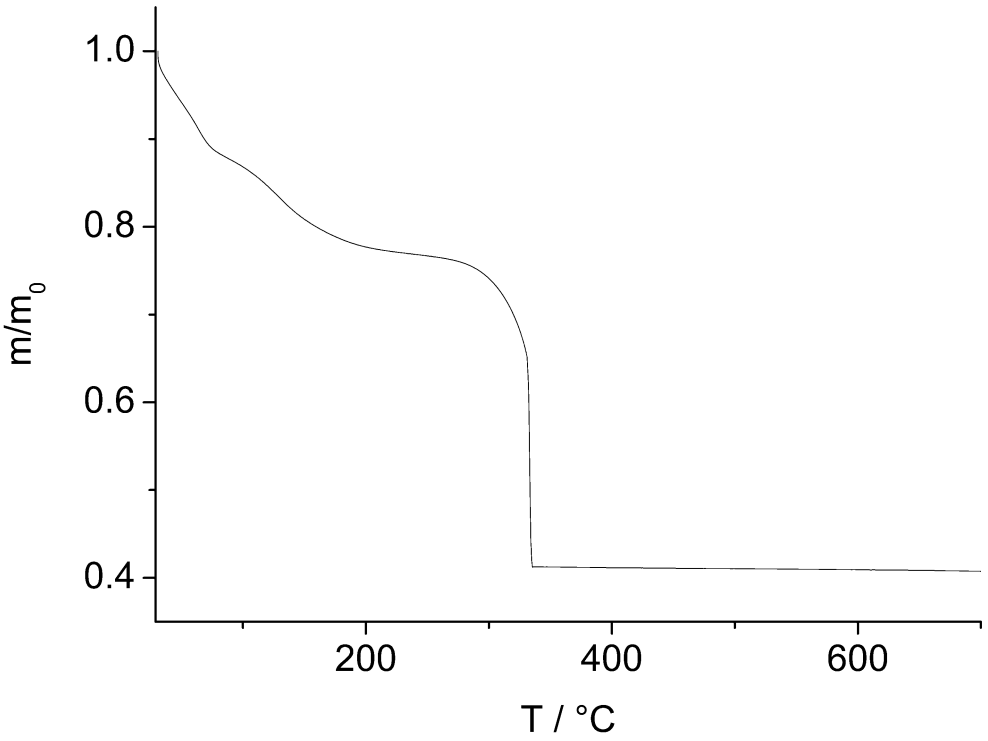

Figure S5: TG-curve of **1** measured under oxygen with a heating rate of 10 K/min.

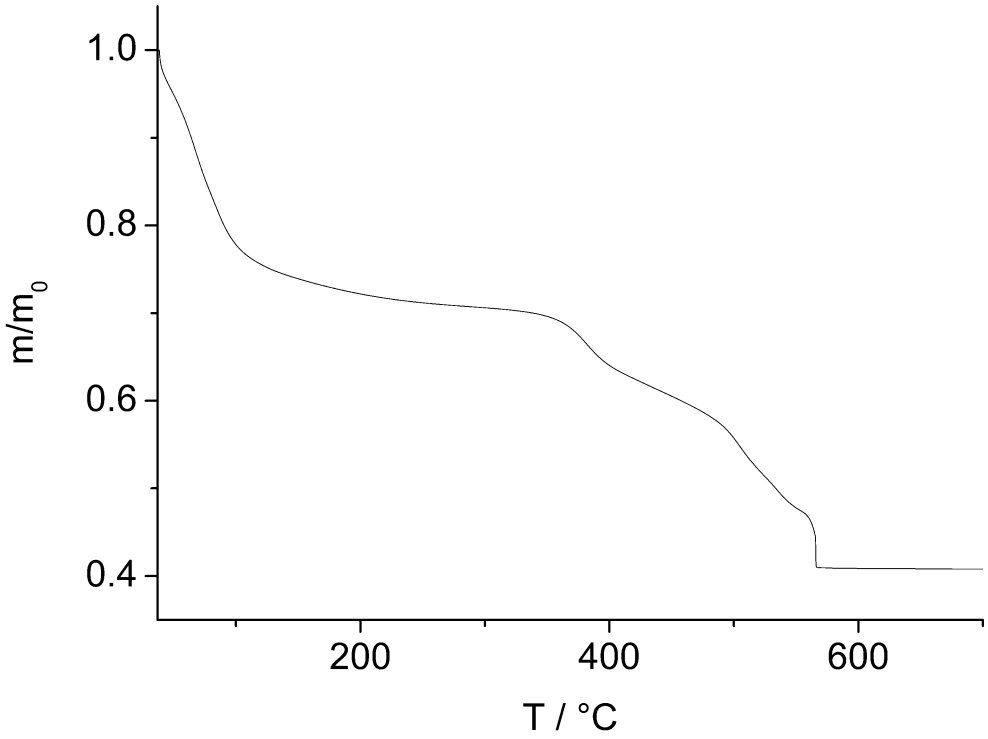

Figure S6: TG-curve of **2** measured under oxygen with a heating rate of 10 K/min.

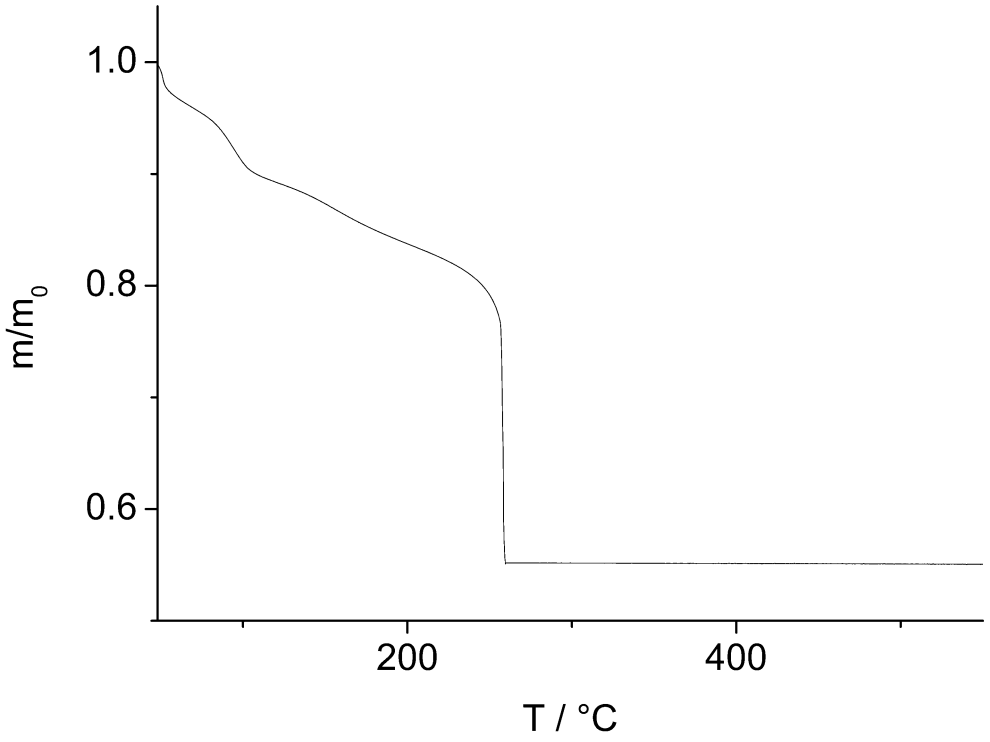

Figure S7: TG-curve of **3** measured under oxygen with a heating rate of 10 K/min.

Table S1: Measured and expected mass losses in the TG-experiments.

compound	(**1**)	(**2**)	(**3**)
mass loss till 100 °C	13 %	22 %	9 %
corresponding to *n* H_2O	≈ 13	≈ 22	≈ 11
mass loss above 100 °C	46 %	37 %	36 %
expected mass loss above 300°C	40 %	41 %	35 %

Crystallographic Information:

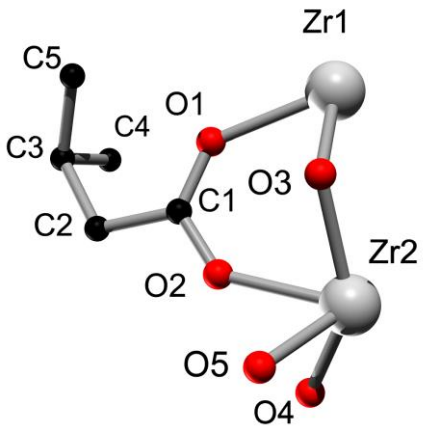

Figure S8: Asymmetric unit of **1** with numbering scheme used in Tab S1. Guest molecules are omitted.

Table S2: Some relevant bond distances in the structure of **1**. The linker molecule was treated as rigid body therefore no standard uncertainties are given.

Zr1	O3	2.076(11)
	O1	2.161(9)
Zr2	O4	2.121(31)
	O3	2.155(11)
	O5	2.167(12)
	O2	2.174(9)
	O3	2.198(11)
O1	C1	1.248(8)
O2	C1	1.250(7)
C1	C2	1.504
C2	C3	1.586
C3	C5	1.508
	C4	1.513
	C3	1.554

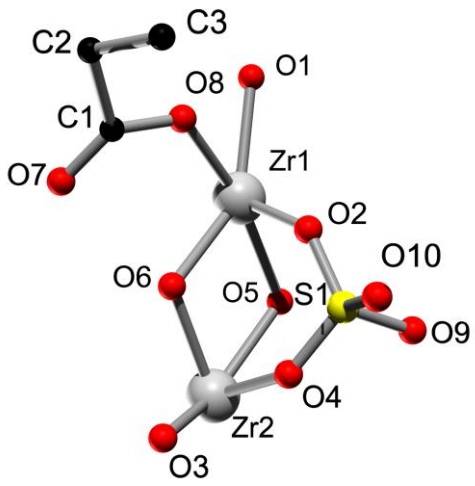

Figure S9: Asymmetric unit of **2** with numbering scheme used in Tab S2. Guest molecules are omitted.

Table S3: Some relevant bond distances in the structure of **2**.

Zr1	O5	2.054(25)
	O5	2.086(32)
	O2	2.154(21)
	O7	2.227(15)
	O1	2.272(26)
	O8	2.274(18)
	O6	2.283(22)
Zr2	O4	2.137(20)
	O3	2.221(37)
	O5	2.223(25)
	O6	2.262(22)
S1	O10	1.459(22)
	O4	1.465(23)
	O2	1.498(21)
	O9	1.532(25)
C1	O7	1.280(26)
	O8	1.282(31)
C1	C2	1.582(26)
C2	C3	1.568(43)
C3	C3	1.531(29)

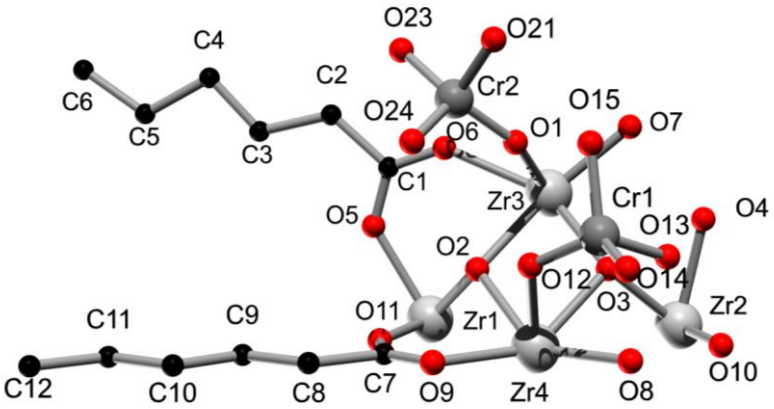

Figure S10: Asymmetric unit of **3** with numbering scheme used in Tab S3. Guest molecules are omitted.

Table S4: Some relevant bond distances in the structure of **3**

Zr1	O5	2.201(28)		O1	1.624(20)
	O2	2.251(20)		O21	1.641(23)
	O11	2.257(16)		O24	1.667(18)
Zr2	O10	2.089(18)	C1	O6	1.224(27)
	O4	2.193(16)		O5	1.242(28)
	O3	2.230(21)	C6	O7	1.250(23)
Zr3	O7	2.122(18)		O4	1.266(26)
	O2	2.250(20)	C7	O9	1.247(28)
	O3	2.257(21)		O11	1.271(23)
	O6	2.286(21)	C12	O8	1.251(25)
	O1	2.290(12)		O10	1.260(23)
Zr4	O8	2.155(21)	C1	C2	1.567(31)
	O2	2.201(21)	C2	C3	1.547(34)
	O12	2.204(15)	C3	C4	1.485(35)
	O3	2.231(20)	C4	C5	1.576(24)
	O9	2.278(27)	C5	C6	1.565(26)
Cr1	O14	1.558(33)	C7	C8	1.587(25)
	O12	1.653(26)	C8	C9	1.540(22)
	O15	1.678(17)	C9	C10	1.526(31)
	O13	1.784(31)	C10	C11	1.573(28)
Cr2	O23	1.586(24)	C11	C12	1.593(29)

Cif-files:

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