Supporting information for

Transformation of molecular compounds with Ba(Sr)/Al/Si and Ca(Sr, Ba)/Ti(Zr, Hf)/Si heteroelements as new efficient route to metal silicate materials

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Crystallographic Data for Compounds 1-9.

Table S1. Crystal and data collection parameters for compounds **1-5.**

Crystal	**3**·THF	**3**·2C_7H_8	**4**·2THF	**5**·1.6C_7H_8	**5**·4THF
Chemical formula	$C_{106}H_{138}O_{26}Si_4Sr_4Ti_2$	$C_{116}H_{146}O_{25}Si_4Sr_4Ti_2$	$C_{110}H_{147}ClO_{27}Si_4Sr_4Zr_2$	$C_{113.2}H_{144.8}O_{26}Si_4Sr_4Hf_2$	$C_{118}H_{164}Hf_2O_{30}Si_4Sr_4$
Formula Mass	2386.80	2498.96	2582.00	2741.32	2882.30
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$C2/c$
a/Å	14.926 (4)	13.359 (4)	11.599 (4)	11.641 (2)	26.366 (10)
b/Å	14.964 (4)	15.235 (6)	23.593 (5)	23.511 (3)	23.735 (6)
c/Å	15.660 (4)	15.870 (6)	21.871 (6)	21.993 (5)	21.213 (7)
α/°	107.74 (3)	112.91 (3)			
β/°	95.45 (2)	93.04 (3)	98.86 (3)	98.79(2)	103.96 (4)
γ/°	118.92 (3)	90.47 (3)			
Unit cell volume/Å^3	2790(2)	2970(2)	5914 (3)	5948.6 (2)	12883 (8)
Temperature/K	100(2)	85(2)	100(2)	80(2)	80(2)
Z	1	1	2	2	4
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα
Absorption coefficient, μ/mm^{-1}	2.147	2.020	2.093	3.627	3.356
No. of reflections measured	23340	22615	34598	58858	26475
No. of independent reflections	13134	12686	16589	14293	12045
No. of observed reflections (I> 2σ(I))	9024	9912	8910	11070	7080
R_{int}	0.0621	0.0265	0.0677	0.0642	0.0541
Final R_1 values (I> 2σ(I))	0.0647	0.0375	0.0709	0.0424	0.0628
Final wR(F^2) values (I> 2σ(I))	0.1421	0.0785	0.1141	0.1033	0.1324
Final R_1 values (all data)	0.1025	0.0589	0.1584	0.0651	0.1239
Final wR(F^2) values (all data)	0.1684	0.0877	0.1415	0.1218	0.1602
Goodness of fit on F^2	1.034	1.038	1.009	1.086	1.013
Δρmax/eÅ^{-3}	1.06	0.58	0.74	1.12	1.19
Δρmin/eÅ^{-3}	-1.27	-0.46	-0.78	-1.54	-1.17

Table S2. Crystal and data collection parameters for compounds **5-9.**

Crystal	**6**·4THF	**7**·1.8C_7H_8·0.2CH_2Cl_2	**8**·2C_7H_8·2H_2O	**9**·14C_7H_8
Chemical formula	$C_{112}H_{148}Hf_2O_{25}Si_4Sr_3$	$C_{108.8}H_{134.8}Ca_2Cl_{0.4}O_{22}Si_4Zr_2$	$C_{110}H_{140}Ca_2Hf_2O_{24}Si_4$	$C_{290}H_{344}Ba_8Cl_8O_{40}Si_8Zr_4$
Formula Mass	2626.50	2183.71	2395.71	6441.55
Crystal system	Monoclinic	Triclinic	Triclinic	Orthorhombic
Space group	*C*2/*c*	*P*$\bar{1}$	*P*$\bar{1}$	*Pbcn*
a/Å	25.601 (3)	11.421 (3)	11.394 (4)	40.661 (6)
b/Å	16.596 (3)	14.263 (4)	14.120 (4)	20.363 (3)
c/Å	29.699 (6)	19.107 (5)	19.167 (5)	36.720 (5)
α/°		103.64 (4)	100.03 (2)	
β/°	96.88 (3)	95.93 (4)	102.58 (3)	
γ/°		113.43 (4)	112.84 (3)	
Unit cell volume/Å^3	12527 (4)	2706.7 (18)	2656.4 (17)	30403 (8)
Temperature/K	85(2)	101(2)	80(2)	100(2)
Z	4	1	1	4
Radiation type	MoKα	MoKα	MoKα	MoKα
Absorption coefficient, μ/mm^{-1}	3.022	0.409	2.167	1.313
No. of reflections measured	37786	21235	17022	73581
No. of independent reflections	13505	10648	9682	31025
No. of observed reflections ($I > 2\sigma(I)$)	9206	7403	8831	24888
R_{int}	0.0487	0.0846	0.0361	0.0431
Final R_1 values ($I > 2\sigma(I)$)	0.1086	0.0681	0.0494	0.0695
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.2418	0.1459	0.1206	0.1819
Final R_1 values (all data)	0.1490	0.1060	0.0553	0.0861
Final $wR(F^2)$ values (all data)	0.2675	0.1688	0.1247	0.1923
Goodness of fit on F^2	1.154	1.042	1.092	1.123
Δρmax/eÅ^{-3}	3.16	0.58	3.66	3.07
Δρmin/eÅ^{-3}	-5.08	-1.06	-1.90	-1.50

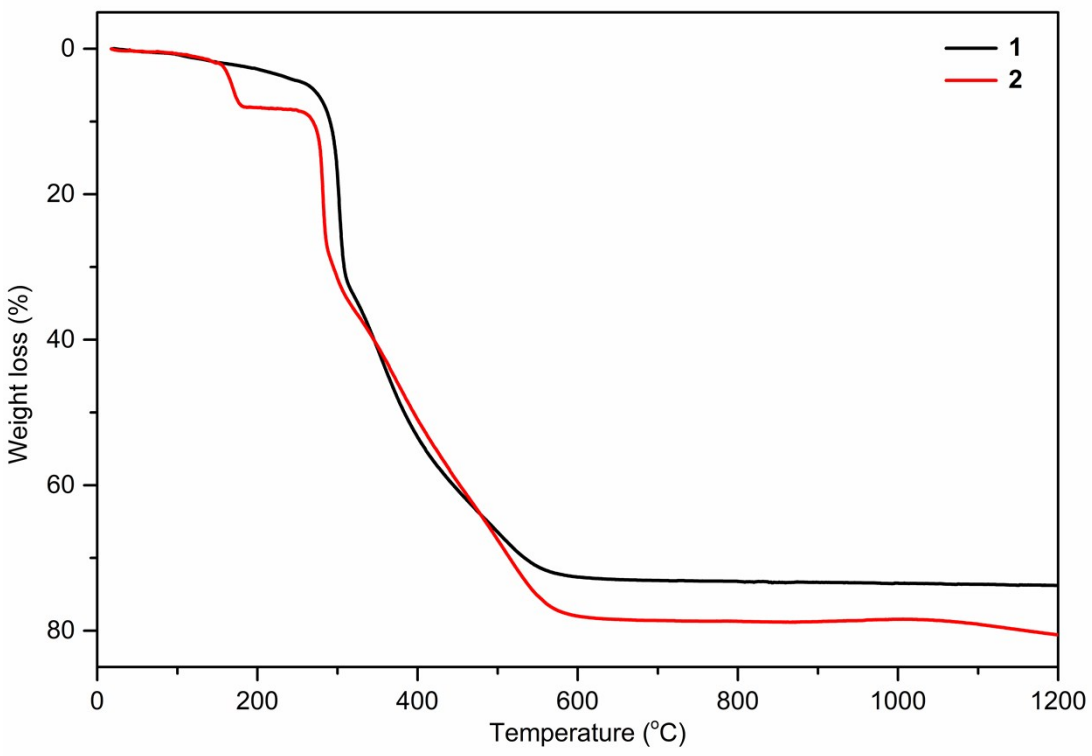

Fig.S1 TGA curves for **1**–**2** under N_2 with a heating rate of 10 °C min^{-1}.

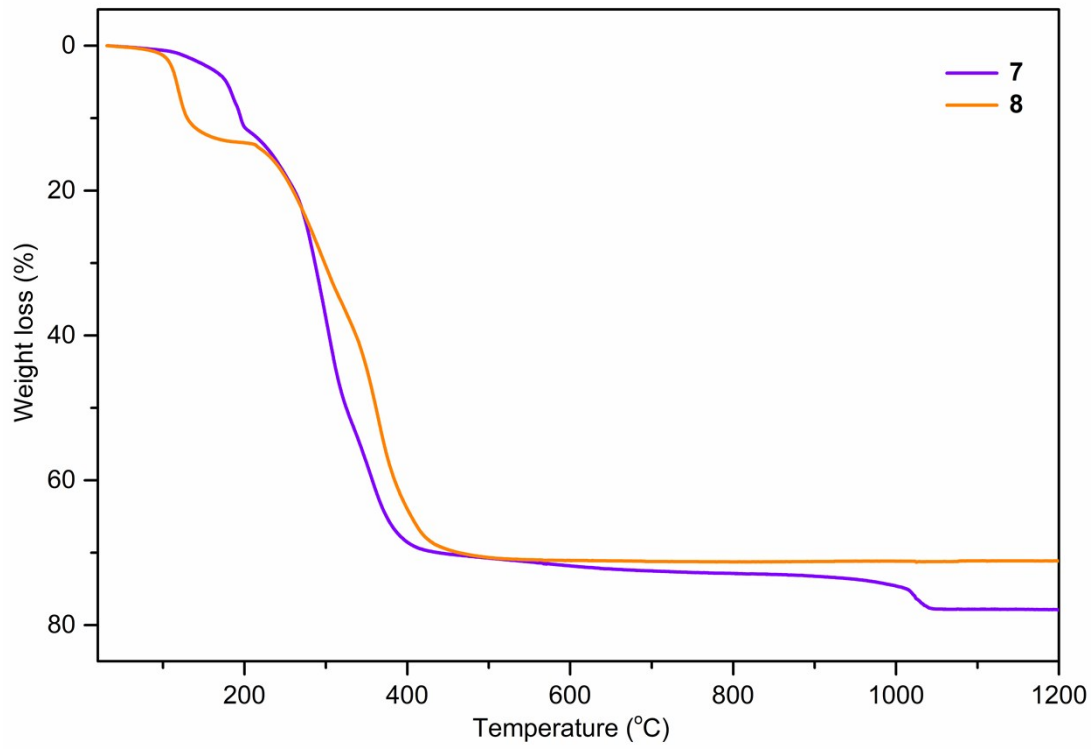

Fig.S2 TGA curves for **7**–**8** under N_2 with a heating rate of 10 °C min^{-1}.