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Supporting Information (SI)

Impact of Zn source on the RSN-type zeolite formation

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Energy Dispersive X-Ray Fluorescence (ED-XRF) spectra fitting. The resulting X-ray spectra were fitted using the Quantitative X-ray Analysis System (QXAS) software developed by International Atomic Energy Agency (IAEA) in order to obtain characteristic line intensities.[20] Characteristic line intensities of Si and Zn, in case of a monochromatic source, for the i-th sample can be written as:

$$I_i(Si) = w_i(Si)C(Si)A_i(Si)\left(1 + S_i(Si)\right) \tag{1}$$

$$I_i(Zn) = w_i(Zn)C(Zn)A_i(Zn) \tag{2}$$

where $w_i(Si)$ and $w_i(Zn)$ are mass fractions of Si and Zn in the i-th sample; $C(Si)$ and $C(Zn)$ are constants depending on fundamental parameters and on experimental setup; $A_i(Si)$ and $A_i(Zn)$ are absorption correction factors; and $S_i(Si)$ is the enhancement of Si line intensity due to secondary emission. $A_i(Si)$, $A_i(Zn)$ and $S_i(Si)$ depend on fundamental parameters and on sample composition. By fundamental parameters we refer to quantities such as cross sections that can be calculated with sufficient precision from theory or from empirical formulae.

$A_i(Si)$ can be expressed as:

$$A_i(Si) = \frac{1 - e^{-\mu_i\left(E_0,E(Si)\right)d}}{\mu_i\left(E_0,E(Si)\right)} \tag{3}$$

where d is sample thickness in g/cm^2 and $\mu_i\left(E_0,E(Si)\right)$ is:

$$\mu_i\left(E_0,E(Si)\right) = \frac{\mu_i(E_0)}{\cos\vartheta_{in}} + \frac{\mu_i(E(Si))}{\cos\vartheta_{out}} \tag{4}$$

$\mu_i(E_0)$ and $\mu_i(E(Si))$ are mass absorption coefficients for the i-th sample at the incoming beam energy E_0 (K_α line for Rh) and K_α line energy for Si, $E(Si)$; ϑ_{in} and ϑ_{out} are incident and take off angles, with respect to the sample surface normal. The analogous expressions hold for $A_i(Zn)$.

The sample is said to be infinitely thick if the sample thickness is big enough so that the second part of numerator in Equation (3) can be neglected. In our measurement that was the case and it was checked by weighting the samples with a microbalance Mettler Toledo XA105 Dual Range (readability 10 μg). For infinitely thick sample the enhancement due to secondary emission is [2]:

$$S_i(Si) = \sum_{j=K,Zn} w_i(j)D_j\left[\ln\left(1 + \frac{\mu_i(E_0)}{\mu_i(E(j))\cos\vartheta_{in}}\right)\frac{\cos\vartheta_{in}}{\mu_i(E_0)} + \ln\left(1 + \frac{\mu_i(E(Si))}{\mu_i(E(j))\cos\vartheta_{out}}\right)\frac{\cos\vartheta_{out}}{\mu_i(E(Si))}\right] \tag{5}$$

where the sum goes over all the elements in the sample that have characteristic line energies high enough to produce characteristic line of Si (in our case K and Zn). D_j ´s are constants depending on fundamental parameters.

It is difficult to obtain constant $C(Si)$ from Equation (1) with sufficient precision. The sensitivity of experimental setup is very low for Si and therefore the uncertainty due to efficiency determination is large. Fortunately, it was sufficient to calculate the ratio of Zn to Si mass fractions in the i-th sample relative to the mass fraction ratio in the crystal material (index c in following equations) with known composition:

$$R_i^W \overset{\text{def}}{=} \frac{w_i(Zn)\, w_c(Si)}{w_i(Si)\, w_c(Zn)} \qquad (6)$$

In this way constants $C(Zn)$ and $C(Si)$ cancel out and from Equations (1) and (2) it follows

$$R_i^W = \frac{R_i^I}{R_i^A R_i^S} \qquad (7)$$

where R_i^I, R_i^A and R_i^S are double ratios for the intensity, absorption and secondary emission correction:

$$R_i^I \overset{\text{def}}{=} \frac{I_i(Zn)\, I_c(Si)}{I_i(Si)\, I_c(Zn)} \qquad (8)$$

$$R_i^A \overset{\text{def}}{=} \frac{A_i(Zn)\, A_c(Si)}{A_i(Si)\, A_c(Zn)} \qquad (9)$$

$$R_i^S \overset{\text{def}}{=} \frac{1 + S_c(Si)}{1 + S_i(Si)} \qquad (10)$$

Corrections for absorption and secondary emission depend, via mass absorption coefficients, on mass fractions of all elements present in the sample (equations (3), (4) and (5)). In general it is therefore impossible to calculate them just from measurements. Absorption correction can be huge and even secondary emission can be significant (up to 50%). Nevertheless, overall correction factor from Equation (7) should be close to 1. It was estimated by assuming the following fractions.

$$w_i(Si) = w_c(Si)\frac{I_i(Si)}{I_c(Si)} \qquad (11)$$

$$w_i(K) = w_c(K)\frac{I_i(K)}{I_c(K)} \qquad (12)$$

$$w_i(Zn) = w_c(Zn)\frac{I_i(Zn)}{I_c(Zn)} \qquad (13)$$

$$w_i(O) = \left(1 - w_i(Si) - w_i(K) - w_i(Zn)\right)\frac{w_c(O)}{w_c(O) + w_c(Na)} \qquad (14)$$

$$w_i(Na) = \left(1 - w_i(Si) - w_i(K) - w_i(Zn)\right)\frac{w_c(Na)}{w_c(O) + w_c(Na)} \qquad (15)$$

For Si, K and Zn, whose characteristic lines are present in the spectra, it was assumed that mass fractions are proportional to line intensities (Equations (11), (12) and (13)), while for invisible O and Na it was assumed that ratio of their mass fractions is the same in all samples. Equations (14) and (15) are then derived using the constraint that sum of all mass fractions must be equal to one. With these assumptions overall correction was negligible in majority of samples i.e. it was smaller than the estimated overall uncertainty. The biggest correction was about 20%. Uncertainty of the correction factor was estimated by varying mass fractions of Si and K by ±20%, mass fraction of Zn by ±10% and mass fraction of Na by ±30%. Obtained correction factors differed only slightly, by a few percent. Therefore, uncertainty of the correction factor was estimated to be about 3%.

Uncertainty of the final result, Equation (6), was estimated to be about 8% and it was dominated by uncertainties of determining line intensities for Si, $I_i(Si)$ and $I_c(Si)$ which were estimated to be about 5%.

Characterization data

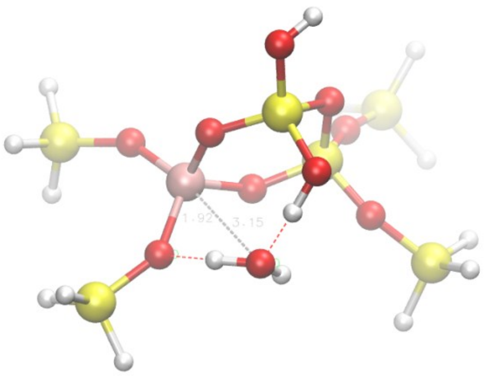

Figure S1. Model used in the calculations.

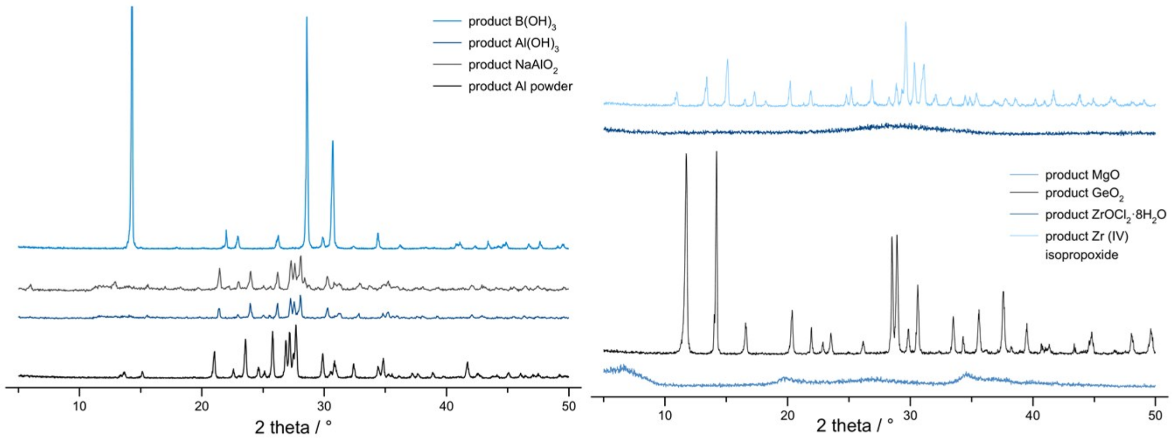

Figure S2. XRD patterns of the solids obtained after hydrothermal treatment at 180 °C of reaction mixtures containing various potential T atoms.

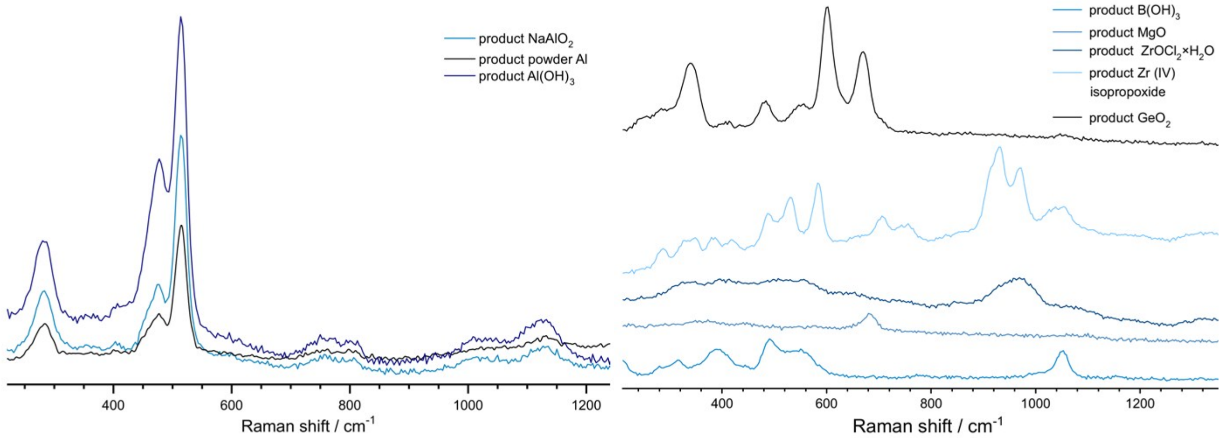

Figure S3. Raman spectra of the solids obtained after hydrothermal treatment at 180 °C of reaction mixtures containing various potential T atoms.

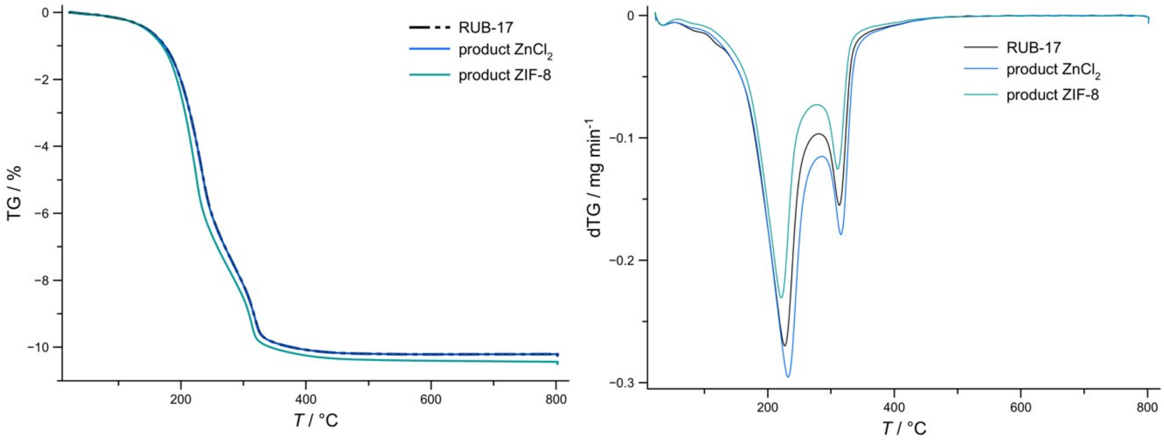

Figure S4. TG and dTG curves of the final products obtained after hydrothermal treatment at 180 °C using different Zn sources.

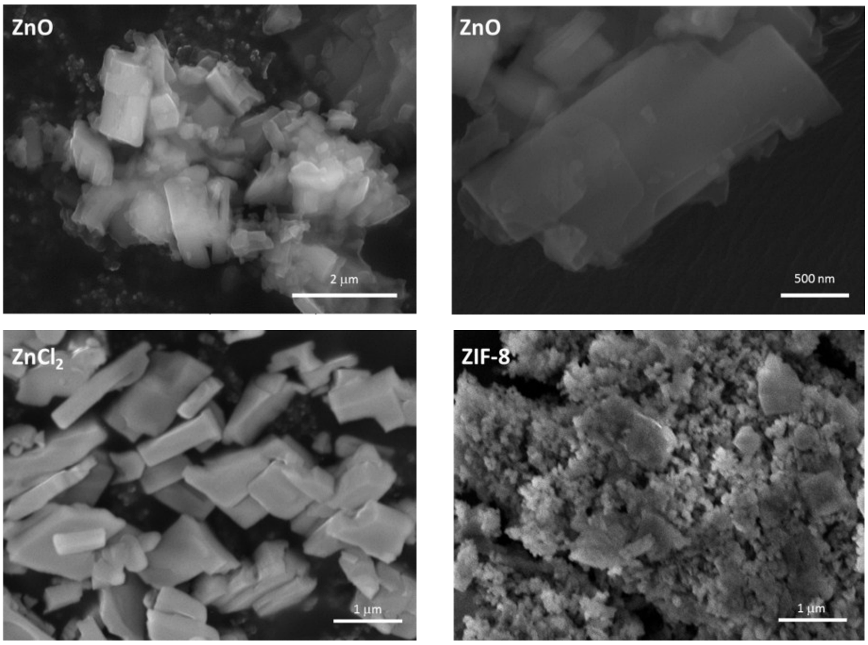

Figure S5. SEM images of RSN-type material crystals prepared from systems containing ZnO, $ZnCl_2$ and ZIF-8 as zinc source.

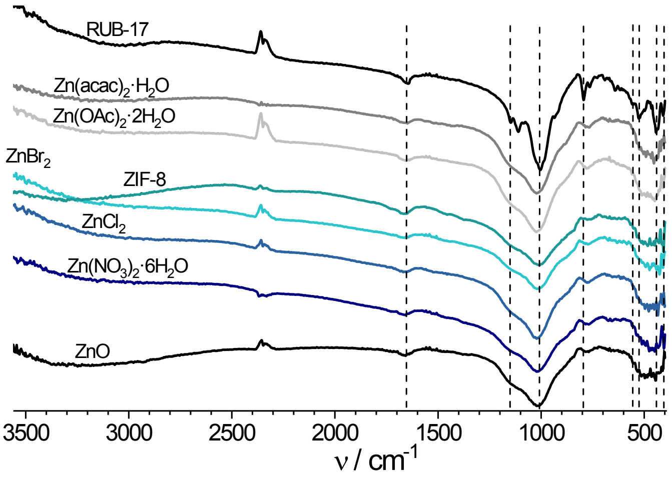

Figure S6. FTIR spectra of the completely crystalline RUB-17 and the precursors taken after 8 h of the hydrothermal treatment at 180 °C of the reaction mixtures with different Zn sources.

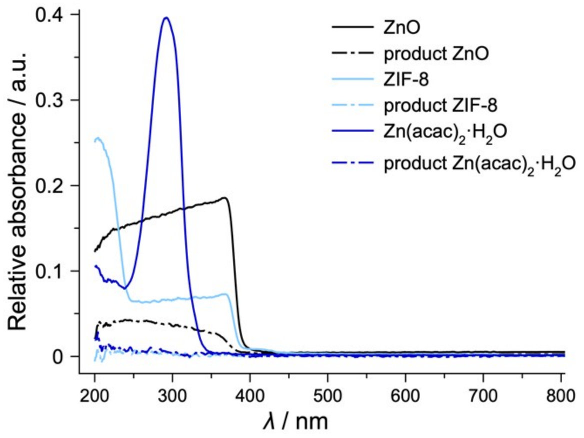

Figure S7. Solid state UV/VIS spectra of the selected initial Zn source chemicals and of the final product material obtained from corresponding Zn sources.

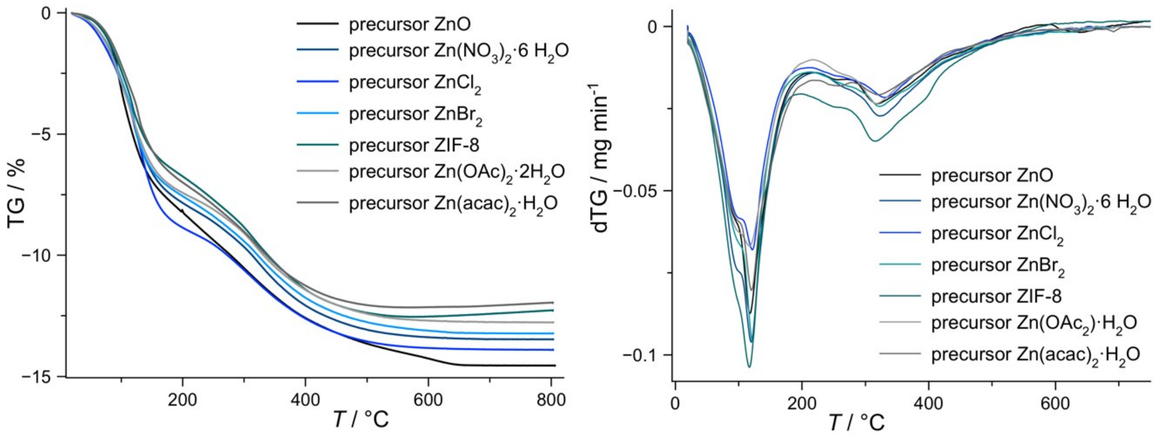

Figure S8. TG (left hand side) and dTG (right hand side) curves of the solid phases of the precursors taken after 8 h of the hydrothermal treatment at 180 °C of the reaction mixtures with different Zn sources.

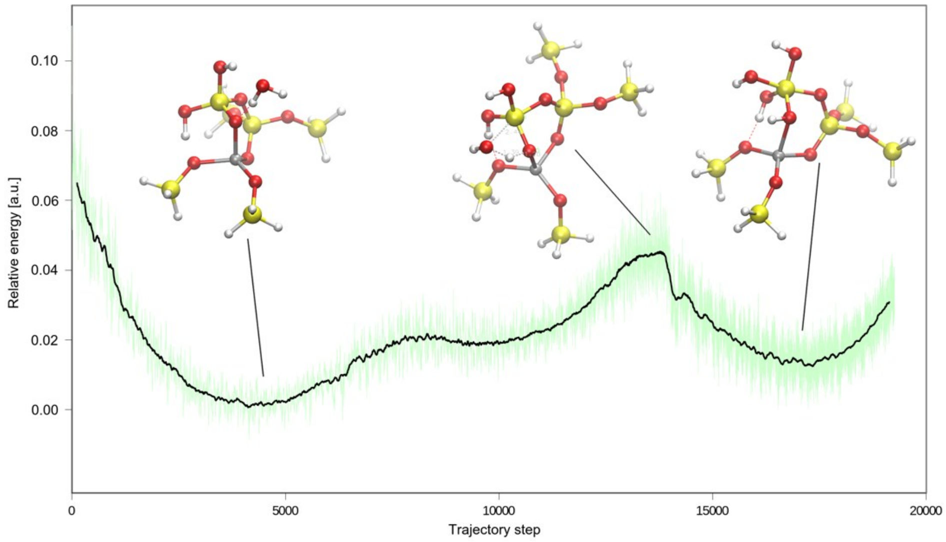

Figure S9. The energy profile of the reaction of the 3-ring formation with the Zn heteroatom in one of the T-sites.

Table S1. Results on the chemical analysis of the final RUB-17 products obtained by hydrothermal treatment at 180 °C of the reaction mixtures with different Zn sources.

Starting chemical	Si/Zn^{XRF} – RUB-17
ZnO	3.63
$Zn(NO_3)_2 \cdot 6H_2O$	3.45
$ZnCl_2$	3.52
$ZnBr_2$	3.30
ZIF-8	3.54
$Zn(OAc)_2 \cdot 2H_2O$	3.39
$Zn(acac)_2 \cdot H_2O$	3.49

Additional references:

1. J. Sherman, *Spectrochim. Acta*, 1955, **7**, 283-306.