

Electronic supplementary information

Luminescent twelve-nuclear rhenium clusters

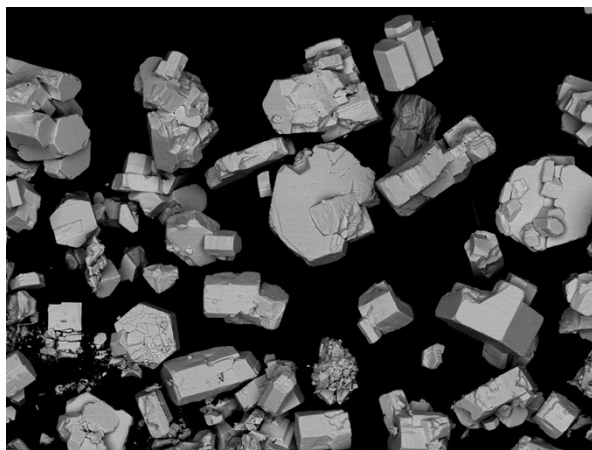
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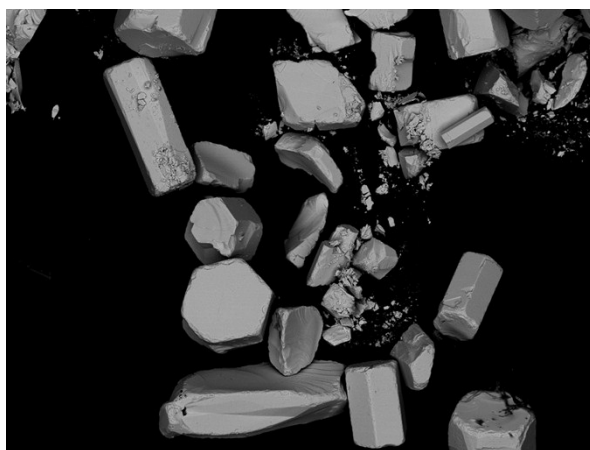
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a)



b)



c)

Figure S1. SEM images of the crystals of compounds **1–3** (*a–c*, respectively).

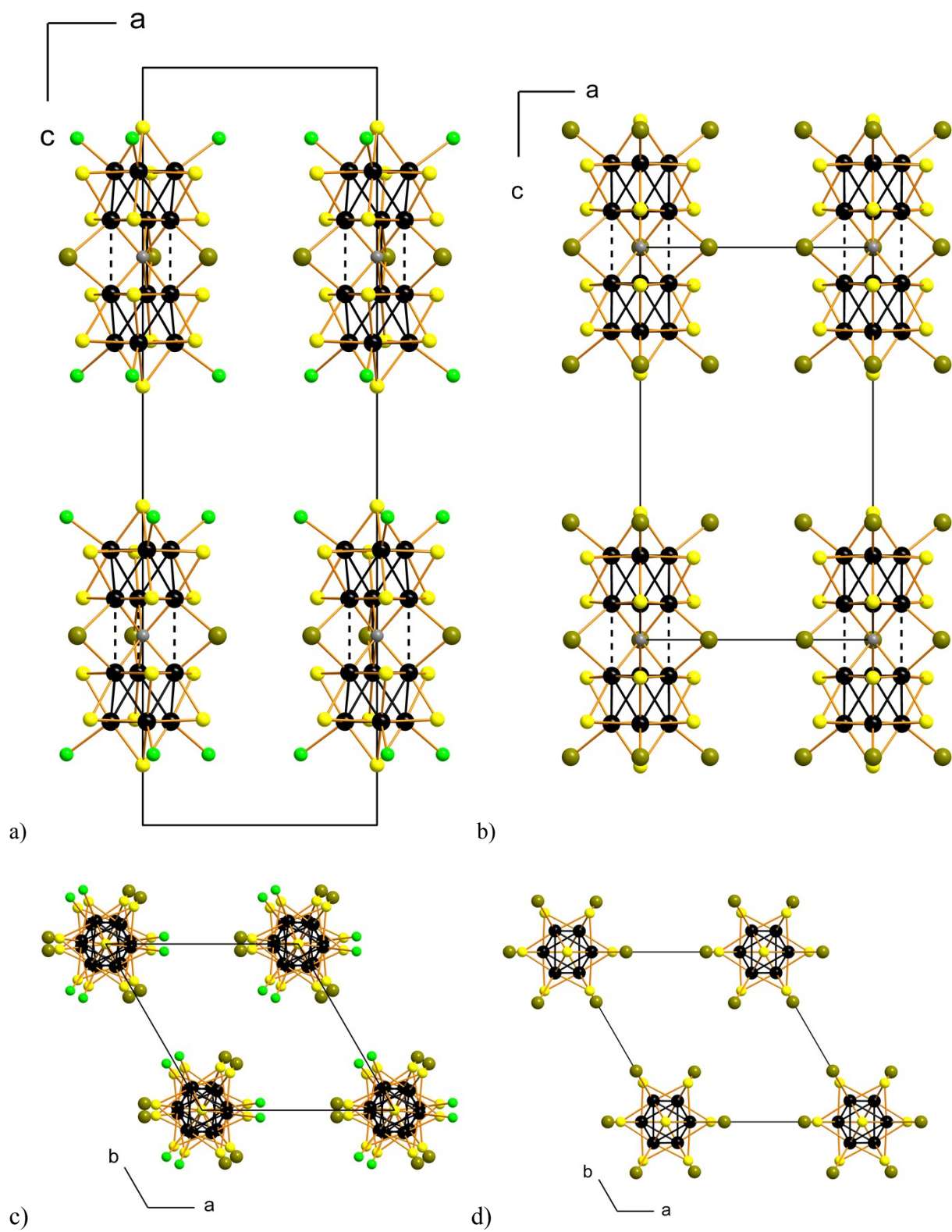


Figure S2. Packing of the cluster anions in the structures of the compounds 2 (a, c) and 3 (b, d).

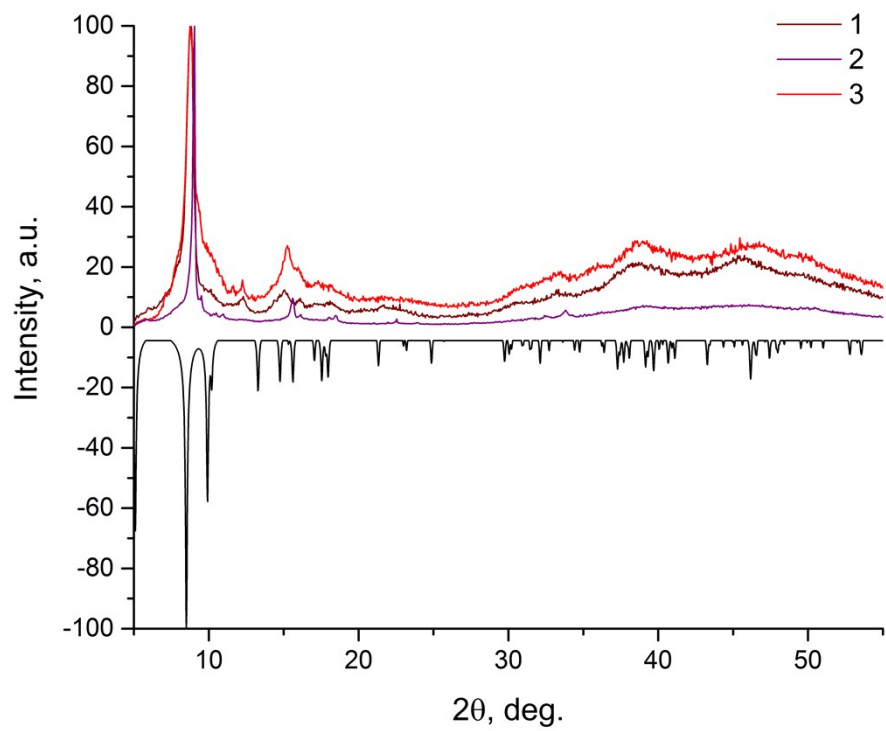
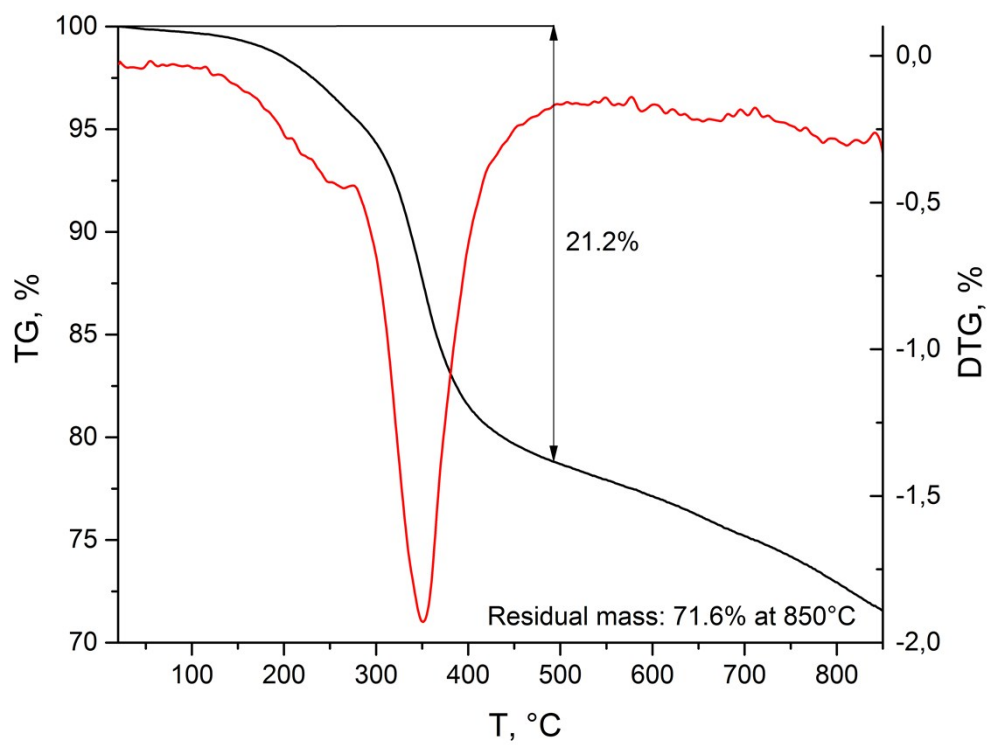


Figure S3. Powder patterns of the samples of compounds **1–3**.



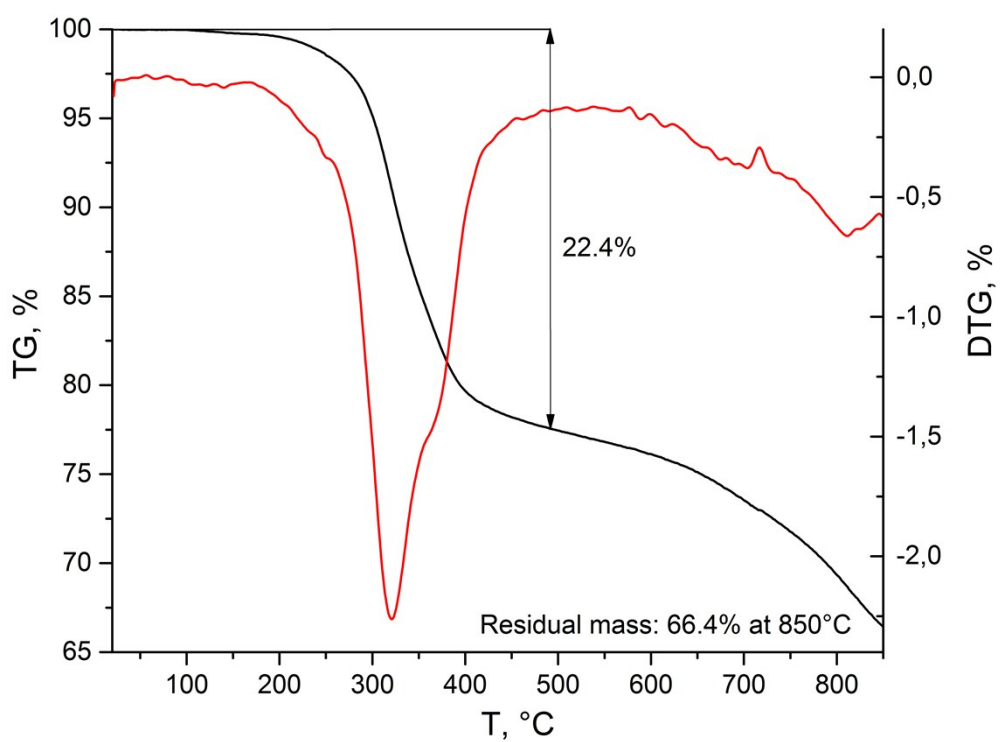
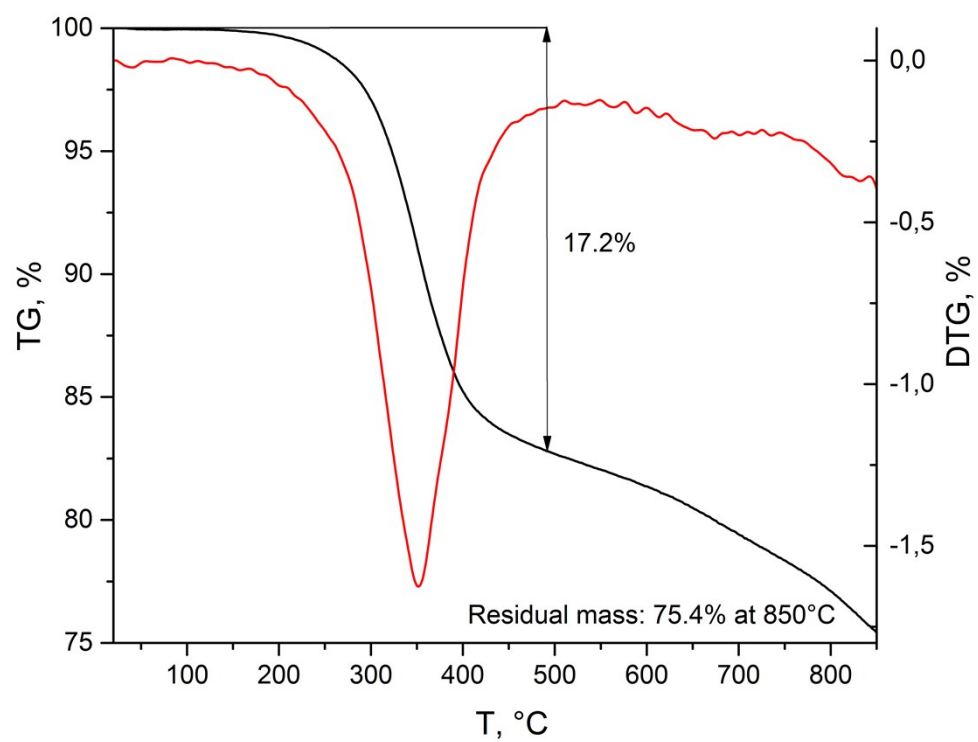


Figure S4. TGA and DTG curves for the samples of compounds **1–3** (a-c, respectively).

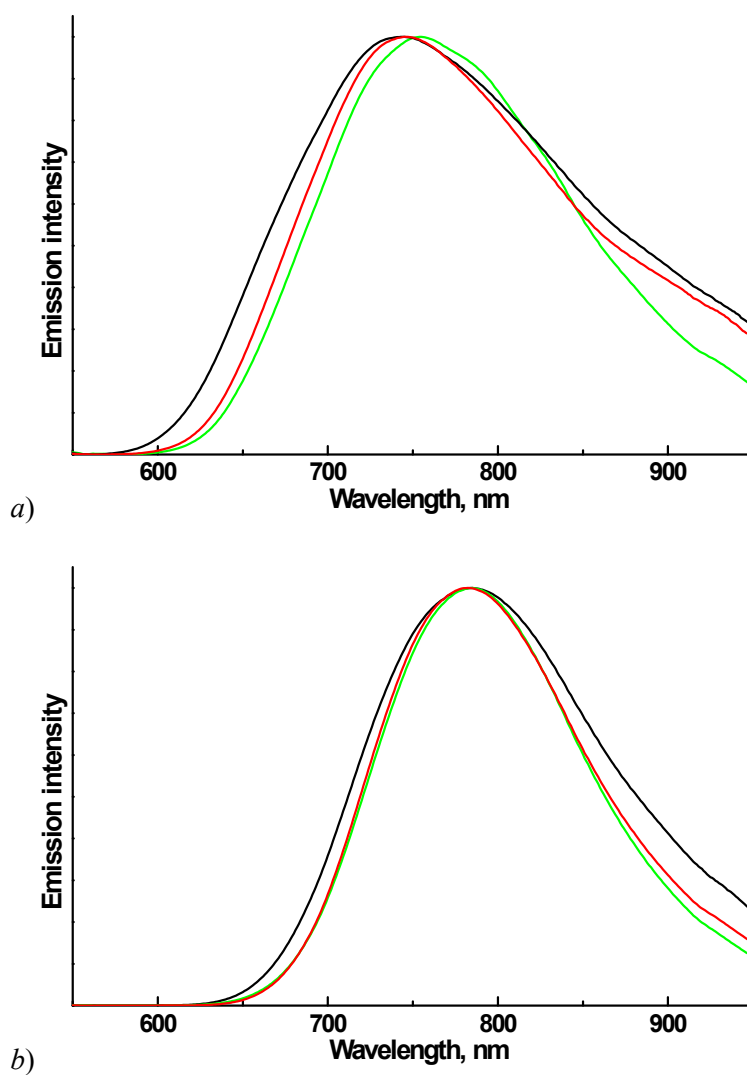


Figure S5. Emission spectra for **1** (black), **2** (red), and **3** (green) in the solid state at 298 K (a) and at 80 K (b). The emission intensities in each figure are normalized to those of the maximum wavelengths.

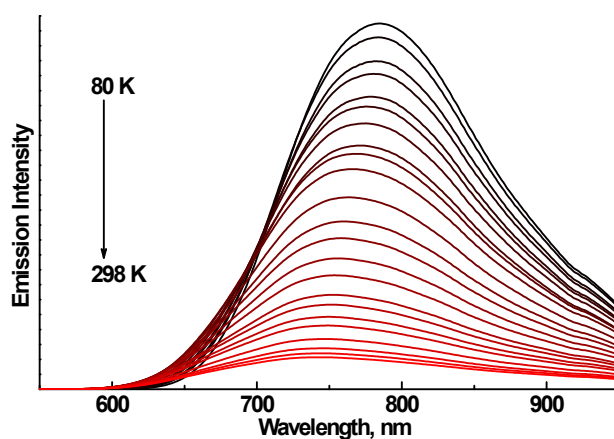


Figure S6. Temperature dependence of the emission spectrum of the solid sample of **1** from 80 to 298 K.

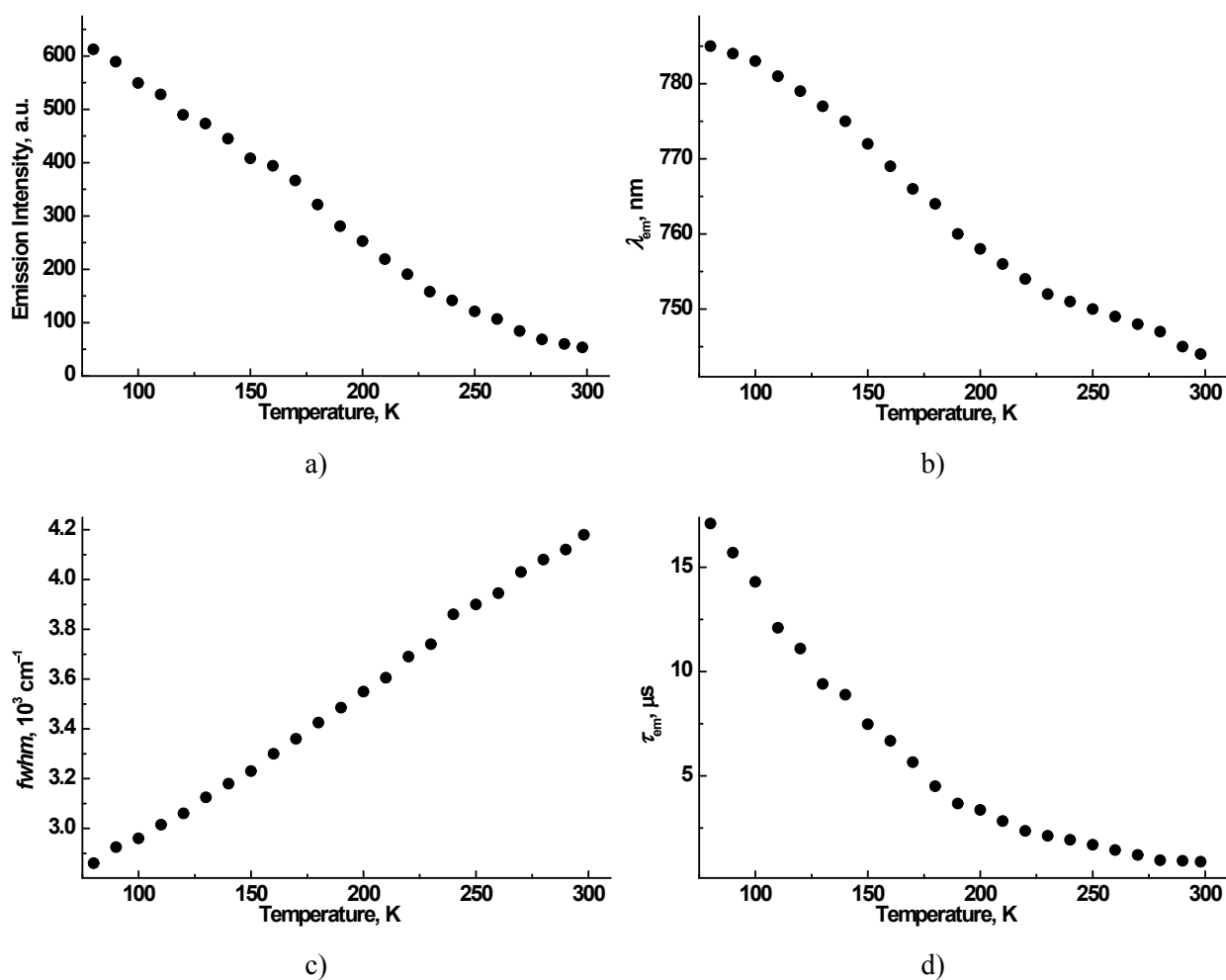


Figure S7. Graphic representation of temperature dependencies of emission intensity (a), emission maximum wavelength (b), fwhm (c) and long-lifetime component (d) of the solid sample of **1** from 80 to 298 K.

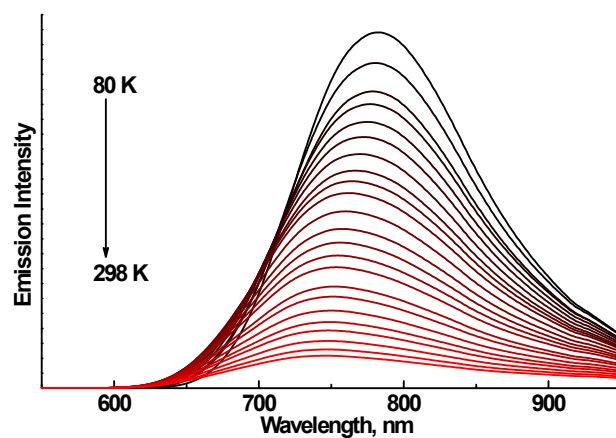


Figure S8. Temperature dependence of the emission spectrum of the solid sample of **2** from 80 to 298 K.

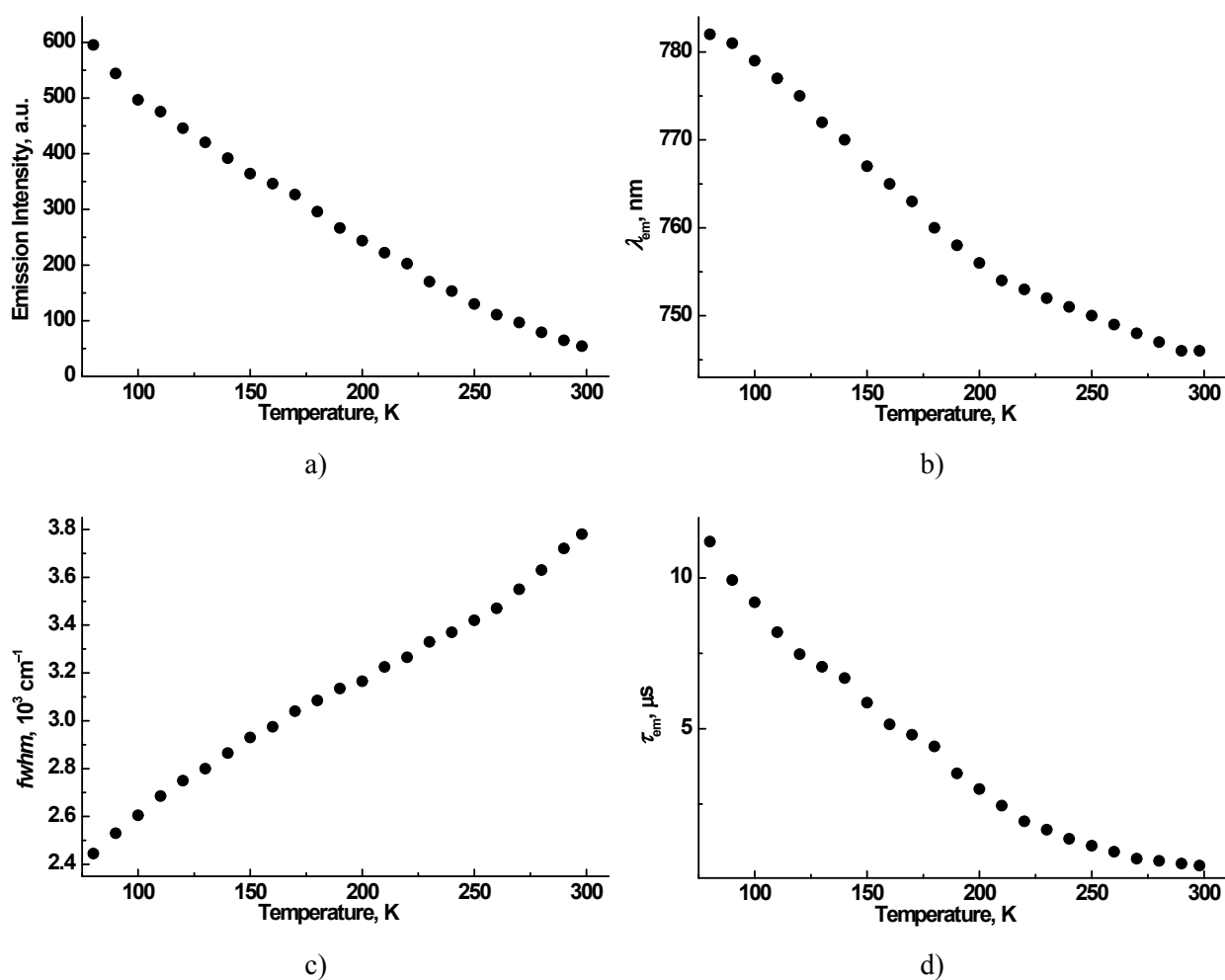


Figure S9. Graphic representation of temperature dependencies of emission intensity (a), emission maximum wavelength (b), fwhm (c) and long-lifetime component (d) of the solid sample of **2** from 80 to 298 K.

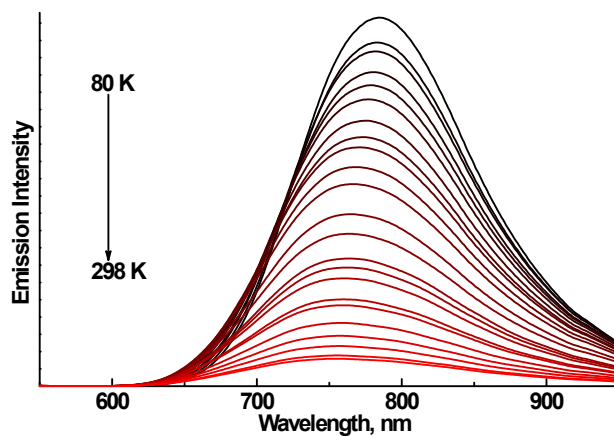


Figure S10. Temperature dependence of the emission spectrum of the solid sample of **3** from 80 to 298 K.

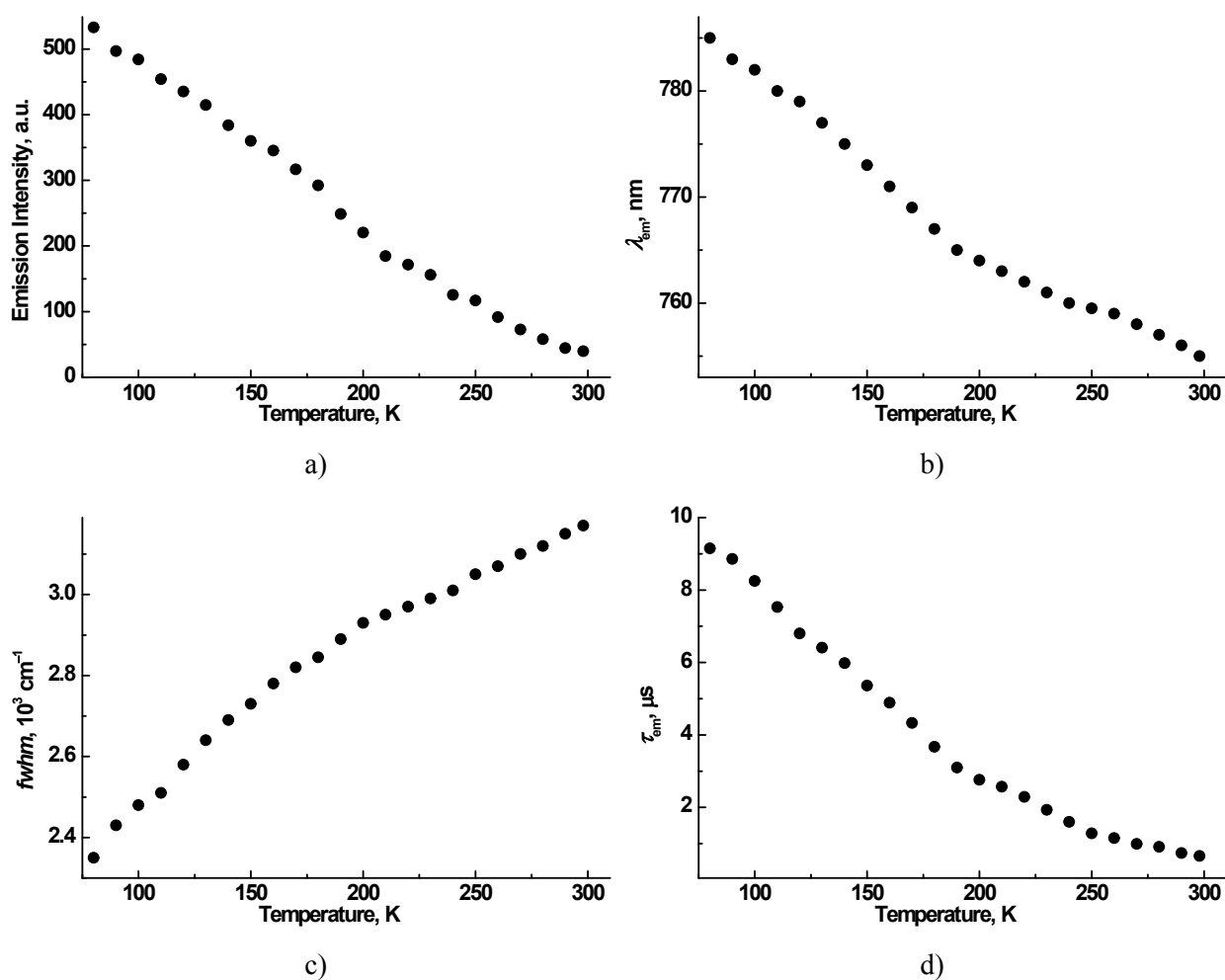


Figure S11. Graphic representation of temperature dependencies of emission intensity (a), emission maximum wavelength (b), fwhm (c) and long-lifetime component (d) of the solid sample of **3** from 80 to 298 K.

Table S1. Energy parameters of the cluster anions at the S12h/TZP//VWN+S12g/TZP level of theory

	$[\text{Re}_{12}\text{CS}_{14}(\mu\text{-Cl})_3\text{Cl}_6]^{5-}$	$[\text{Re}_{12}\text{CS}_{14}(\mu\text{-Br})_3\text{Cl}_6]^{5-}$	$[\text{Re}_{12}\text{CS}_{14}(\mu\text{-Br})_3\text{Br}_6]^{5-}$
$E_{\text{HOMO}} / \text{eV}$	-5.35	-5.19	-5.17
$E_{\text{LUMO}} / \text{eV}$	-1.80	-1.76	-1.76
$\Delta E_{\text{LUMO-HOMO}} / \text{eV}$	3.55	3.43	3.41
$E(\text{S0}) / \text{eV}$	-332.43	-330.58	-326.55
$E(\text{T1}) / \text{eV}$	-330.40	-328.56	-324.55
$E(\text{S0}_{\text{T1}}) / \text{eV}$	-331.84	-329.97	-325.93
$\Delta E(\text{T1-S0}) / \text{eV}$	2.03	2.02	2.00
$\Delta E(\text{T1-S0}) / \text{nm}$	611	614	620
$\Delta E(\text{T1-S0}_{\text{T1}}) / \text{eV}$	1.44	1.41	1.39
$\Delta E(\text{T1-S0}_{\text{T1}}) / \text{nm}$	861	879	892