Supplementary Material

Spin crossover and liquid crystal properties in 2D cyanide-bridged Fe^{II}–$M^{I/II}$ metalorganic frameworks

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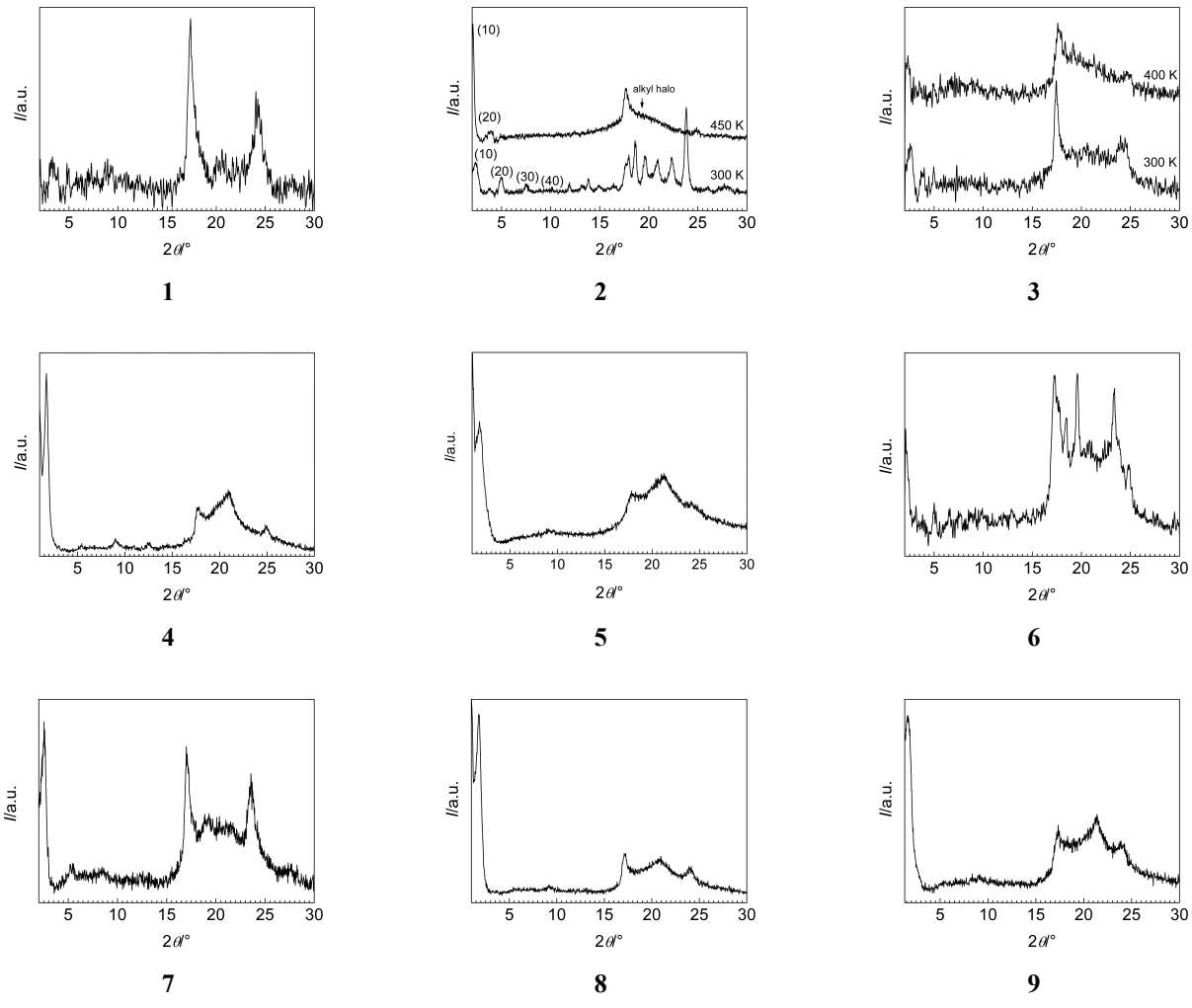
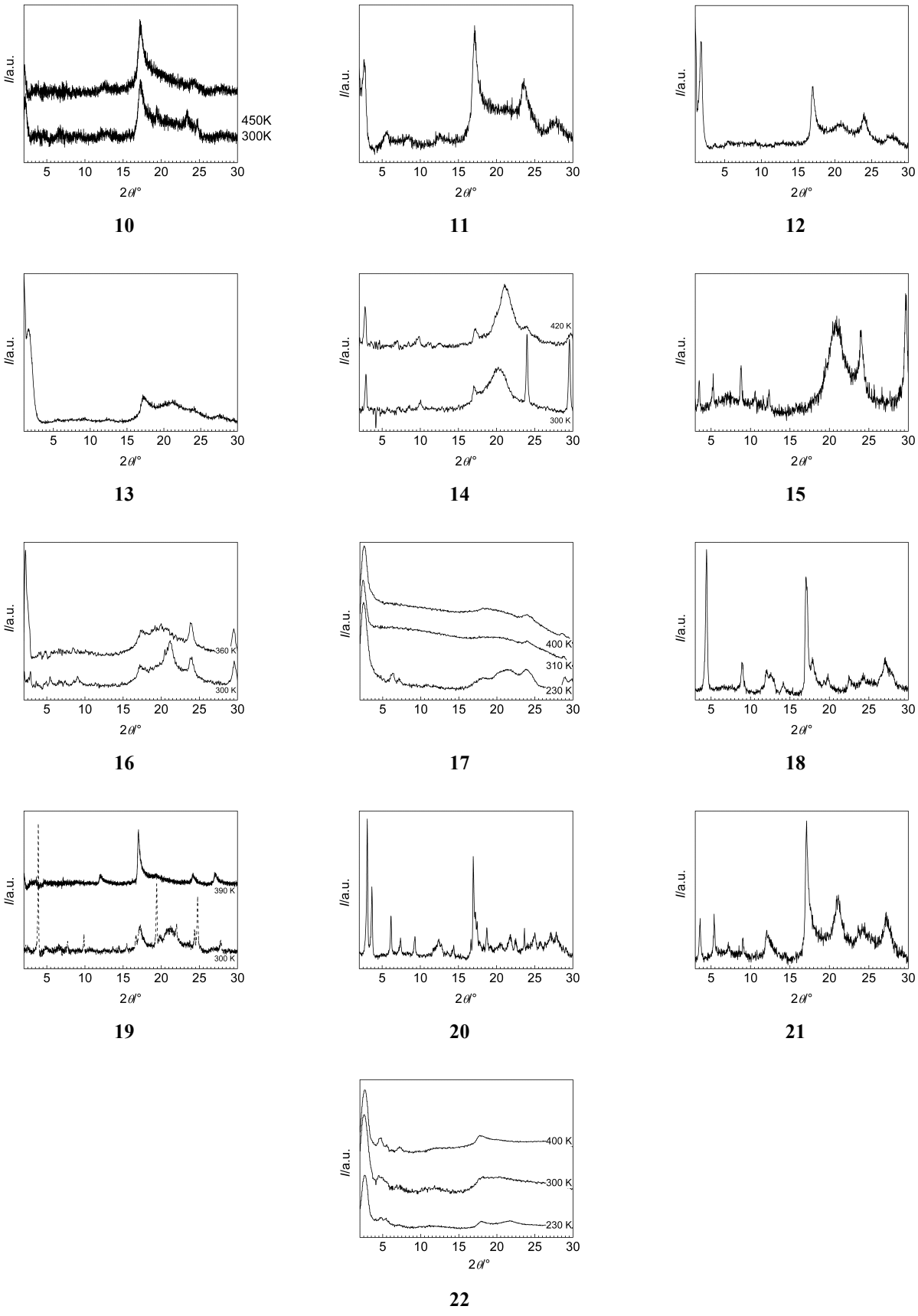
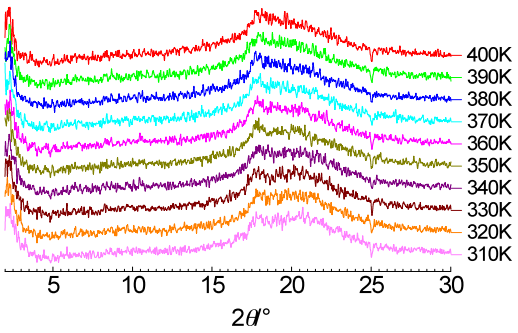
SFigure 1. XRPD patterns of **1–22** at shown temperatures.



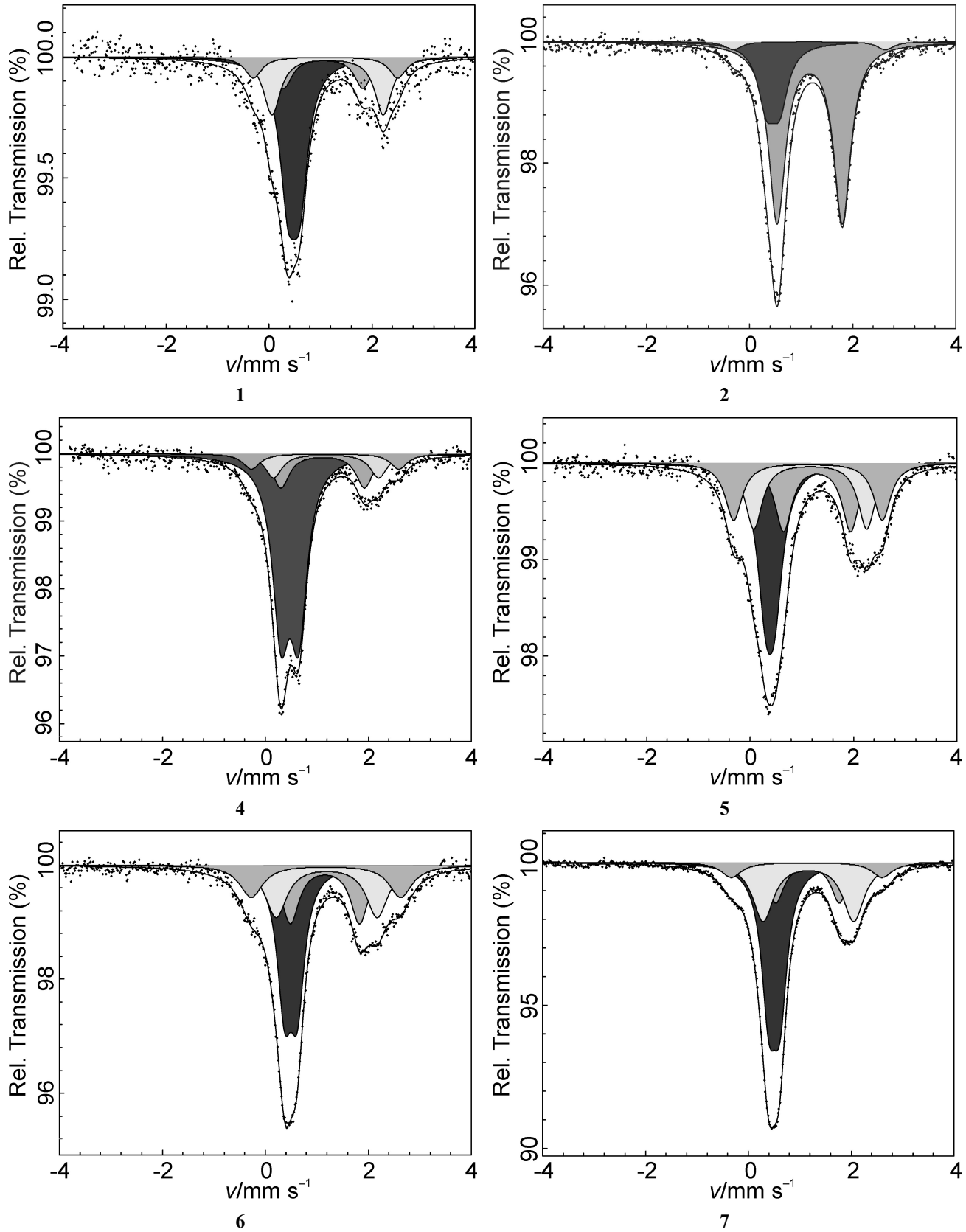


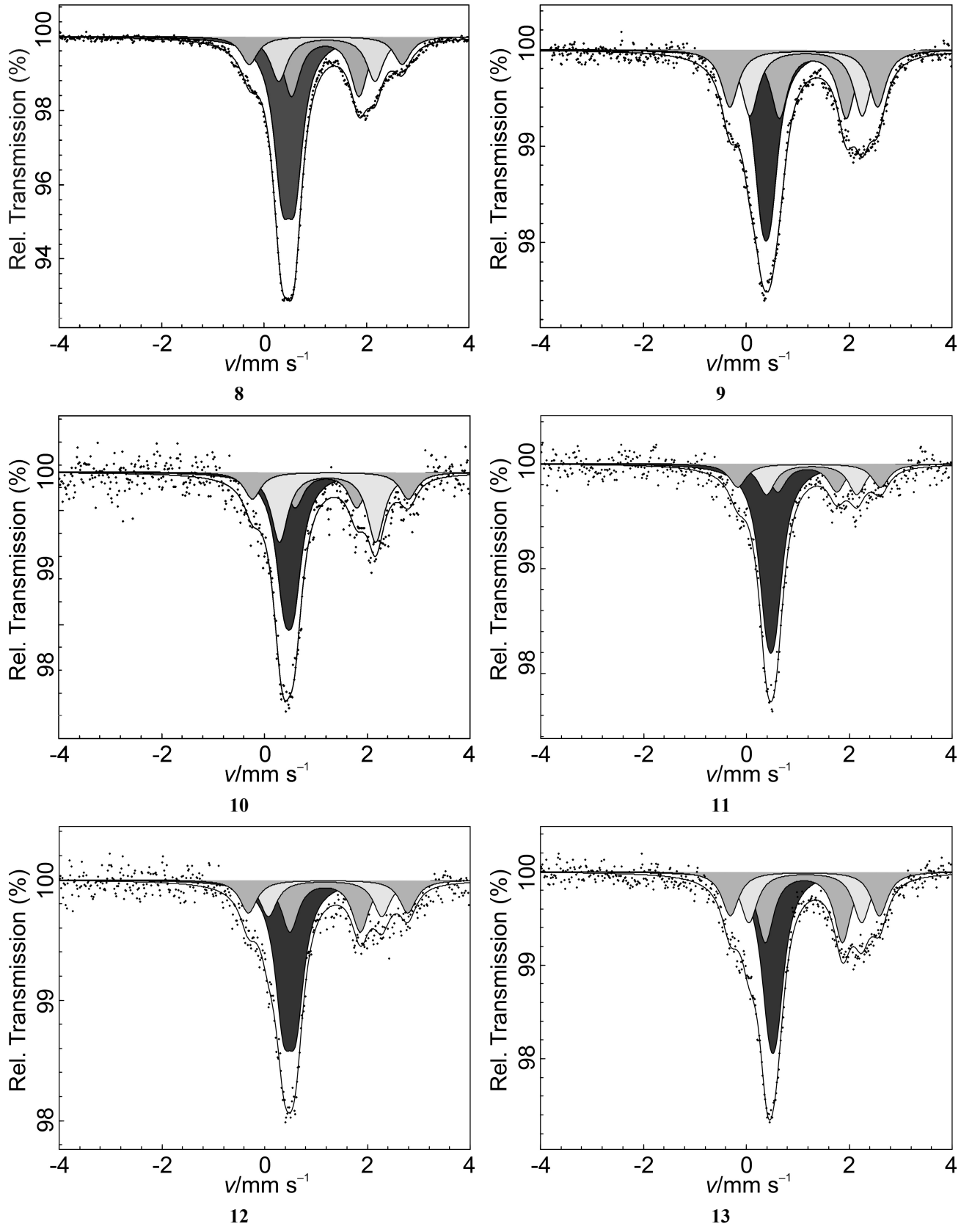
SFigure 1 ***continuation*****.** XRPD patterns of **1–22** at shown temperatures.

SFigure 2. Variation of the XRPD patterns of **5** with temperature.



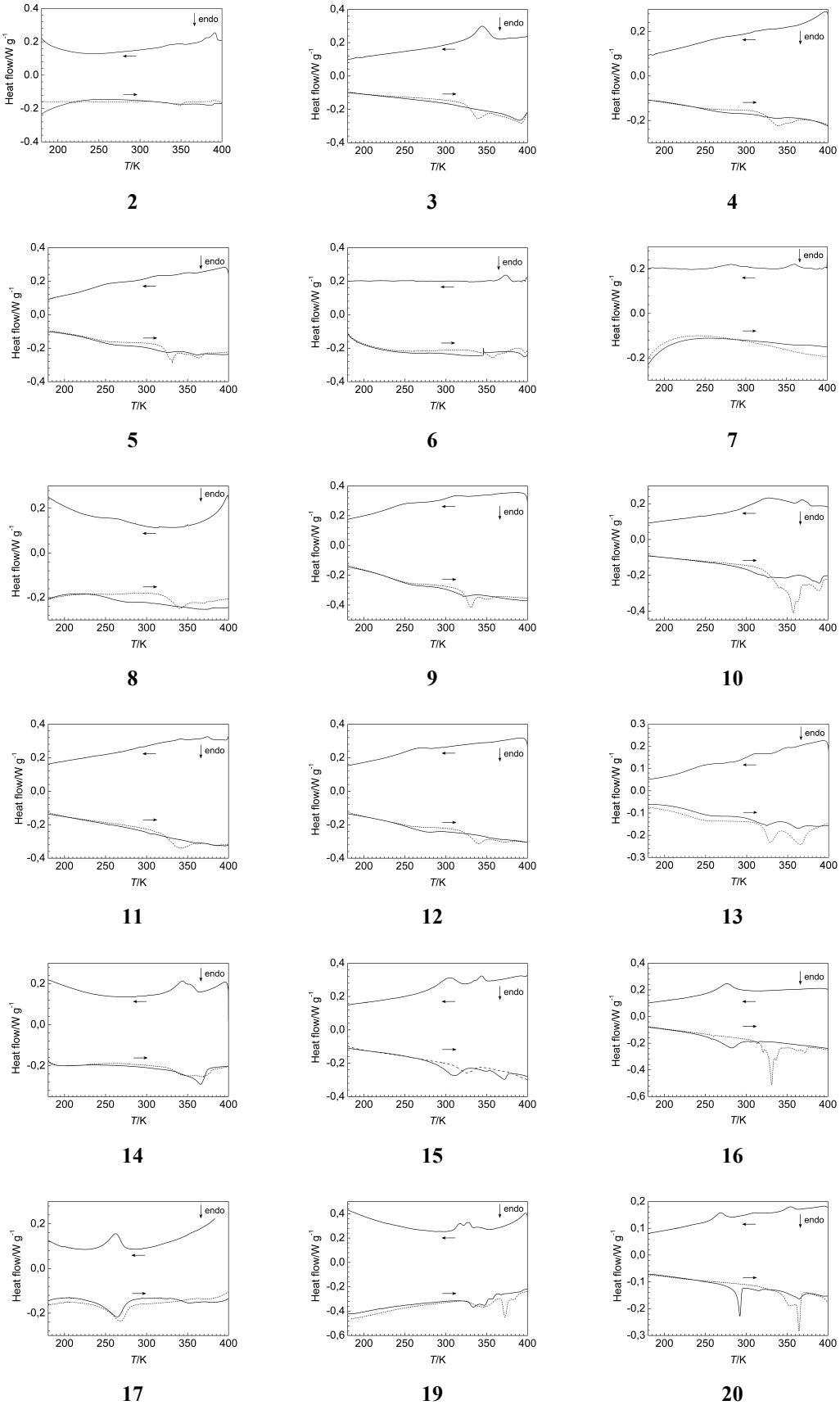
SFigure 3. ^{57}Fe Mössbauer spectrum of **1**-**13** at 80 K.

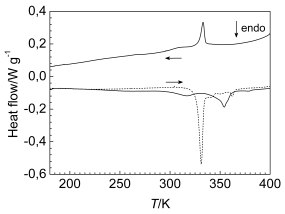




SFigure 3 ***continuation.*** ^{57}Fe Mössbauer spectrum of **1**-**13** at 80 K.

SFigure 4. Differential scanning calorimetry curves for **2-17**, **19–22**. The first run corresponds to the dashed line. The run directions are shown by arrows.





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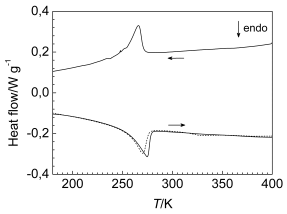

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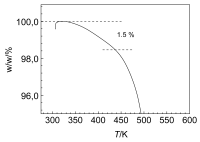
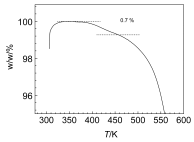
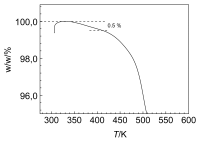
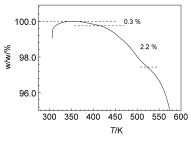
SFigure 4 ***continuation*****.** Differential scanning calorimetry curves for **2-17, 19-22**. The first run corresponds to the dashed line. The run directions are shown by arrows.

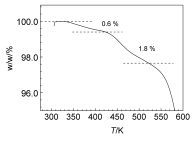
SFigure 5. TGA analysis for **1**-**22**. In parenthesis the temperature is shown at which the dehydration process is centered



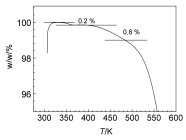


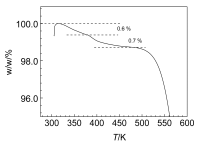


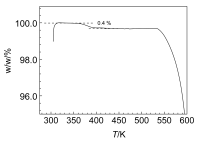


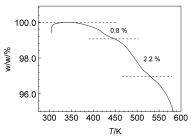


	1	**2**	**3**	**4**	**5**
%	1.5 (390 K)	0	0.5 (390 K)	0.3 (410 K)	0.6 (390 K)
	0	1.3 (420 K)	0	2.2 (470 K)	1.8 (470 K)
	0.6	0	0.3	0.2	0.5
	0	0.8	0	1.5	1.7
total	0.6	0.8	0.3	1.7	2.2
rounded *n*	**1**	**1**	**0.5**	**2**	**2**

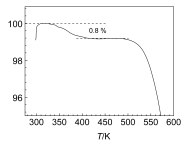


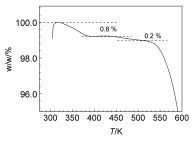


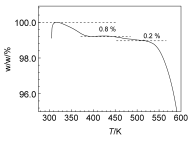


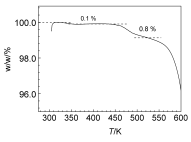


	6	**7**	**8**	**9**
%	0.2 (360 K),	0.6 (345 K)	0.4 (390 K)	0.8 (410 K)
	1.8 (470 K)	0.7 (420 K)	0	2.2 (480 K)
	0.1	0.7	0.3	0.8
	1.1	0	0	1.9
total	1.2	0.7	0.3	2.7
rounded *n*	**1**	**1**	**0.5**	**3**

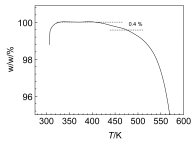
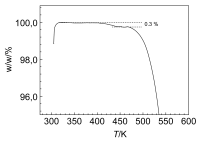
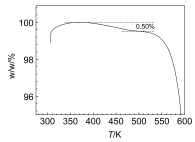
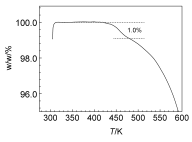


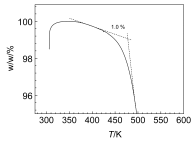
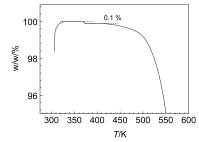
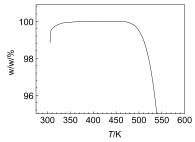
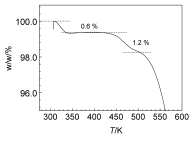
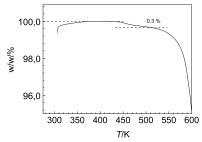






	10	**11**	**12**	**13**
%	0.8 (370 K)	0.9 (360 K)	0.8 (360 K)	0.1 (360 K)
	0	0.6 (460 K)	0.4 (470 K)	1.5 (470 K)
	0.5	0.5	0.6	0.1
	0	0.3	0.3	1.5
total	0.5	0.8	0.9	1.6
rounded *n*	**1**	**1**	**1**	**2**

					
	14	**15**	**16**	**17**	
%	0	0	0	0	
	0.4 (440 K)	0.3 (440 K)	0.5 (440 K)	1.0 (470 K)	
$n$$H_2O$	0	0	0	0	
	0.4	0.3	0.7	1.4	
total	0.4	0.3	0.7	1.4	
rounded n	**0.5**	**0.5**	**1**	**2**	

					
	18	**19**	**20**	**21**	**22**
%	0	0.1 (370 K)	0	0.6 (320 K)	0
	1.0 (420 K)	0	0	1.2 (470 K)	0.3 (460 K)
$n$$H_2O$	0	0.1	0	0.7	0
	0.8	0	0	1.3	0.5
total	0.8	0.1	0	2.0	0.5
rounded n	**1**	**0.5**	**0**	**2**	**0.5**

STable 1. Enthalpy of the Cr↔S_x transition estimated from the DSC data.

Compound	**Δ*H*/kJ mol^{-1}**	***T*/K**	**Compound**	**Δ*H*/kJ mol^{-1}**	***T*/K**
2	10.0	380	**12**	7.0	270
3	16.0	360	**13**	7.1	315
4	3.3	335		7.0	255
5	8.2	254	**14**	1.8	354
	3.2	312	**15**	3.2	343
	1.2	350		8.9	303
6	5.6	380	**16**	5.8	280
7	5.2	267	**17**	23.3	265
	4.6	365	**19**	3.6 m	330
8	1.1	264	**20**	3.9	294
9	1.0	254		1.2	310
	3.3	315		6.3	360
	5.7	355	**21**	2.3	313
10	43.1 m	330		14.9	353
	10	370	**22**	50.9	270
11	1.0	340			
	0.7	365			