Exploring the effects of Synthetic and Post-Synthetic Grinding on the properties of Spin Crossover Materials

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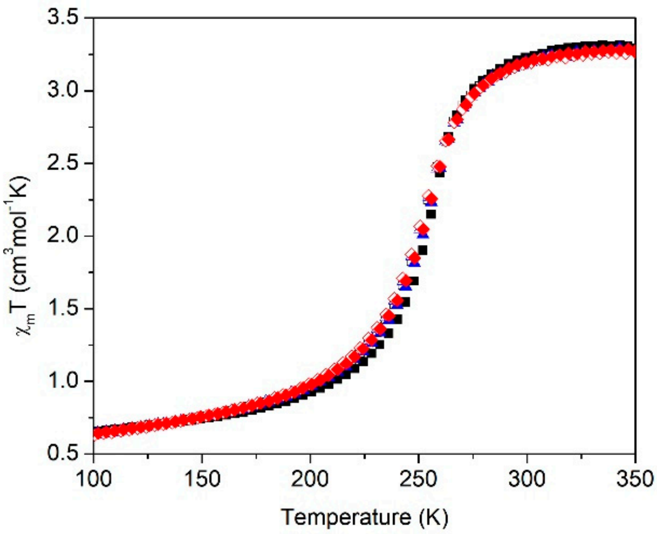

Figure S1: Plots of $\chi_M T$ vs T for compound **1-Sol** three cycles. First cycle: heating , cooling . Second cycle: heating , cooling . Third cycle: heating ▲ and cooling △.

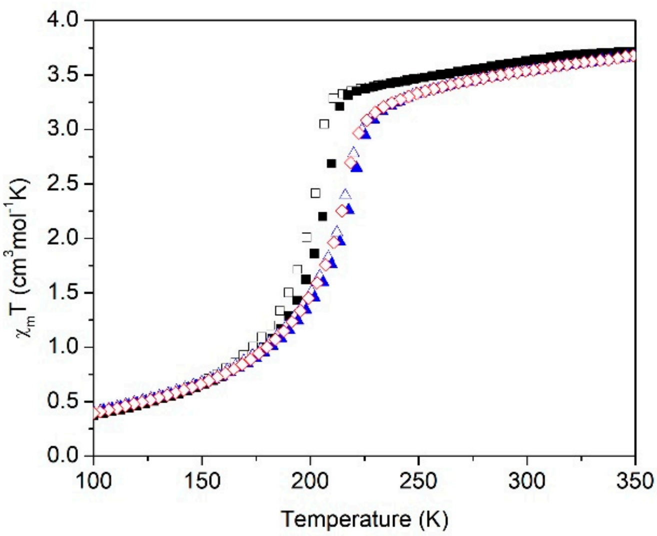

Figure S2: Plots of $\chi_M T$ vs T for compound **1-Mech** three cycles. First cycle: heating , cooling . Second cycle: heating , cooling . Third cycle: cooling △.

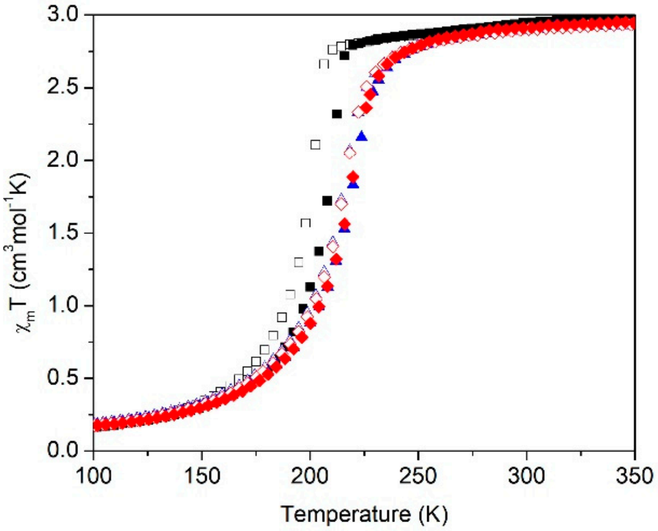

Figure S3: Plots of $\chi_M T$ vs T for compound **1-BM10** three cycles. First cycle: heating , cooling . Second cycle: heating , cooling . Third cycle: heating ▲ and cooling △.

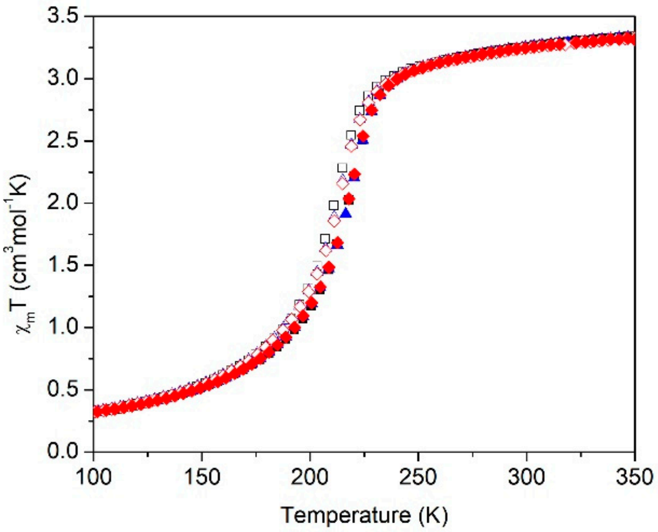

Figure S4: Plots of $\chi_M T$ vs T for compound **1-BM90** three cycles. First cycle: heating , cooling . Second cycle: heating , cooling . Third cycle: heating ▲ and cooling △.

Table S1: Coordination spheres, interionic distances (R), variance of the absorber-scatterer distances (σ^2), energy shift (E_f) and quality of fit (R-fit) of the EXAFS data for (**1-Sol**, **1-Mech**, **1-BM10** and **1-BM90**).

Sample	Neighbour	N	R / Å	σ^2 x10^3 / Å^2	E_f / eV	AFAC	R-fit
1-Sol	N	6	2.19(1)	7.4(11)	8.3(6)	0.88(8)	0.0135
	C	6	3.17(1)	7.7(28)			
	N	6	3.18(1)	10.8(28)			
	Fe	2	3.90(5)	25.6(146)			
1-Mech	N	6	2.20(1)	6.4(12)	8.1(7)	0.85(9)	0.0189
	C	6	3.16(1)	7.9(40)			
	N	6	3.17(1)	10.1(31)			
	Fe	2	3.89(6)	17.4(85)			
1-BM10	N	6	2.20(1)	6.5(12)	8.4(6)	0.81(8)	0.0178
	C	6	3.17(1)	7.5(35)			
	N	6	3.18(1)	10.2(29)			
	Fe	2	3.91(6)	16.6(75)			
1-BM90	N	6	2.20(1)	6.2(12)	8.3(7)	0.80(8)	0.0176
	C	6	3.16(1)	7.7(39)			
	N	6	3.18(1)	9.6(29)			
	Fe	2	3.89(6)	16.4(75)			

The fitting artefact identified in the main text is due to the different K-weighting used in fitting EXAFS data. Different K-weightings are used in data fitting in order to assist in distinguishing different atom types. However, fitting parameters have different k-dependences. As a result, fitting is done with attempts to minimise the differences in raw data and fit for all stated K-weightings. The peak of interest at 3.5 Å exhibits a different peak structure for each of the three K weightings. As the K-weight is increased, part of the peak increases in intensity which indicates the shell the peak represents may include atoms with larger atomic number, such as the Fe-Fe shell. Due to part of the peak decreasing with increase K-weight, it is likely the peak represents at least two shells; where the second shell corresponds to atoms with smaller atomic number, such as the Fe-C shell. Although the K^3-weighted plot could be visually improved by modifying the fitting parameters, this decreases the accuracy of the overall fit. The artefact is visible due to standard practice in the field being to represent the data using the K^3 weighted pseudo-RDF plot.

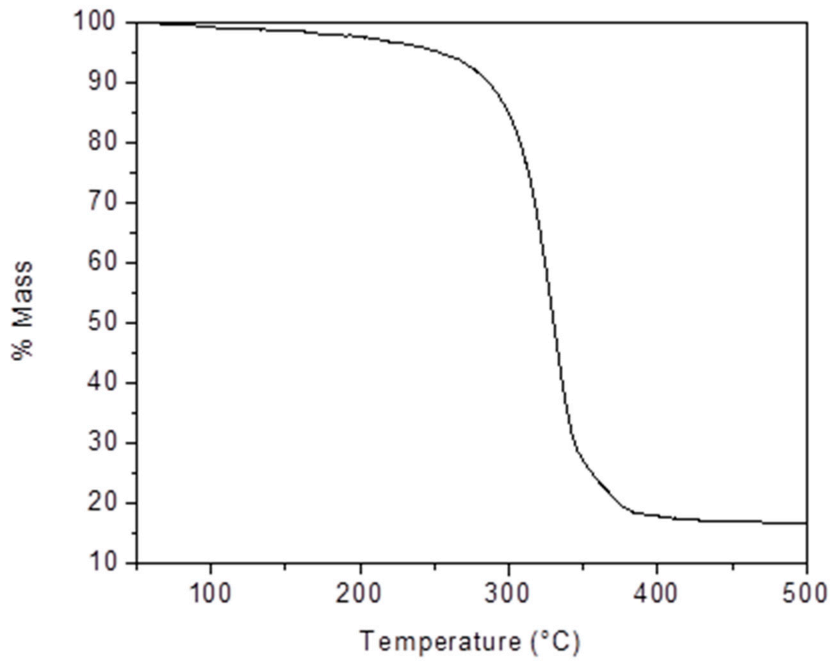

Figure S5: TGA plot of % mass vs temperature for **1-Sol**. Collected between 50-500 °C with a heating rate of 10 K/min.

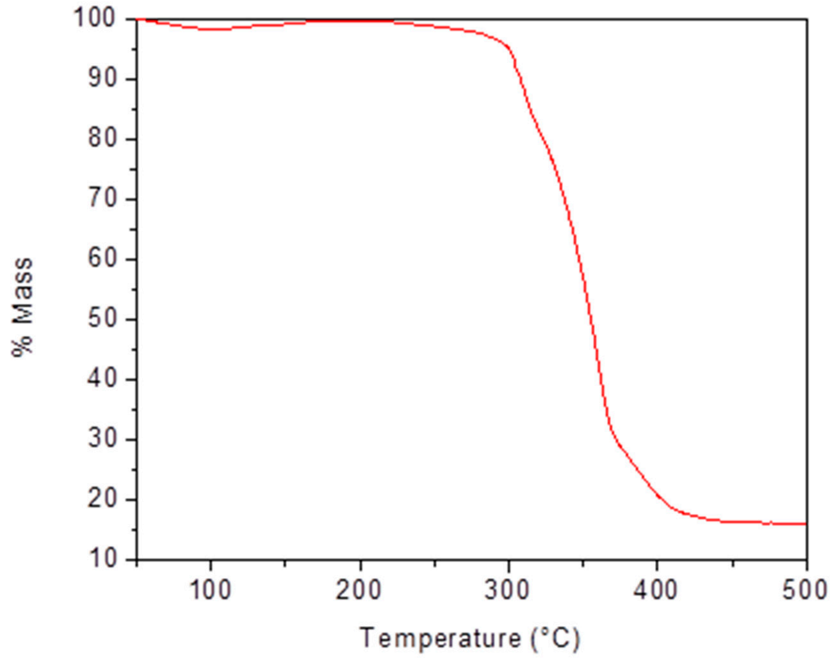

Figure S6: TGA plot of % mass vs temperature for **1-BM10**. Collected between 50-500 °C with a heating rate of 10 K/min.

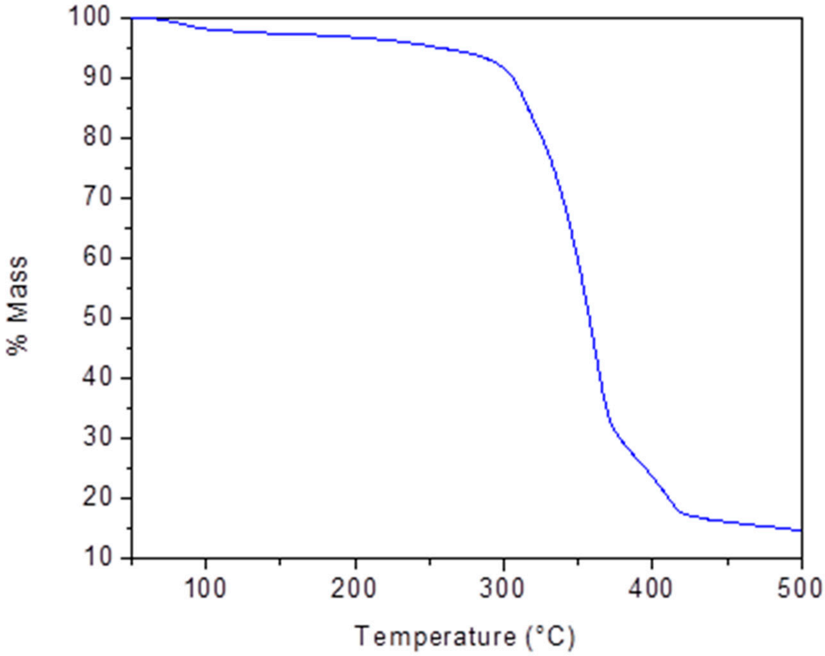

Figure S7: TGA plot of % mass vs temperature for **1-BM90**. Collected between 50-500 °C with a heating rate of 10 K/min.

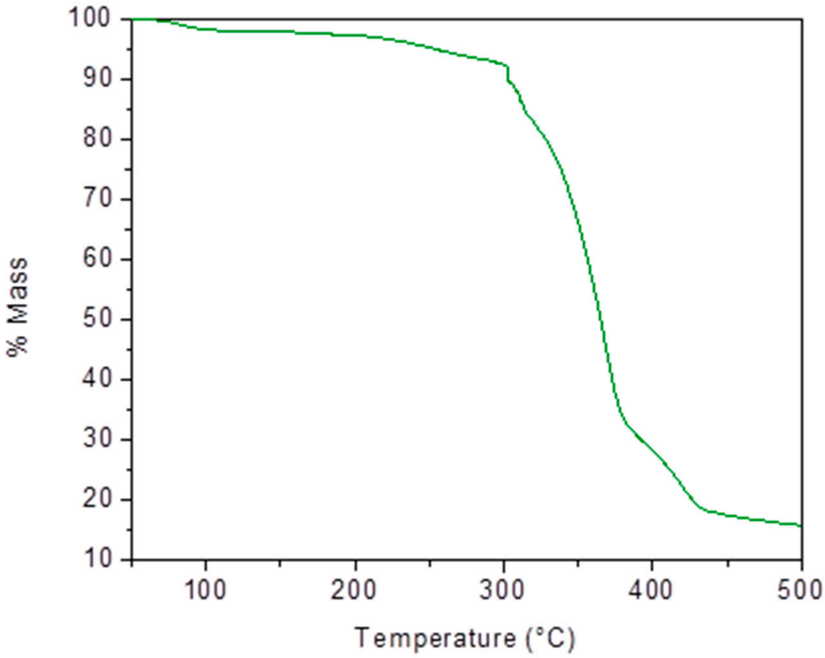

Figure S8: TGA plot of % mass vs temperature for **1-Mech**. Collected between 50-500 °C with a heating rate of 10 K/min.

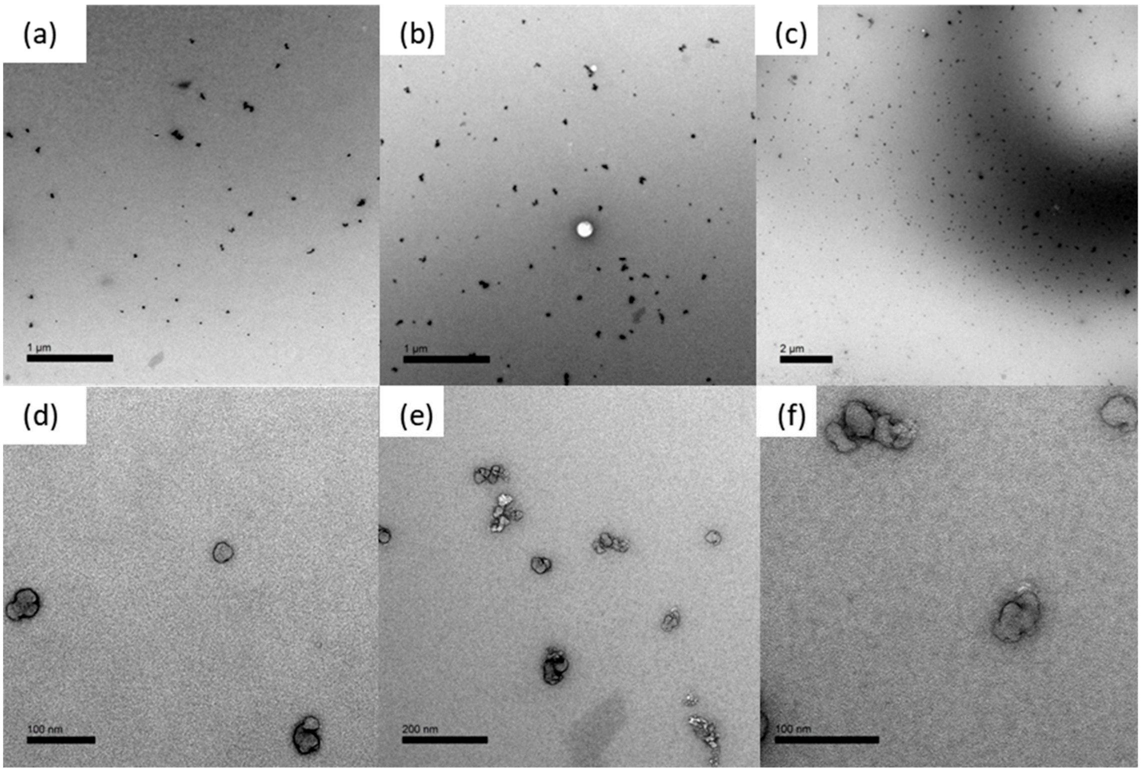

Figure S9: Additional TEM images for **1-Sol**.

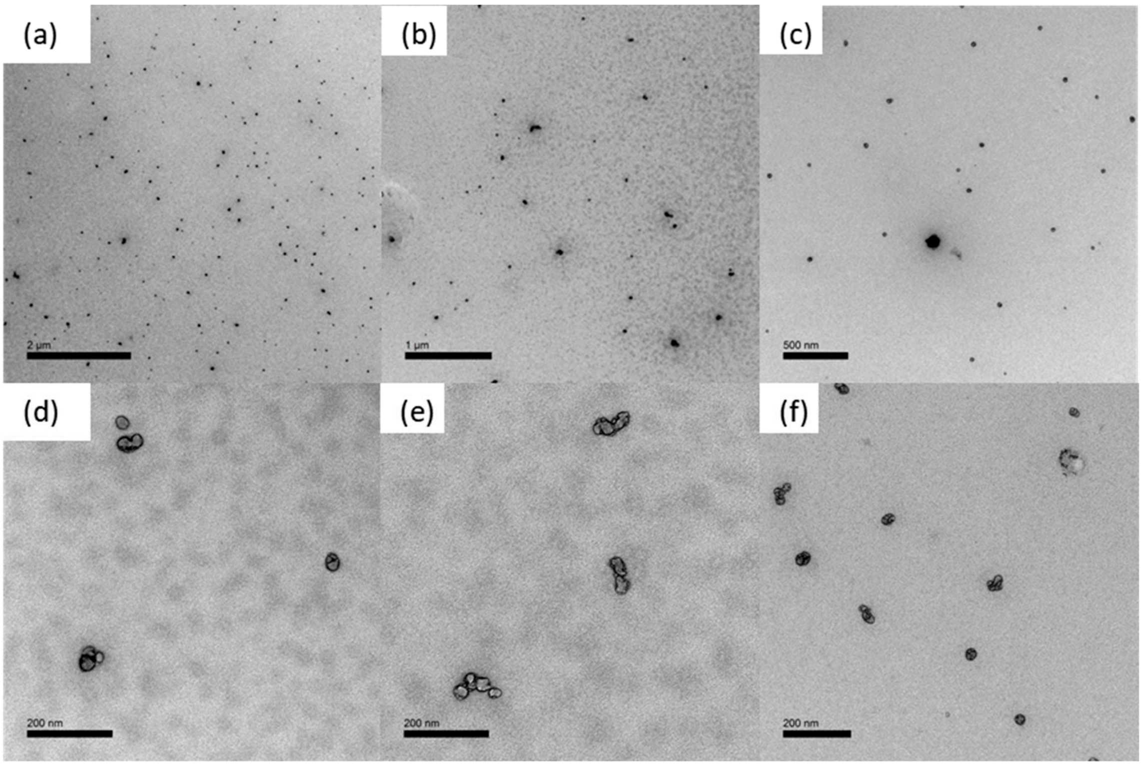

Figure S10: Additional TEM images for **1-Mech**.

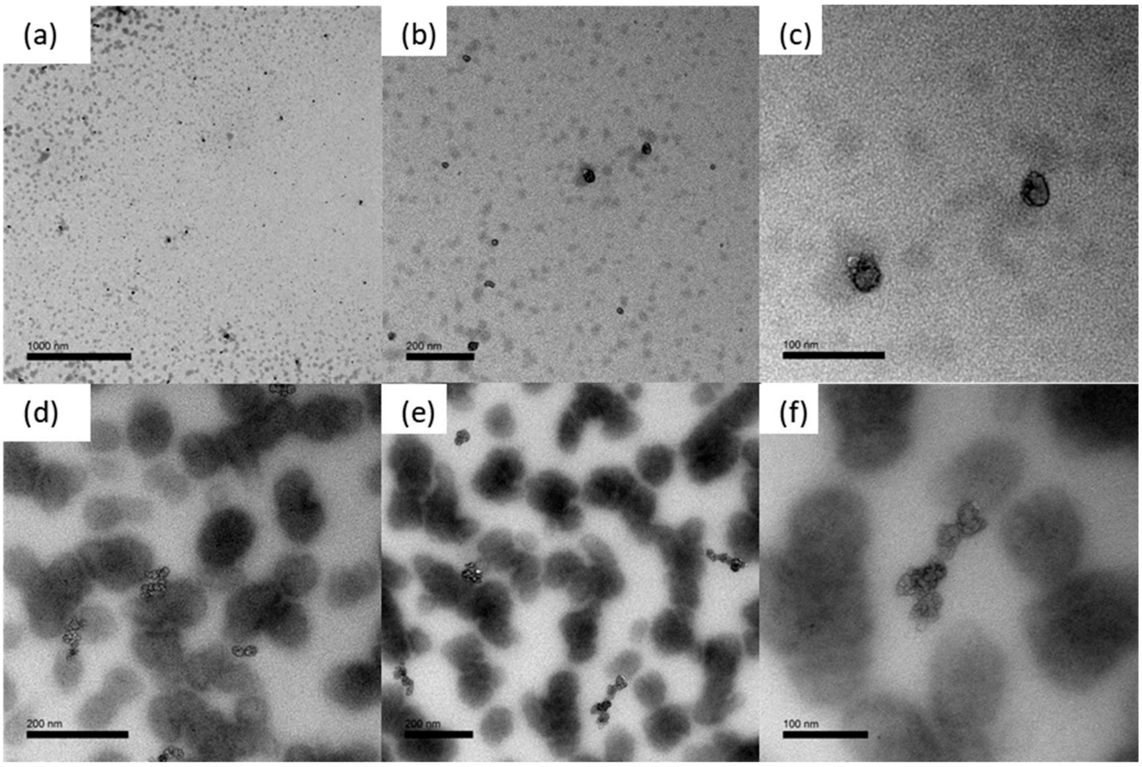

Figure S11: Additional TEM images for **1-BM10**.

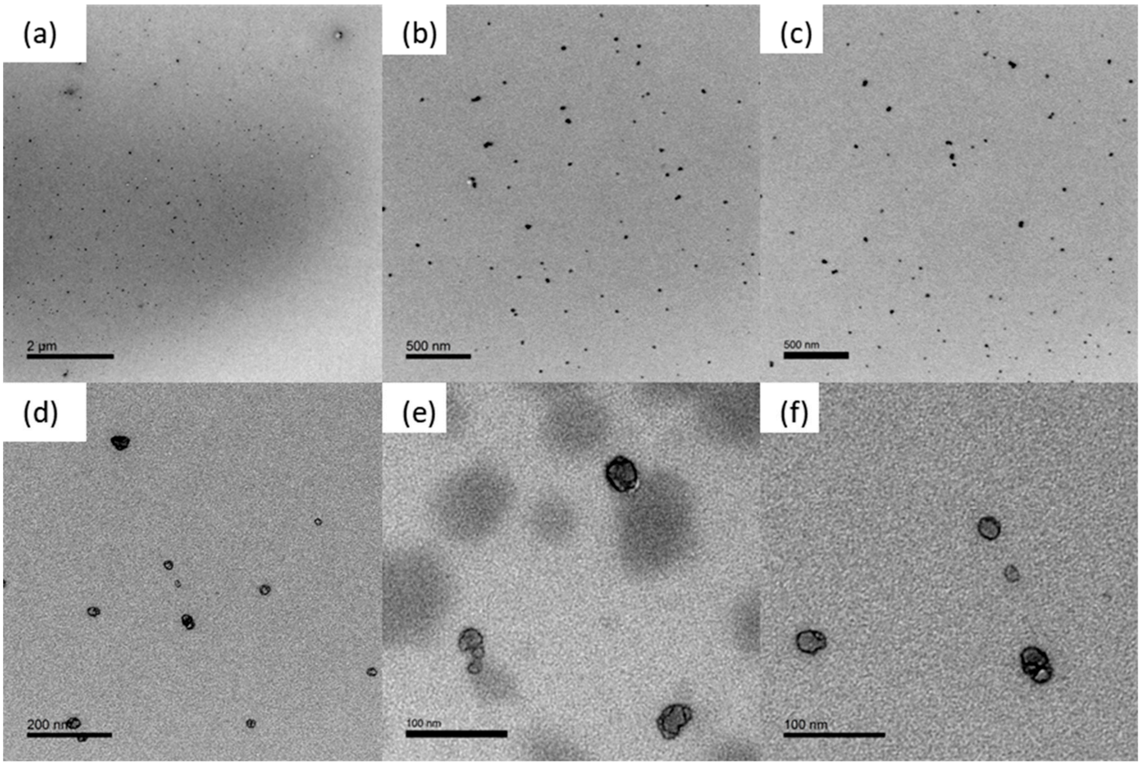

Figure S12: Additional TEM images for **1-BM90.**

Post Synthetic Grinding

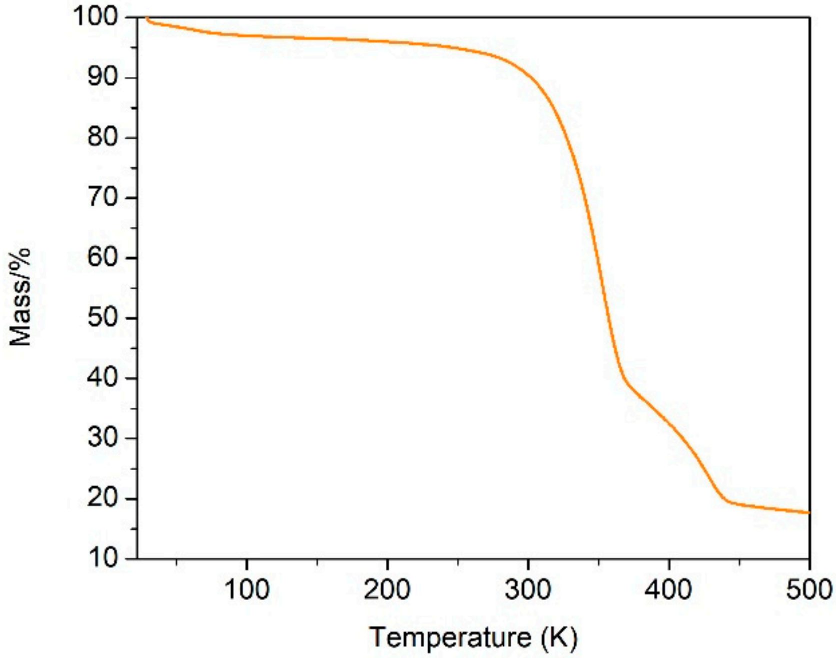

Figure S13: TGA plot of % mass vs temperature for **1-Sol-10**. Collected between 50-500 °C with a heating rate of 10 K/min.

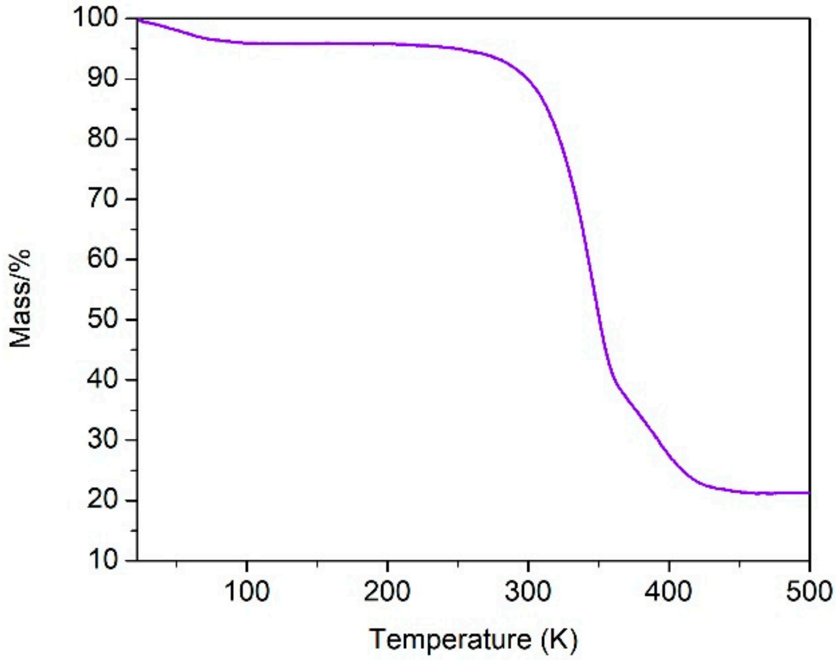

Figure S14: TGA plot of % mass vs temperature for **1-Sol-30**. Collected between 50-500 °C with a heating rate of 10 K/min.