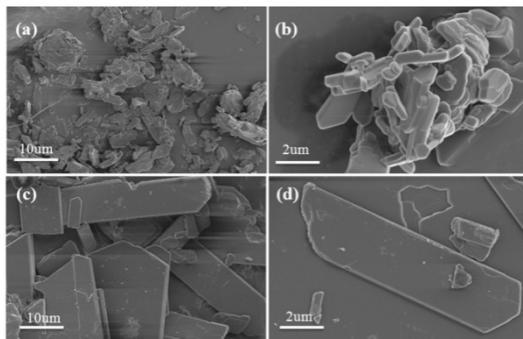


Effects of metal organic complex Ni(Salen) on thermal decomposition of 1,1-diamino-2,2-dinitroethylene (FOX-7)

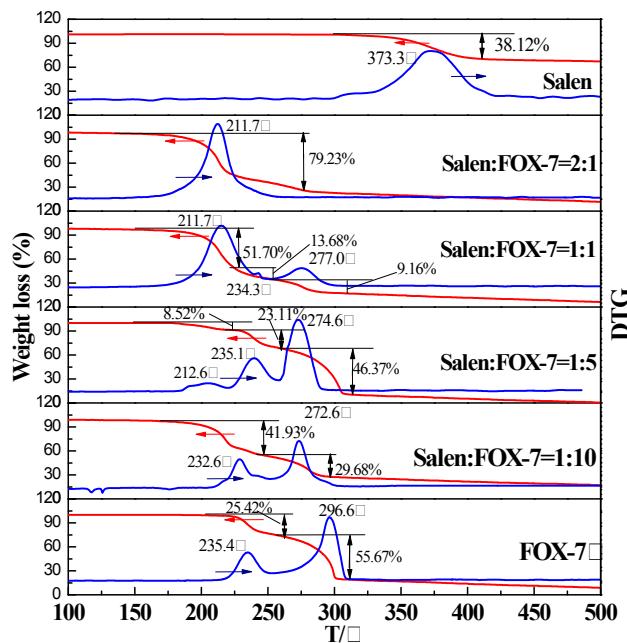
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Ming Zhang^a, Zhicun Feng^b

Supporting Information



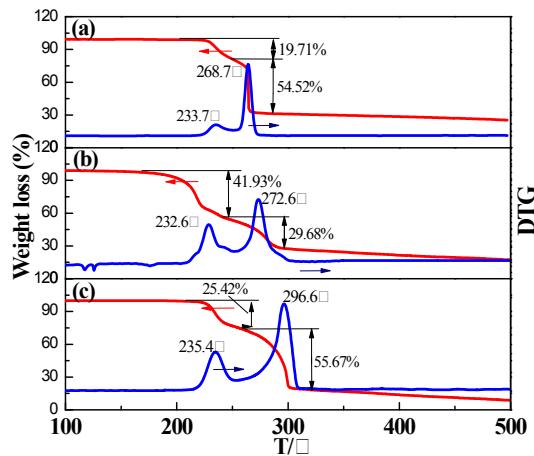
S.1 SEM images of Salen (a, b) and Ni(Salen) (c, d)

The morphology and the microstructures of Ni(Salen) were characterized by SEM and compared with Salen (S.1). The Salen sample is found to be composed of irregular particles with diameters of 1~3μm, and the agglomeration of the particles is also observed. As for Ni(Salen), the sheets with length of dozens of micrometers and width of several micrometers are observed on the image. The sheet surfaces are noticed to be relatively smooth. As stated above, Ni(Salen) has a 2D layered structure, and the layers are connected via intermolecular forces. The layered crystal structures of Ni(Salen) are believed to be closely related to its morphology.



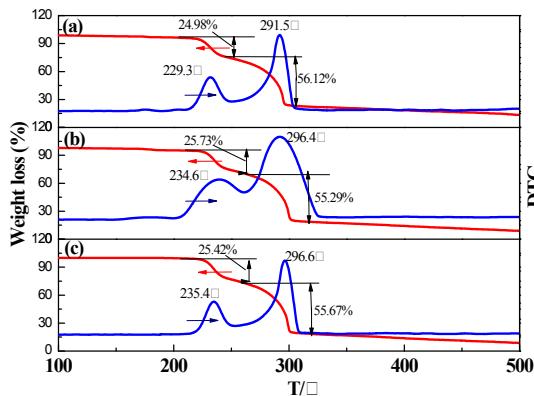
S.2 TG-DTG curves of FOX-7/ Salen mixture at different mass ratios, FOX-7 and Salen ligand

The effect of Salen ligand on the decomposition of FOX-7 was studied by DSC to reveal the role of Salen in the thermal decomposition of FOX-7 / Ni (Salen) system. In addition, in order to further analyze its role in the FOX-7 decomposition process, TG-DTG data was tested and analyzed. The as-prepared Salen was mixed uniformly with FOX-7 at different mass ratios (Salen:FOX-7=1:10, 1:5, 1:1, 2:1), and then subjected to TG-DTG analysis. The results are shown in S. 2. For a mixture with a mass ratio of 1:10, two weight loss events were observed, with weight loss of 41.93% and 29.68%, respectively. Compared to 25.42% and 55.67% of the original FOX-7, the amount of the second weight loss process was reduced, which indicates that the Salen ligand can effectively promote the decomposition of FOX-7. For a mixture with a mass ratio of 1: 5, although a similar phenomenon was observed, a new weight loss process occurred at a lower temperature on the TG-DTG curve compared with the sample with a mass ratio of 1:10. Upon further increase of the ratio to 1:1, the two-stage weightlessness of the original FOX-7 became weaker, and the new weightlessness process at low temperatures became more apparent. In addition, with a higher mass ratio of 2: 1, only a single newly occurring weightless process was detected. The analysis shows that the weightlessness process at low temperature is attributed to the decomposition process of the intermediate organic active agent produced by the interaction between FOX-7 and the ligand Salen. This is consistent with the conclusion of the interaction between the ligand Salen and FOX-7 analyzed by DSC in the original manuscript. It was further proved that the reaction product between Salen and FOX-7 will promote the thermal decomposition of the remaining FOX-7 and lead to a reduced decomposition temperature.



S.3 TG-DTG curves of FOX-7/ Ni(Salen) mixture (a), FOX-7/ Salen mixture (b) and FOX-7 (c)

A comparison was made between the weightlessness behavior of the FOX-7/Ni(Salen) system and the FOX-7/Salen system both with mass ratios of 10:1. As shown in Figure 6 in the original manuscript, it is interesting to noticed that for both systems, the first step of decomposing the weightless process is similar. However, for the FOX-7 / Ni (Salen) system, the second step decomposition is completed at a temperature lower than the FOX-7 / Salen system. Obviously, Ni (Salen) is more active than Salen in promoting the second-step decomposition of FOX-7, which also confirms the conclusions obtained in the original manuscript.



S.4 TG-DTG curves of FOX-7/ NiO mixture (a), FOX-7/ Ni mixture (b) and FOX-7 (c)

For the purpose of understanding the role of Ni^{2+} in Ni(Salen), nano Ni and nano NiO were added to FOX-7, and the weightlessness behavior of the mixtures(Ni/NiO:FOX-7=1:10) were recorded. As shown in Figure. 7 in the original manuscript, when compared with the pure FOX-7, the TG-DTG result of the FOX-7/Ni mixture indicates that the metallic Ni shows no effects on the weightlessness of FOX-7. Compared

with pure FOX-7, the addition of NiO can complete the weight loss earlier, which proves that Ni^{2+} can promote the decomposition of FOX-7. Therefore, it can be considered that the active material NiO produced by the thermal decomposition of Ni (Salen) can significantly promote the decomposition of FOX-7 in the FOX-7 / Ni (Salen) system.