Supporting information

Nanocrystalline Zinc peroxide mediated unprecedented nitrene transfer: an expeditious access to aziridines.

Sanny Verma and Suman L. Jain

Chemical Sciences Division, CSIR-Indian Institute of Petorleum

Mohkampur, Dehradun-248005 (India)

Email: suman@iip.res.in

Synthesis and characterization of Nanocrystalline ZnO_2

***Synthesis of nanocrystalline ZnO_2*[1]:** A solution of $Zn(CH_3COO)_2.2H_2O$(1g) in deionized water (50 mL) was added H_2O_2 (5 mL, 30 wt %). The resulting mixture was stirred overnight at room temperature and then separated by filtration. The resulting fine powder was washed with deionized water and dried at 60 °C for 3 days to afford nanocrystalline ZnO_2 .

The synthesized nanocrystalline zinc peroxide was characterized with various techniques. The FT-IR spectrum[2] of nanocrystalline ZnO_2 is presented in Figure 1, which reveals the characteristic band of Zn-O at 430 cm^{-1}. The signature band of the O-O stretching is observed at 1020 cm^{-1} and the presence of bands in the range of 3431.4 cm^{-1} and 1573.1 cm^{-1} attributed to the OH stretching and bending modes of water respectively.

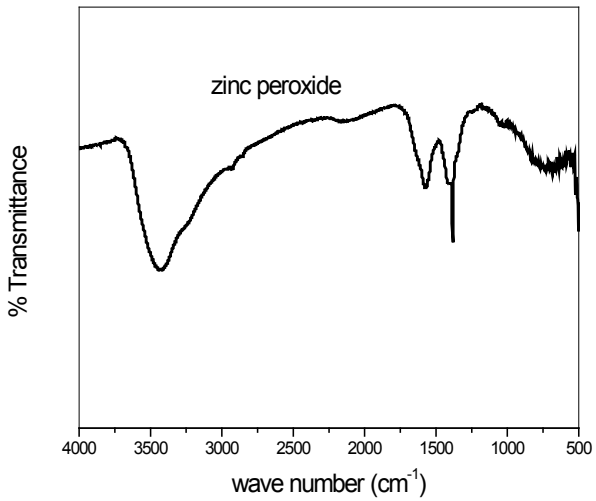


Fig. 1: FTIR of nanocrystalline zinc peroxide

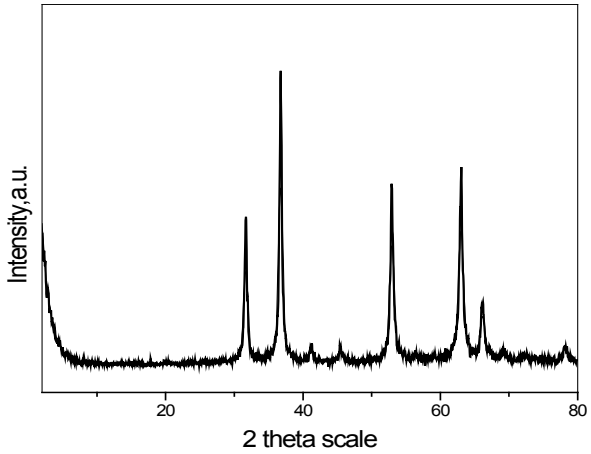


Fig.2 XRD pattern of nanocrystalline zinc peroxide

Figure 2 shows the XRD pattern of the synthesized nanocrystalline zinc peroxide which was found to be similar to the XRD pattern as described in literature.[2,3]

The morphological feature of the prepared nanocrystalline material was determined by Field Emission Scanning Electron Microscopy (FESEM).The FE-SEM images shown in Figure 3

shows, the nanoparticles of zinc peroxide are approximately 50-100 nm and are of aggregated type.[2]

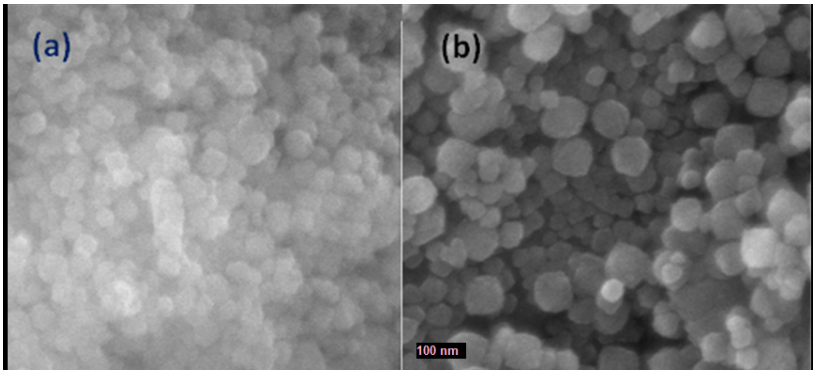


Figure 3: (a) Low- and (b) high-magnification FE-SEM images of nanocrystalline zinc peroxide

The thermal behavior of the as-prepared ZnO_2 nanocrystals was investigated by TG–DSC analysis. The TG curve in Fig. 4 shows that the weight loss below 180 °C was about 12%, which was attributed to the release of surface-adsorbed/bound water. The major weight loss was found in the range of 180–350 °C in the TG curve, which could be due to the decomposition of ZnO_2 into ZnO and oxygen ($2ZnO_2$) = $2ZnO + O_2$) as suggested in the literature.[2] In addition, the DSC curve in Fig. 4 exhibited a strong exothermic peak at around 244 °C, corresponding to the decomposition of ZnO_2 into ZnO and O_2. It is very important to recognize that anionic substitution of ZnO_2 at high temperature cannot be performed easily as it is known to liberate oxygen violently on heating at around 244°C.[2]

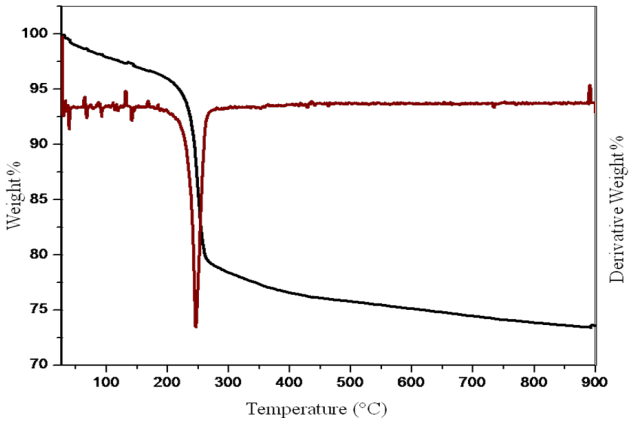
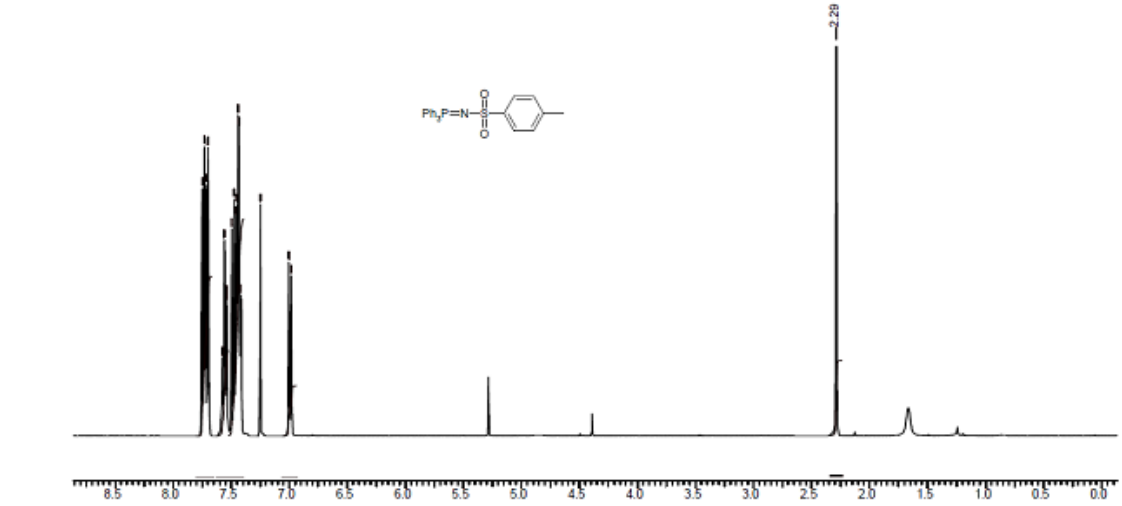


Fig. 4: TG-DSC curve of nanocrystalline ZnO_2

^{1}H and ^{13}C NMR of $Ph_3P{=}NTs$



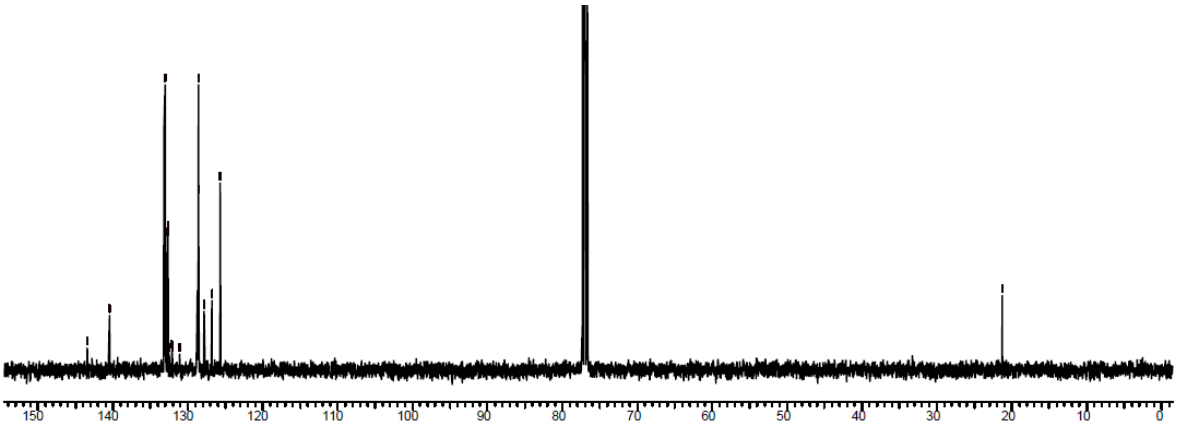


Table 1, entry 12 (Aziridination of *cis*-2-hexene)

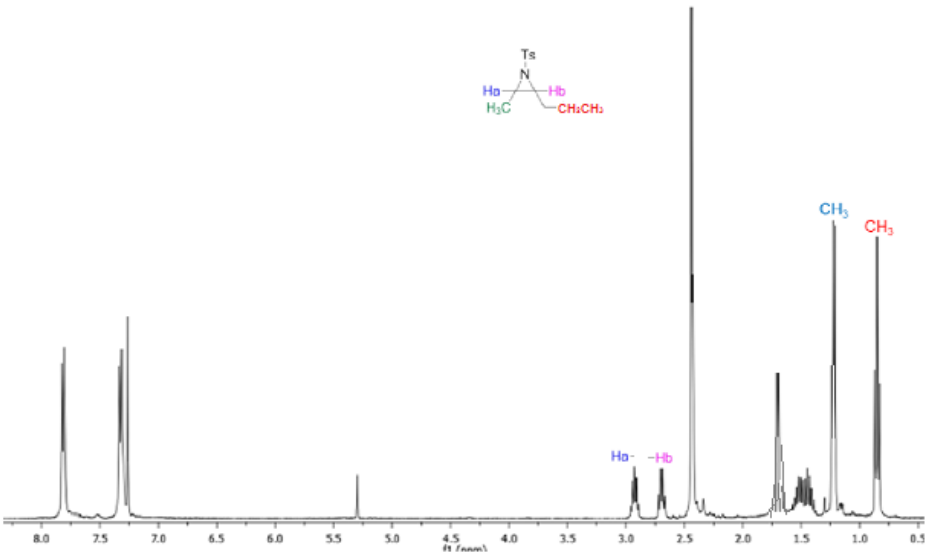
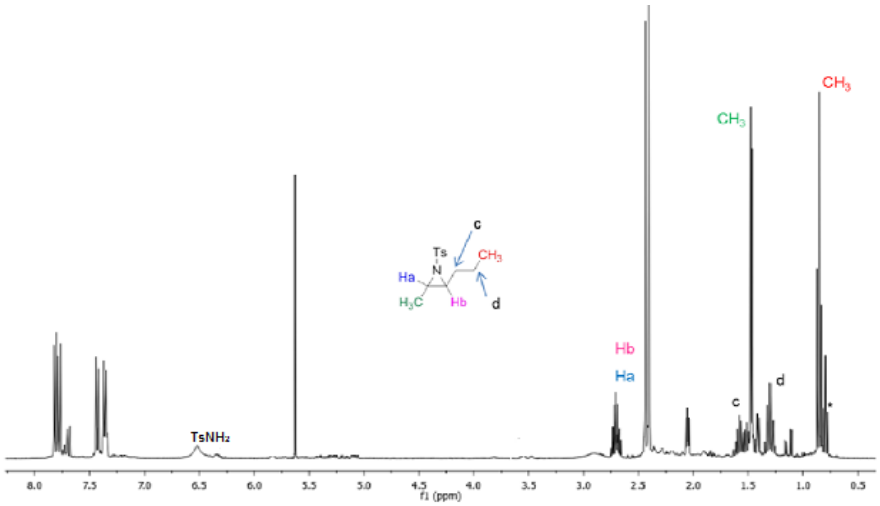


Table 1, entry 13 (Aziridination of *trans*-2-hexene)



References

1. a) Sun, M.; Hao, W.; Wang, C.; Wang, T. *Chem. Phys. Lett.* **2007**, 443, 342–346.; b) Ahmad, S.; Kharkwal, M.; Govind, N. R. *J. Phys. Chem. C* **2011**, 115, 10131–10139.
2. Cheng, S. ; Yan, D.; Chen, J. T.; Zhuo, R. F ; Feng, J. J. ; Li, H. J.; Feng, H. T.; Yan, P. X. *J. Phys. Chem. C* **2009**, 113, 13630–13635.
3. Chen, W.; Lu, Y. H.; Wang, M.; Kroner, L.; Paul, H.; Fecht, H.-J.; Bednarcik, J.; Stahl, K.; Zhang, Z. L.; Wiedwald, U.; Kaiser, U.; Ziemann, P.; Kikegawa, T.; Wu, O C. D.; Jiang, J. Z. *J. Phys. Chem. C* **2009**, 113, 1320–1324.