Electronic Supplementary Information

Surface modification of nano-silica with amides and imides for use in polyester nanocomposites

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Calculation of Number of reacted silanol groups per square nanometer on silica surface

Percentage organic content on silica surface after APS modification is 11.8 wt-%.

Silica : Degussa, Aerosil 200®, diameter = 12 nm

Specific surface area of silica particle = 200 m^2/g (from the manufacturer)

Surface Area of a sphere is given by**: $4\pi r^2$**

∴ surface area of silica with 12 nm diameter is:

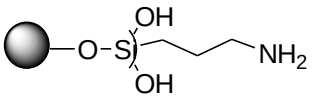
$4 \times 3.14 \times (6\times 10^{-9})^{2} = 4.52 \times 10^{-16}\ m^2$

Since Mass = surface Area / specific surface area

∴ mass of the given silica = $4.52 \times 10^{-16}\ m^2$ / 200 m^2/g

$= 2.26 \times 10^{-18}\ g$

Considering that all the organic content on the silica degrades, including the amino-propyl group and the two-hydroxy groups of the attached APS, the molecular weight of the organic content coming off is **92.11**



Molar mass of organic content on modified silica = molecular weight of the organic content divided by Avogadro's constant

Molar mass of the organic content on modified silica = $92.11 / 6.023 \times 10^{23} = 1.53 \times 10^{-22}$ g

$$\text{Total weight of organic content on silica} = \text{Mass of Silica} \times \left\{ \frac{\% \text{ organic content on silica} / 100}{1 - \% \text{ organic content on silica} / 100} \right\}$$

$$\text{Total weight of organic content on silica} = 2.26\times10^{-18} \times \left\{ \frac{11.8/100}{1-11.8/100} \right\}$$

Total weight of organic content on silica = $2.26 \times 10^{-18} \times 0.13$

Total weight of organic on silica = $2.94 \times 1\ 0^{-19}$ g

Dividing this by the molar mass of the organic content on modified silica (1.53×10^{-22} g calculated from TGA) gives the total number of reacted silanol groups present on silica surface.

∴ Total number of reacted silanol groups on silica surface = $2.94\times10^{-19} / 1.53 \times 10^{-22}$

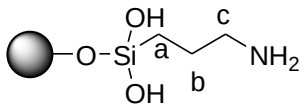
= 1921

Number of reacted silanol groups per square nanometer on silica surface = Total no. of reacted silanol groups present on silica surface / surface area of silica particle

Number of reacted silanol groups per square nanometer on silica surface =

1921 / 452 = **4.2 reacted OH (silanol) groups / nm^2**

Fig. S1 ^{13}C NMR of SiAP



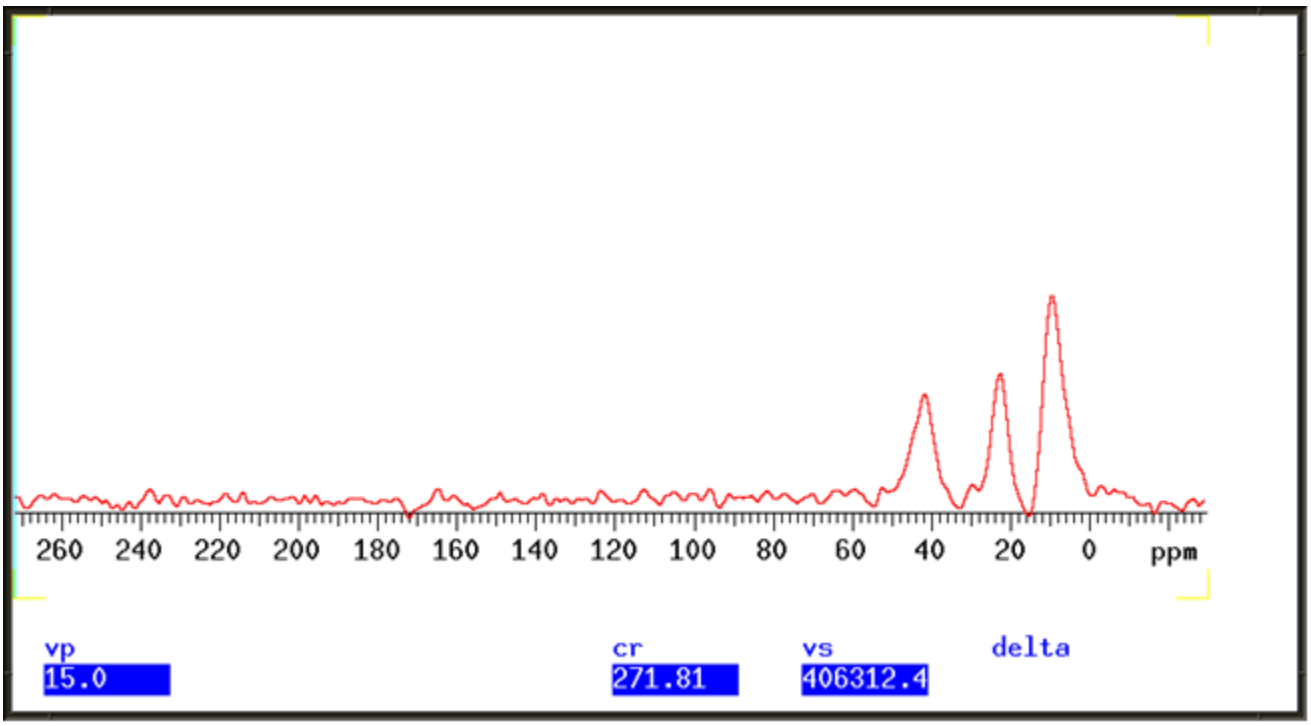
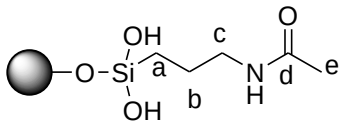


Fig. S2 ^{13}C NMR of SiAc



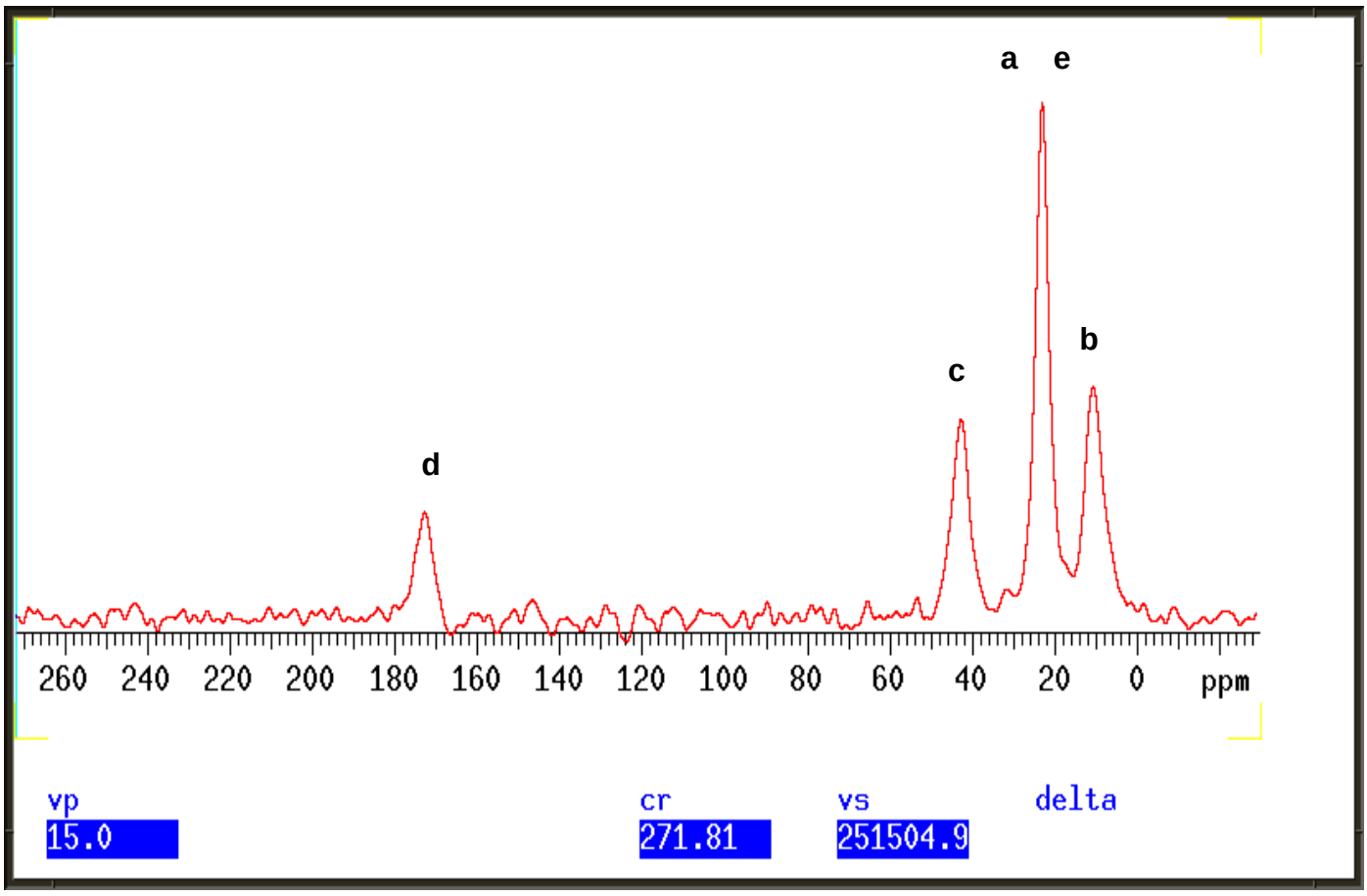
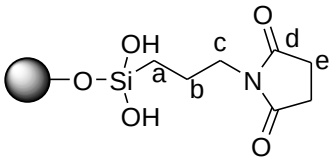


Fig. S3 ^{13}C NMR of SiSA



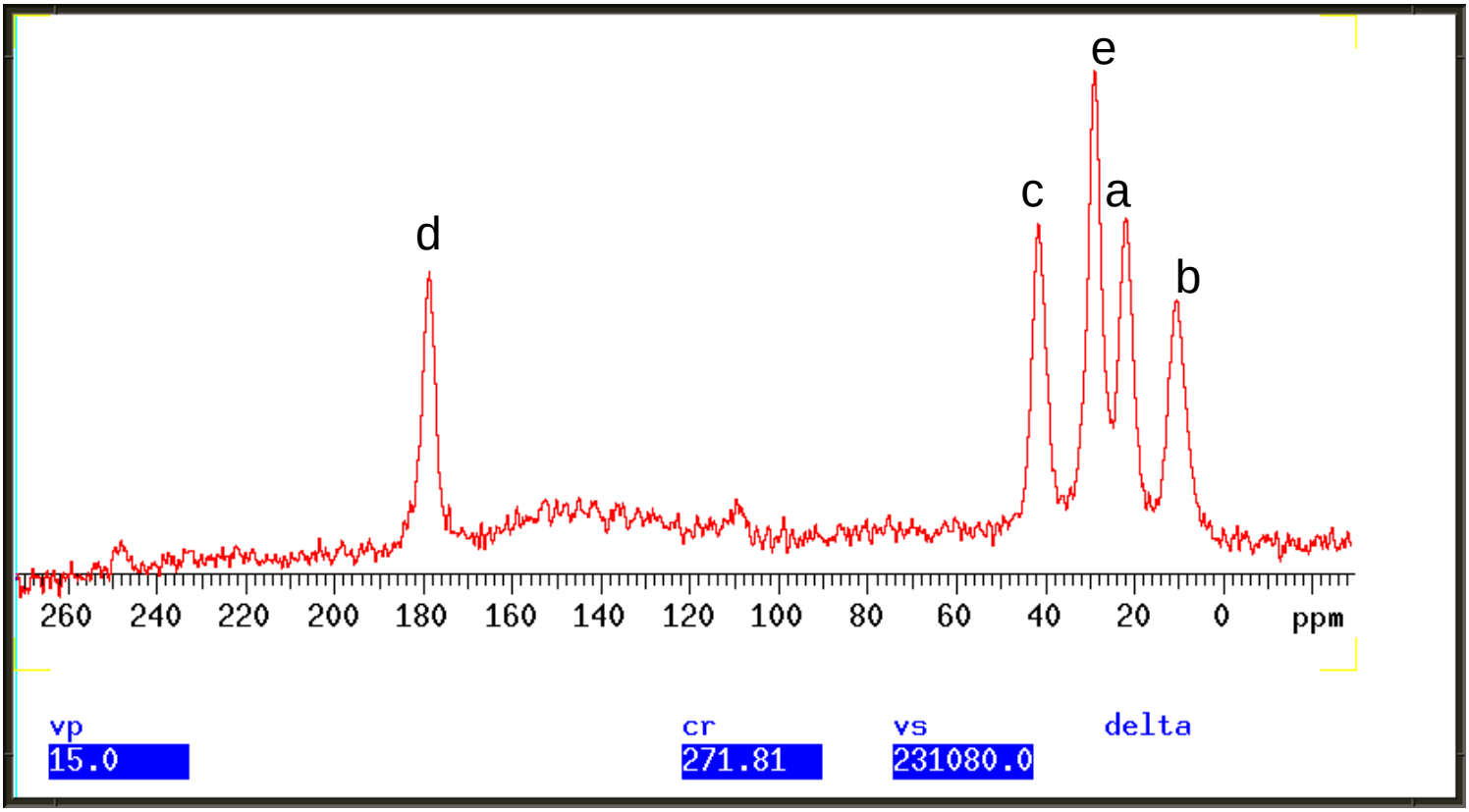
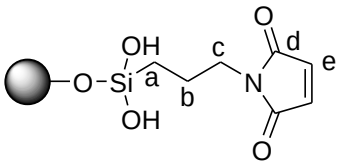


Fig. S4 ^{13}C NMR of SiMA



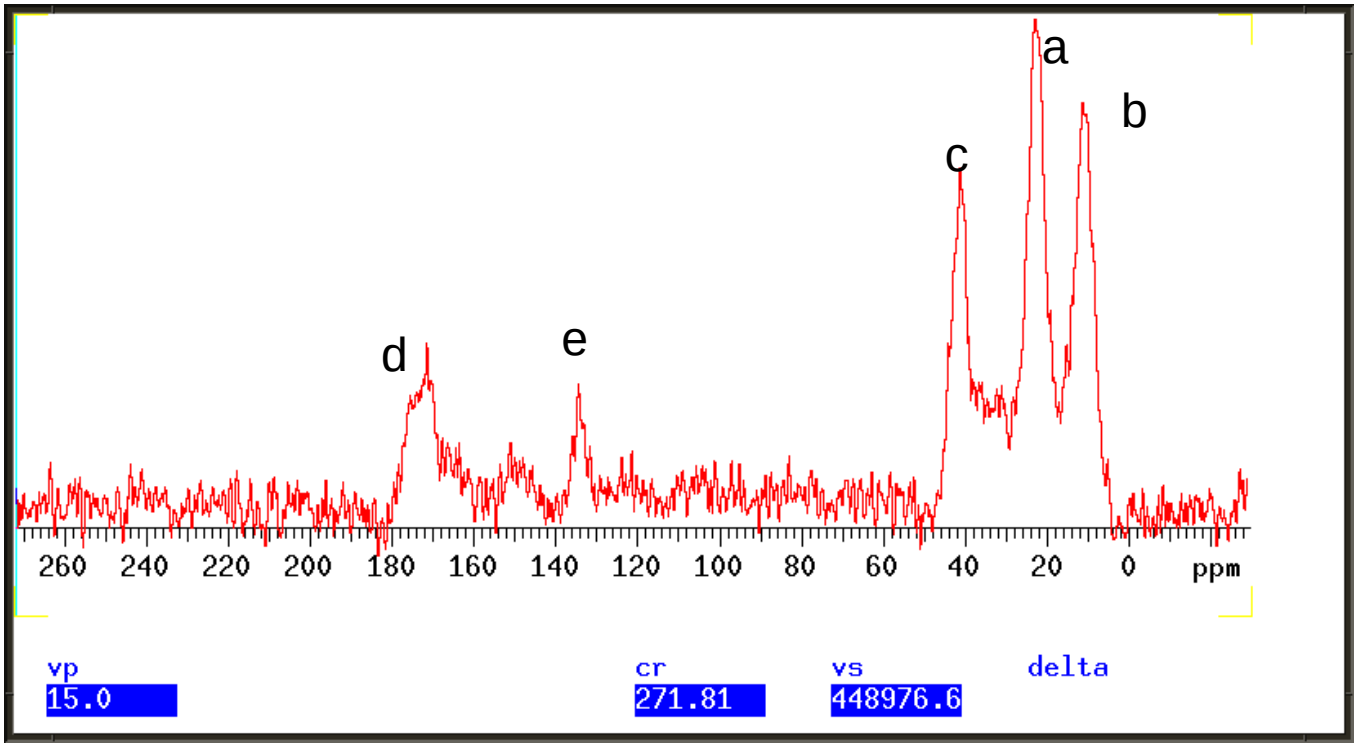


Fig. S5 ^{13}C NMR of SiPA

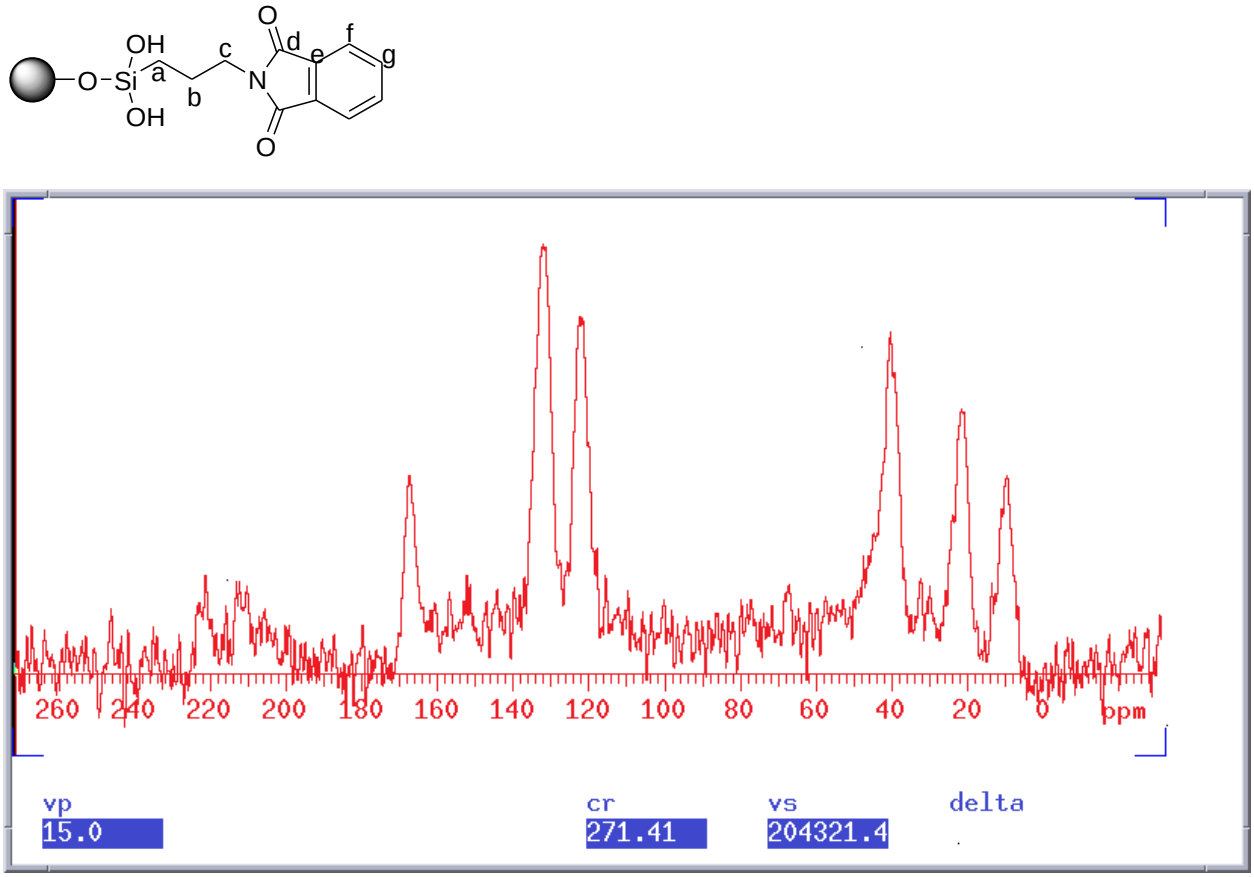
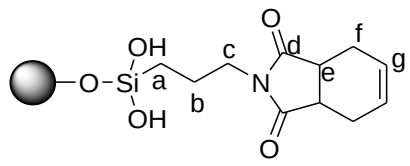


Fig. S6 ^{13}C NMR of SiTPA



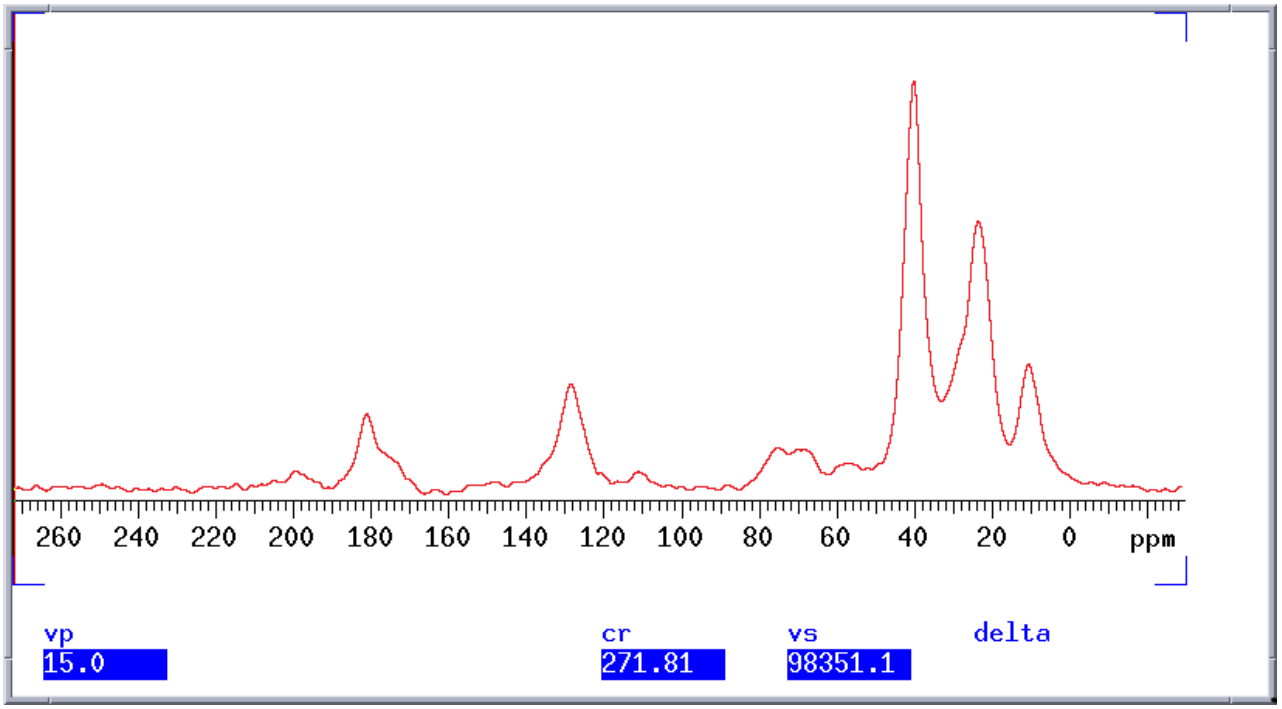


Fig. S7 FT-IR spectra of (1) untreated nano-SiO_2 and after modification with (2) APS, (3) APS/acetic anhydride, (4) APS/succinnic anhydride, (5) APS/maleic anhydride, (6) APS/phthalic anhydride, (7) APS/tetrahydrophthalic anhydride.