

Supplementary Information

Room-temperature reaction of polycarbosilane with iodine under different atmospheres for polymer-derived silicon carbide fibres

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Production of benzene during iodisation of polycarbosilane

The GC-MS and solid-state ^1H NMR analyses (Figures 1 and 4c in the main text) indicate that aromatics, including benzene and toluene, are produced as by-products during the iodisation of polycarbosilane (PCS). Nevertheless, there has been a conflict between the authors on whether the aromatic compounds are (i) derived from solvents (*i.e.*, toluene used for the synthesis of PCS) remaining in PCS or (ii) actually produced by the reaction between PCS and iodine. To confirm this, the room-temperature iodisation of PCS was analysed over time by in-situ solid-state ^1H MAS NMR. PCS and iodine powders were placed in a zirconia rotor and then spun together by the NMR equipment. Although the iodisation rate was expected to be very slow owing to the almost static pressure within the small space, over time, the iodisation reaction occurred, as shown by the decrease in the Si-H signal (~ 4 ppm) in Figure S1. On the other hand, a new peak (~ 7 ppm) ascribable to benzene emerged as the iodisation progressed. This result demonstrates that benzene is a by-product of the iodisation of PCS at ambient temperature.

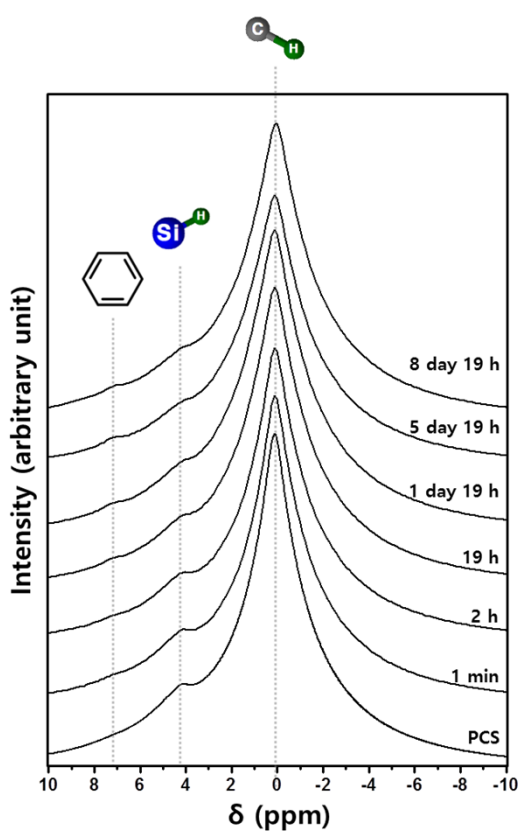


Figure S1. Solid-state ^1H MAS NMR spectra of polycarbosilane (PCS) iodised at room temperature over time, where the PCS and iodine powders were placed in the rotor for a given time (as indicated in the figure) and then spun during the analysis.