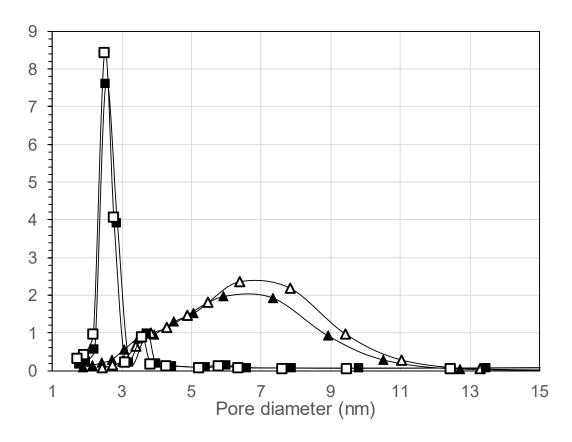
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2022

## **Electronic Supplementary Information**

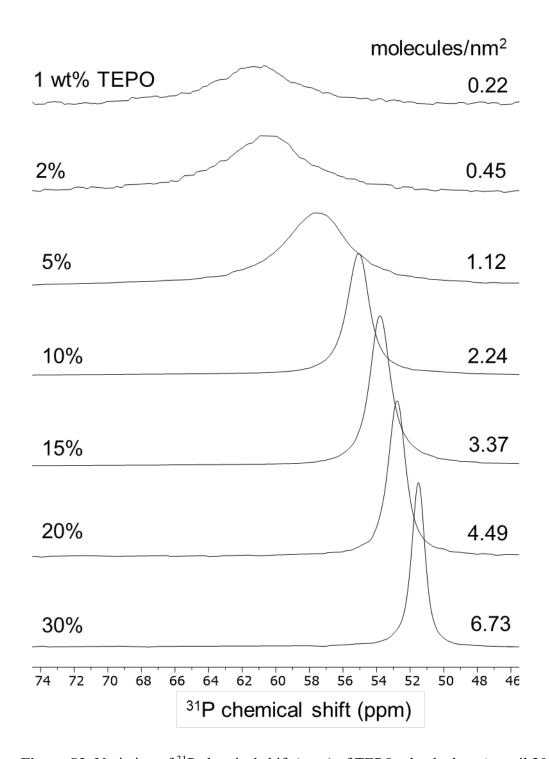
## New insights into the interaction of triethylphosphine oxide with silica surface: exchange between different surface species

Elisabet Pires and José M. Fraile\*

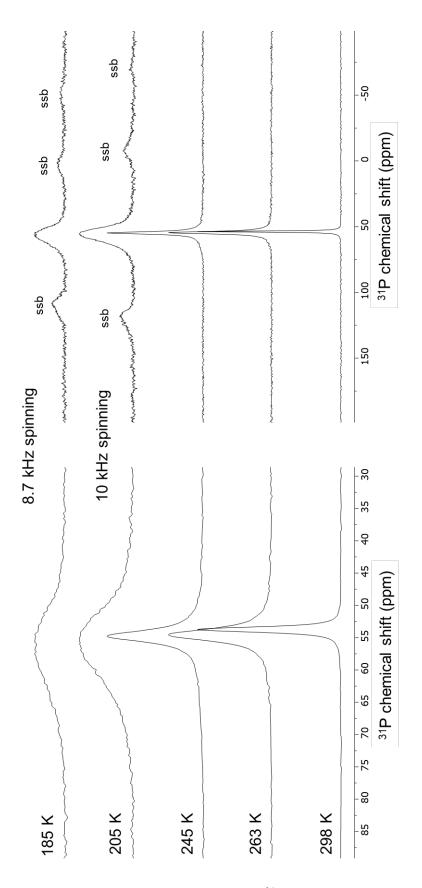
Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC-Universidad de Zaragoza, Facultad de Ciencias, Pedro Cerbuna 12, E-50009 Zaragoza, Spain



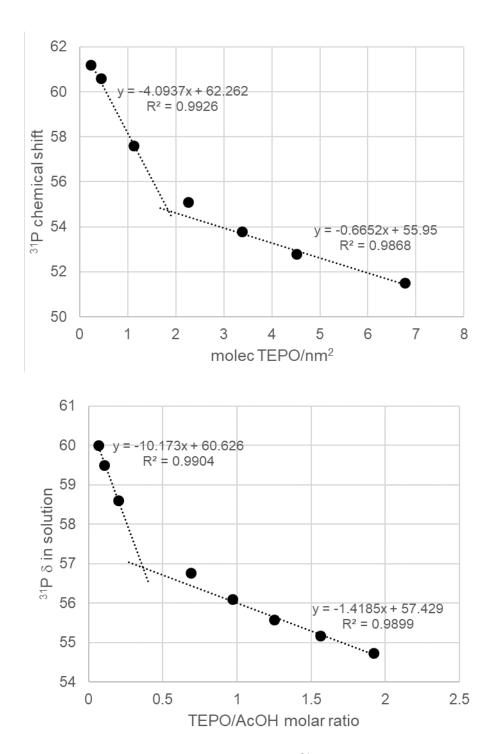
**Figure S1.** Pore size distribution of MCM-41 (squares) and Silia P60 (triangles), pretreated at 200°C (open symbols) and 500°C (filled symbols).



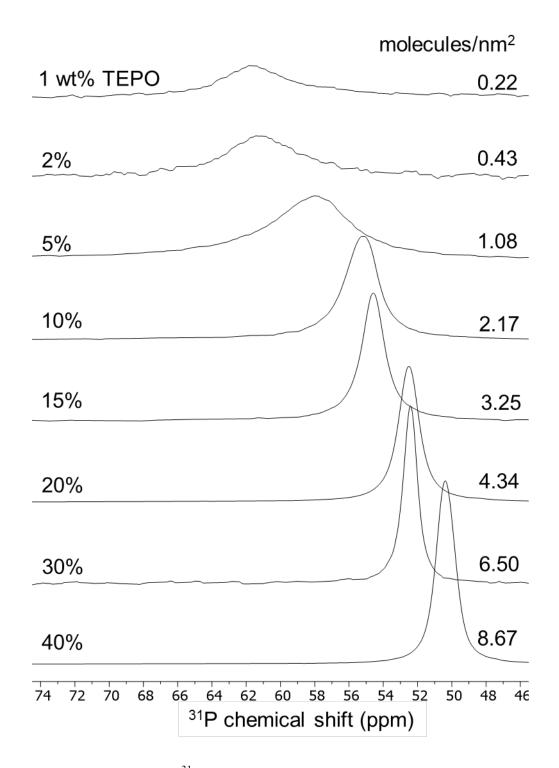
**Figure S2.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on Aerosil 200 calcined at 500°C at different TEPO loadings and the corresponding surface coverage.



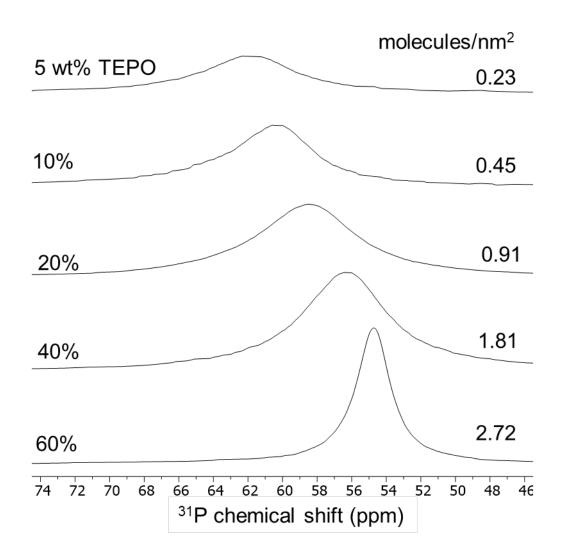
**Figure S3.** Effect of temperature on the <sup>31</sup>P signal of TEPO adsorbed on Aerosil 200 calcined at 500°C at 20 wt% TEPO loading: central signal (left) and full range spectrum (right). SSB = spinning side bands.



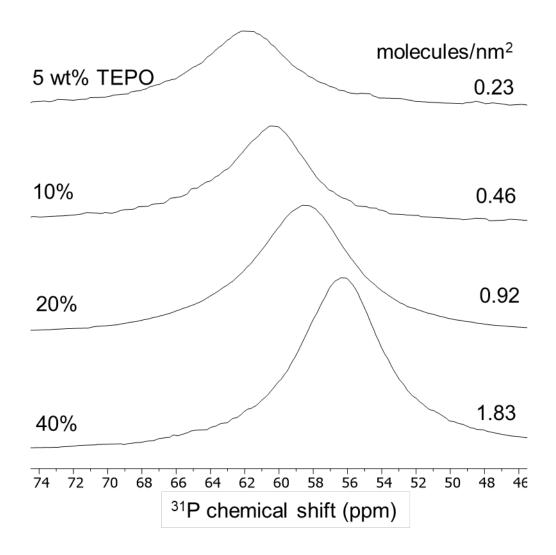
**Figure S4.** Comparison of the variation of <sup>31</sup>P chemical shift (ppm) with TEPO surface coverage on Aerosil 200 calcined at 500°C and in solution with the TEPO/acetic acid molar ratio in CDCl<sub>3</sub> (data taken from reference 13).



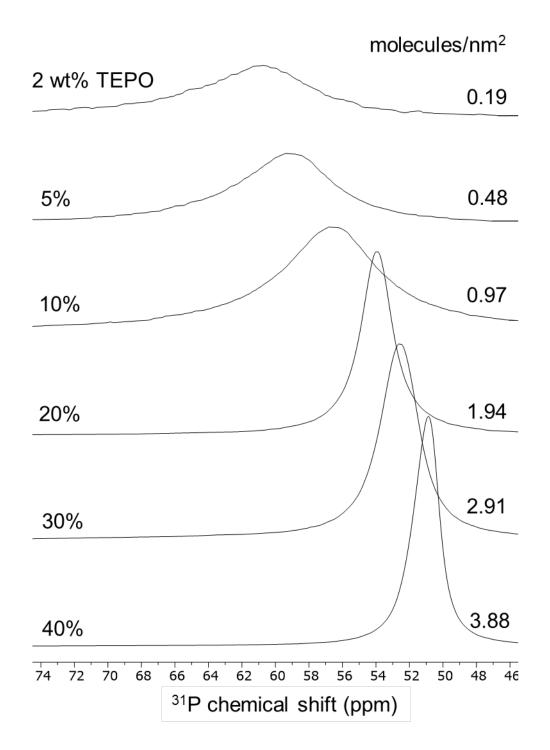
**Figure S5.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on Aerosil 200 calcined at 200°C at different TEPO loadings and the corresponding surface coverage.



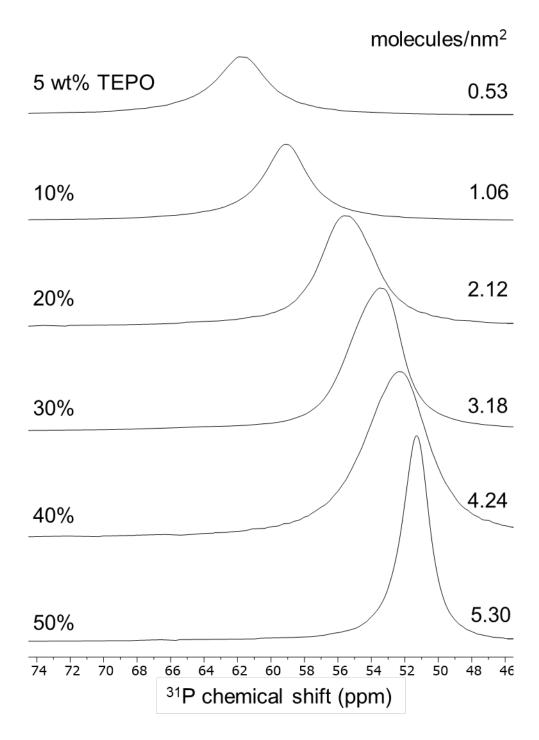
**Figure S6.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on MCM-41 calcined at 500°C at different TEPO loadings and the corresponding surface coverage.



**Figure S7.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on MCM-41 calcined at 200°C at different TEPO loadings and the corresponding surface coverage.



**Figure S8.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on Silia P60 calcined at 500°C at different TEPO loadings and the corresponding surface coverage.



**Figure S9.** Variation of <sup>31</sup>P chemical shift (ppm) of TEPO adsorbed on Silia P60 calcined at 200°C at different TEPO loadings and the corresponding surface coverage.