

Supporting Information

Tin-decorated ruthenium nanoparticles: a way to tune selectivity in hydrogenation reaction

Eric BONNEFILLE,^{a,b} Fernando NOVIO,^{a,b} Torsten GUTMANN,^{a,b} Romuald POTEAU,^c Pierre
LECANTE,^d Jean-Claude JUMAS,^e Karine PHILIPPOT,^{a,b*} Bruno CHAUDRET^{c*}

^{a,b} *Laboratoire de Chimie de Coordination; CNRS; LCC; 205 Route de Narbonne, F-31077 Toulouse, France; Université de Toulouse; UPS, INPT; LCC; F-31077 Toulouse, France*

^c *LPCNO; Laboratoire de Physique et Chimie de Nano-Objets 135, Avenue de Rangueil, F-31077 Toulouse, France*

^d *CNRS ; Centre d'Elaboration de Matériaux et d'Etudes Structurales (CEMES) ; 29, rue Jeanne Marvig, BP 4347, 31055 Toulouse Cedex, France.*

^e *Institut Charles Gerhardt, ICG/AIME (UMR 5253 CNRS), Université Montpellier II CC 15-02, Place E. Bataillon, 34095 Montpellier Cedex 5, France.*

Contents

Figure S1. HREM analysis of Ru/dppb/Sn.	3
Figure S2. Fluorescence X of Ru/dppb/Sn (red line) and standard (green line).	4
Figure S3. IR spectra of Ru/PVP/Sn nanoparticles after reaction with CO prepared with different amounts of tin.	5
Figure S4. IR spectra of Ru/PVP/Sn nanoparticles after reaction with CO prepared with different amounts of tin: enlargement of the area 2300-1530 cm^{-1}	6
Figure S5. ^{13}C NMR Ru/PVP (bottom) and Ru/PVP/Sn (top).	7
Figure S6. ^{13}C MAS (bottom) and ^{13}C CP-MAS (top) NMR Sn-Ru/PVP prepared with 0.05equiv. of tin.	8
Figure S7. IR spectra of Ru/dppb/Sn prepared with 0.1 equiv. of tin.	9
Figure S8. ^{13}C NMR spectra of Ru/dppb (bottom) and Ru/dppb/Sn (top).	10
Figure S9. ^{13}C CP-MAS (bottom) and ^{13}C MAS (top) NMR Sn-Ru/dppb prepared with 0.1 equiv. of tin.	11
Figure S10. ^{31}P CP-MAS NMR Sn-Ru/dppb prepared with 0.1 equiv. of tin before reaction with CO (red line) and after CO reaction (blue line).	12
Figure S11. Top view of SnR_m^* , R'_k^* species adsorbed on Ru(0001).	13

Figure S1. HREM analysis of Ru/dppb/Sn.

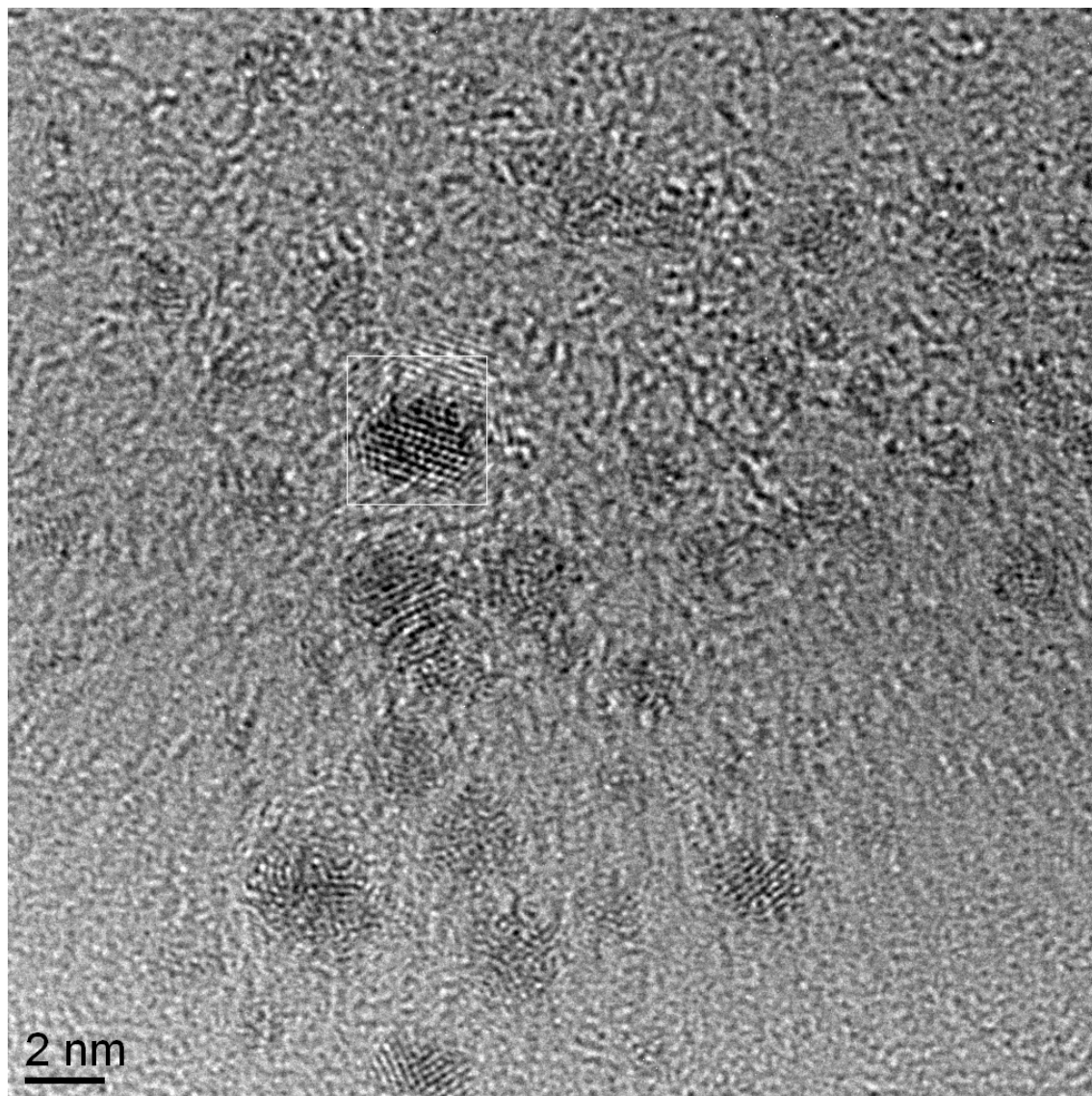


Figure S2. Fluorescence X of Ru/dppb/Sn (red line) and standard (green line).

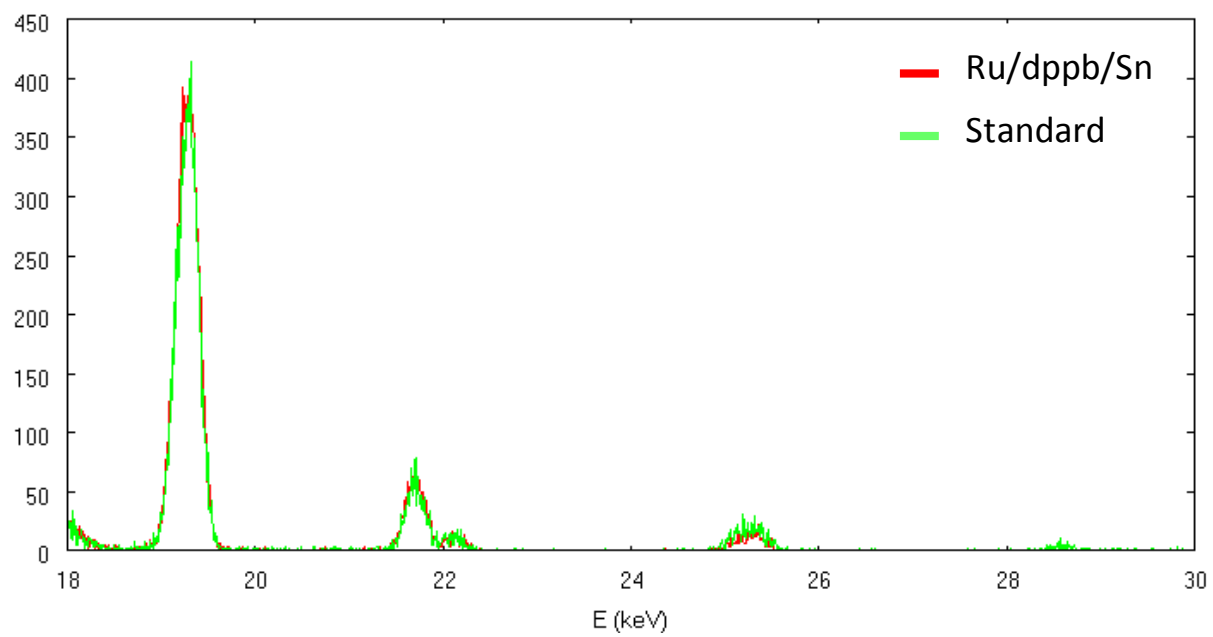


Figure S3. IR spectra of Ru/PVP/Sn nanoparticles after reaction with CO prepared with different amounts of tin.

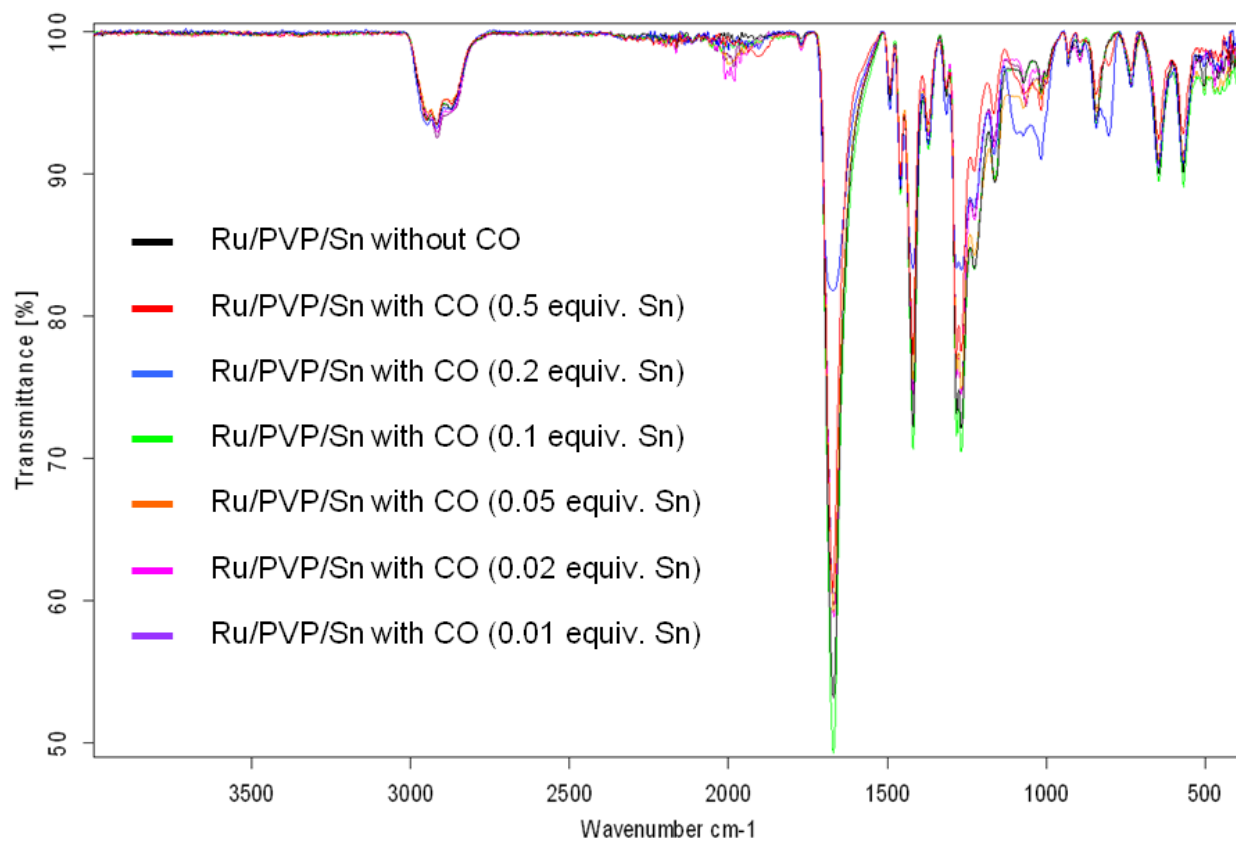


Figure S4. IR spectra of Ru/PVP/Sn nanoparticles after reaction with CO prepared with different amounts of tin: enlargement of the area 2300-1530 cm^{-1}

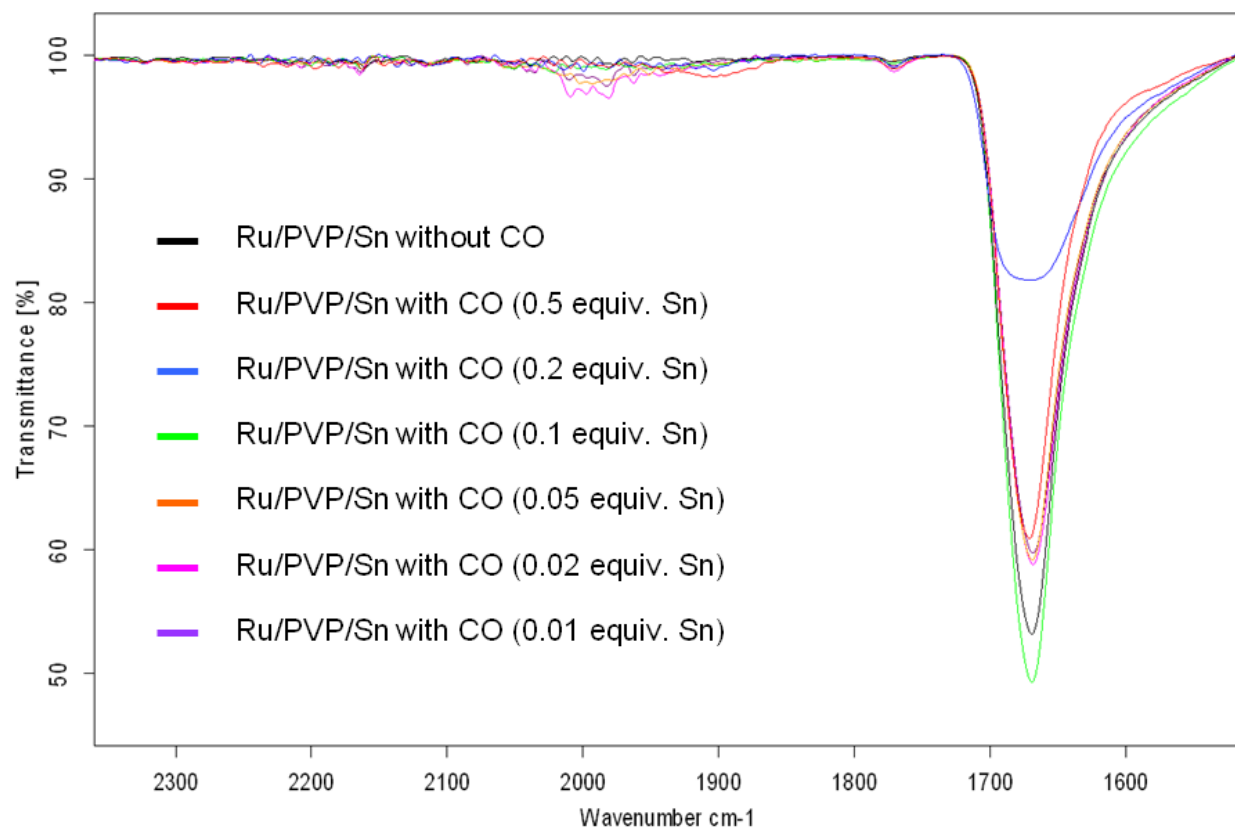


Figure S5. ^{13}C NMR Ru/PVP (bottom) and Ru/PVP/Sn (top).

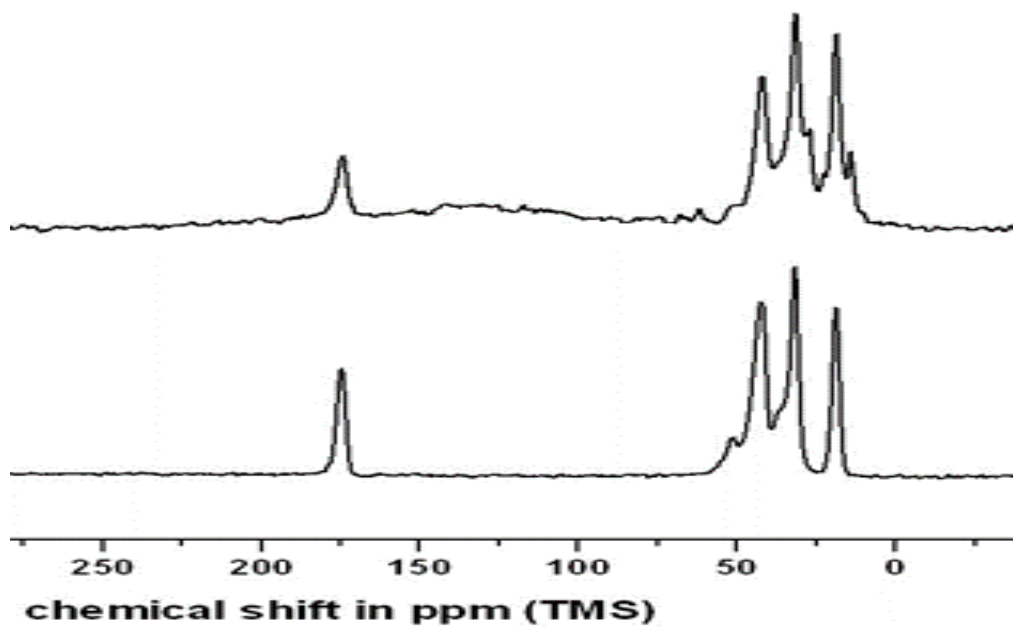


Figure S6. ^{13}C MAS (bottom) and ^{13}C CP-MAS (top) NMR Sn-Ru/PVP prepared with 0.05equiv. of tin.

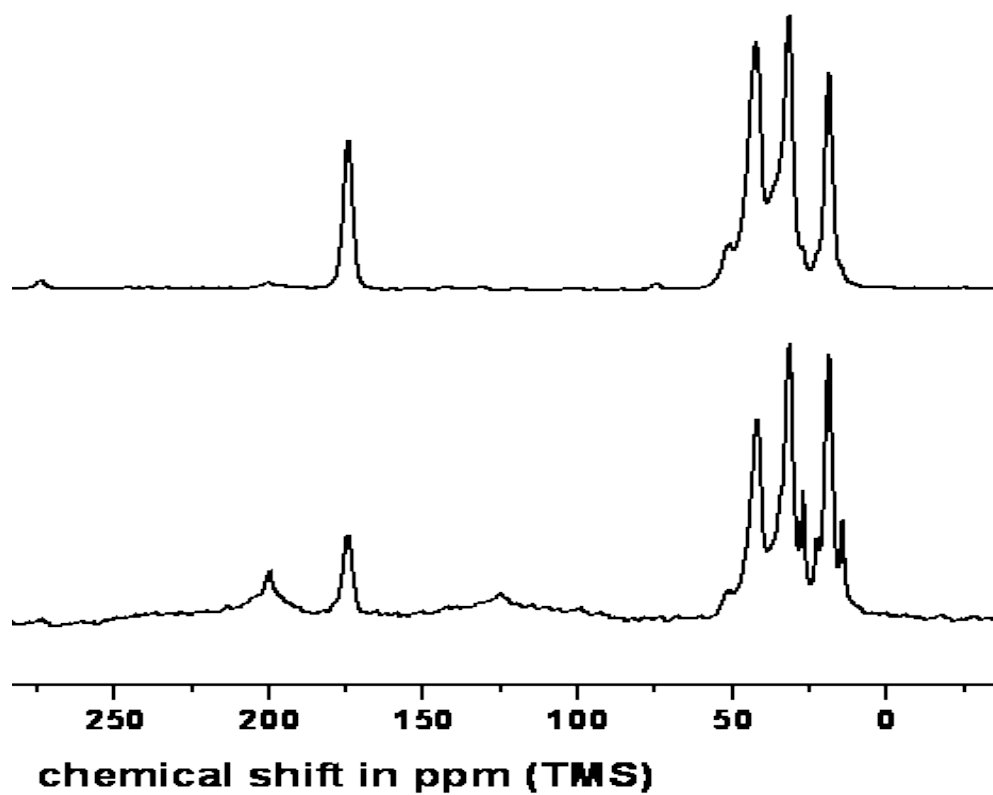


Figure S7. IR spectra of Ru/dppb/Sn prepared with 0.1 equiv. of tin.

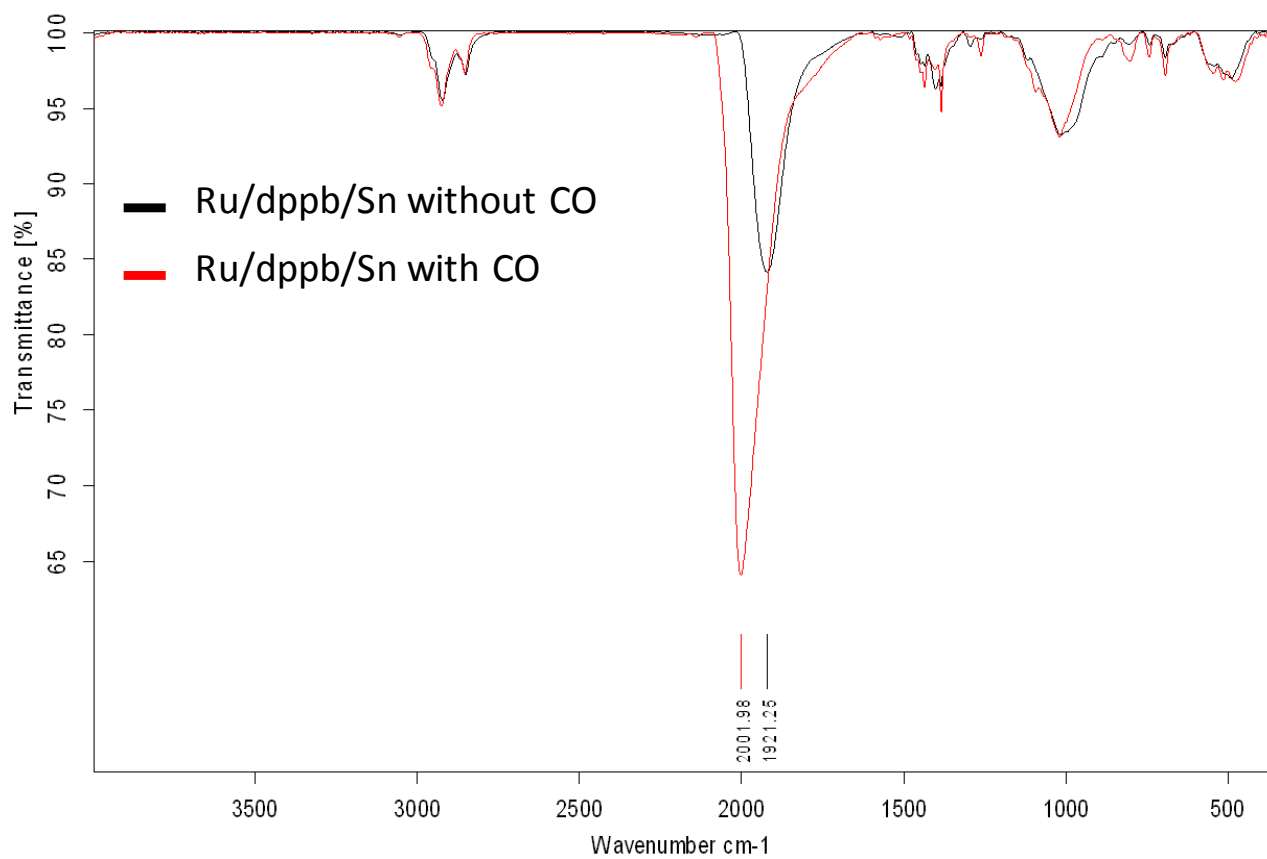


Figure S8. ^{13}C NMR spectra of Ru/dppb (bottom) and Ru/dppb/Sn (top).

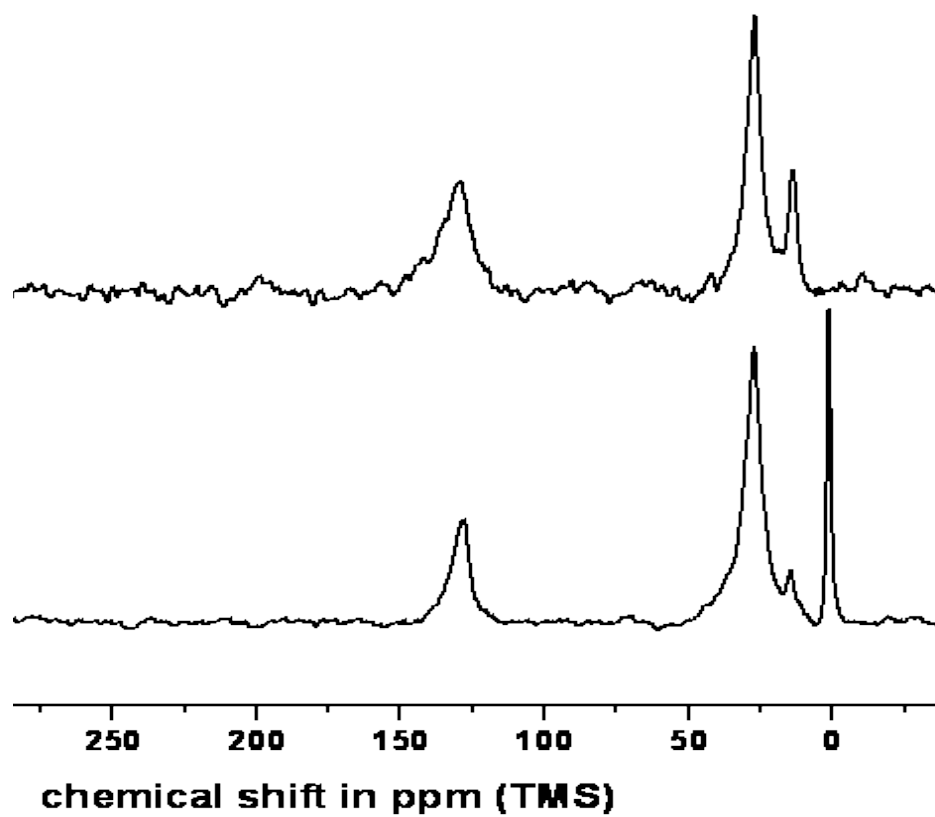


Figure S9. ^{13}C CP-MAS (bottom) and ^{13}C MAS (top) NMR Sn-Ru/dppb prepared with 0.1 equiv. of tin.

* Spinning side bands

* Spinning side bands of Teflon

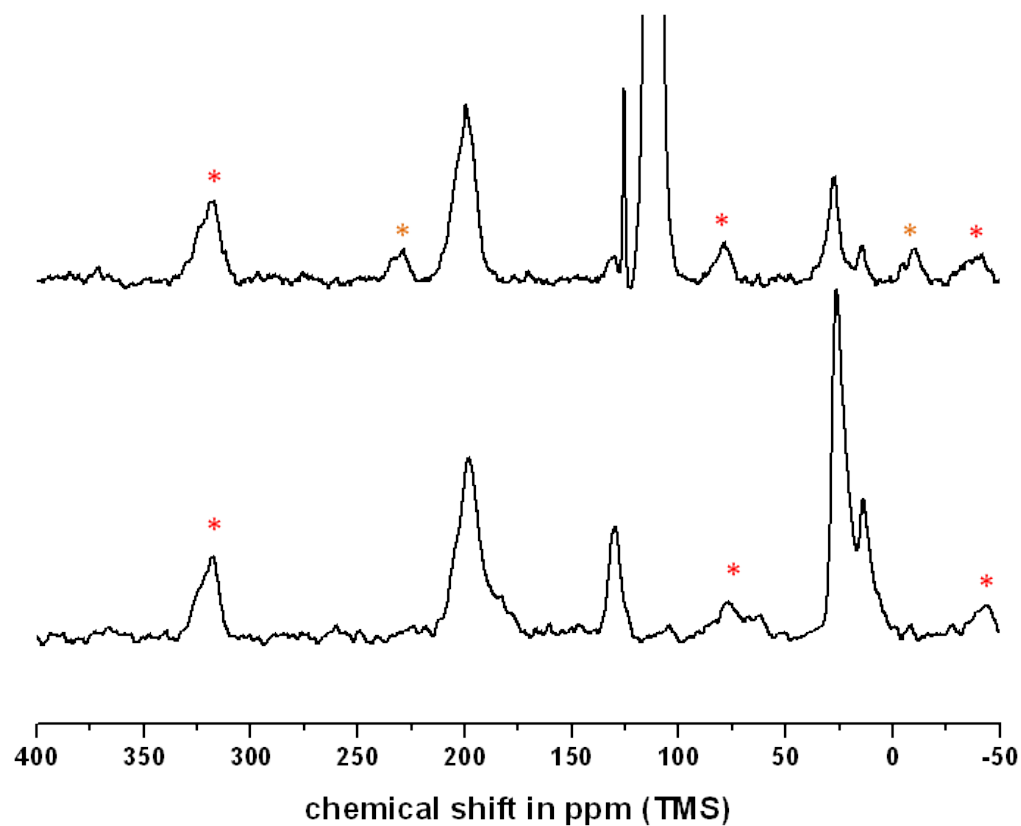


Figure S10. ^{31}P CP-MAS NMR Sn-Ru/dppb prepared with 0.1 equiv. of tin before reaction with CO (red line) and after CO reaction (blue line).

* Spinning side bands

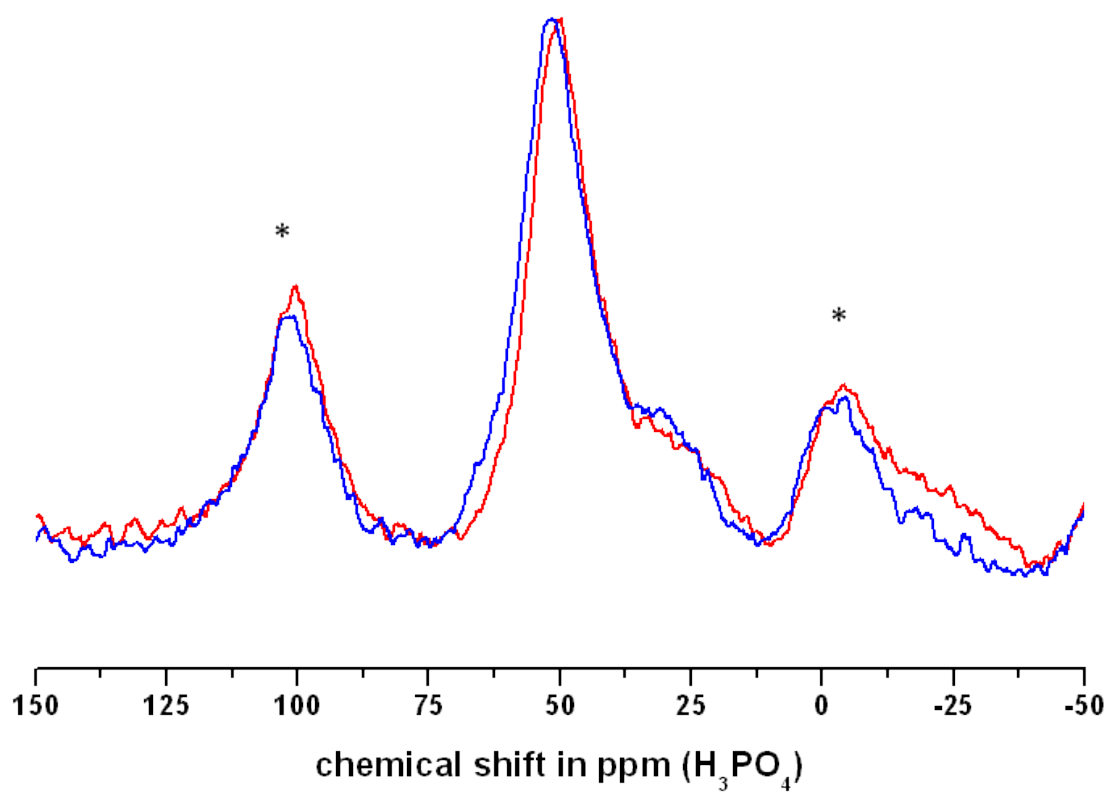
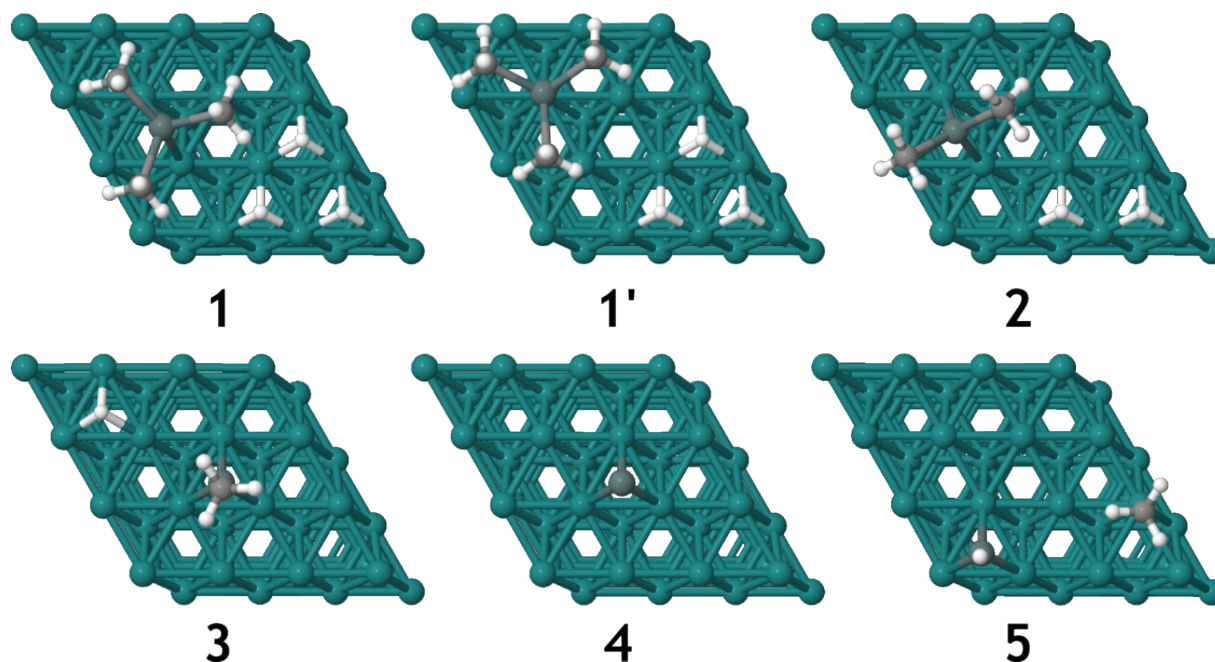


Figure S11. Top view of SnR_m^* , R'_k^* species adsorbed on $\text{Ru}(0001)$. [23]

1: $\mu\text{-SnR}_3^*$, 3H^* ; 1': top-SnR_3^* , 3H^* ; 2: SnR_2^* , 2H^* ; 3: SnR^* , 3H^* ; 4: Sn^* ; 5: SnH^* , Me^* .



[23] *Gaussian 03 (Revision B.05)*. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C. & Pople, J. A. (2003).