

# Influence of Pd and Pt Promotion in Gold Based Bimetallic Catalysts on Selectivity Modulation in Furfural Base-Free Oxidation

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Three different metal loadings were studied: 0.5 wt.%, 1.25 wt.% and 2 wt.%. The ratios between gold and the second metal was varied at 3:1, 1:1 and 1:3.

**Table S1.** DoE procedure applied for the study of bimetallic systems.

Number of catalysts	M-Au/TiO <sub>2</sub>	Ratio M/Au, molar		Matrix			
		M	Au	Run	Blk	A	B
1	0.5	1	1	1	1	-1	-1
2	1.25	1	1	2	1	1	-1
2	1.25	1	1	3	1	-1	1
2	1.25	1	1	4	1	1	1
3	2	1	1	5	1	-1	0
4	0.5	1	3	6	1	1	0
5	1.25	1	3	7	1	0	-1
6	2	1	3	8	1	0	1
7	0.5	3	1	9	1	0	0
8	1.25	3	1	10	1	0	0
9	2	3	1	11	1	0	0

The synthesis of bimetallic catalysts has been conducted in the REALCAT high-throughput equipment by varying the preparation conditions using a DoE. A Response Surface Design (Central Composite) was created. It was designed for 3 factors to model curvature data and identify factor settings that optimize the response. The Central composite design (CCD) was used with 2 factors at three levels of evaluation (low (-1) and high (+1)) and central level (0). The central level was also repeated 3 times to evaluate the error of the DoE model. The aforementioned “levels” are used in CCD to easily represent the minimum, the central and the maximum values of a factor influencing the catalyst activity. In CCD, all the possible combinations of high and low levels are studied for the 2 factors. Hence, the total number of conditions for the CCD was 11 by metals as calculated:  $2n + 3$  repetitions at 0 level (where  $n = 2$ , the number of factors in this study and 3 is the number of levels). As the “Metal” are non-numerical factors, no zero level can be applied for this parameter. Therefore, 2 CCD were conducted one for Pt (11 experiences) and the second one for Pd (11 experiences), 22 experiences for both metal. When varying all the parameters a matrix is built using the “minitab” software.

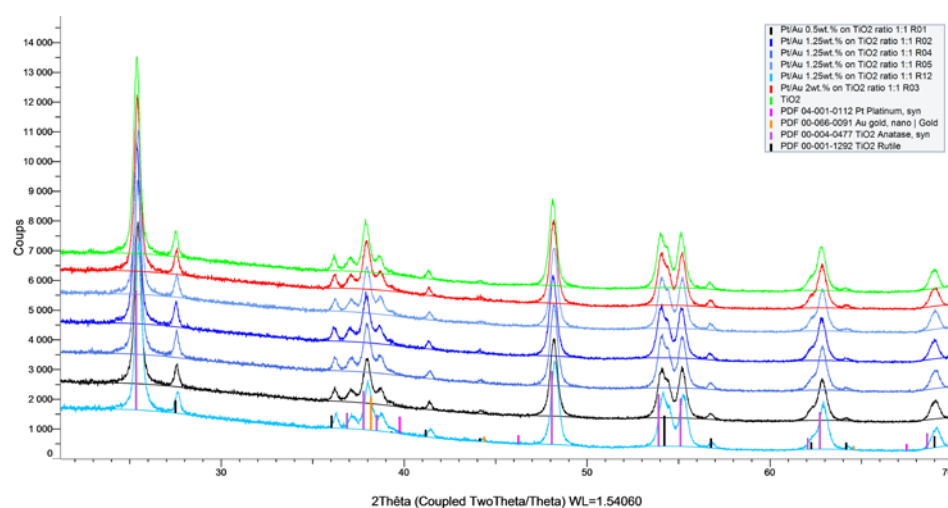


Figure S1. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pt-Au/TiO<sub>2</sub>, ratio 1:1.

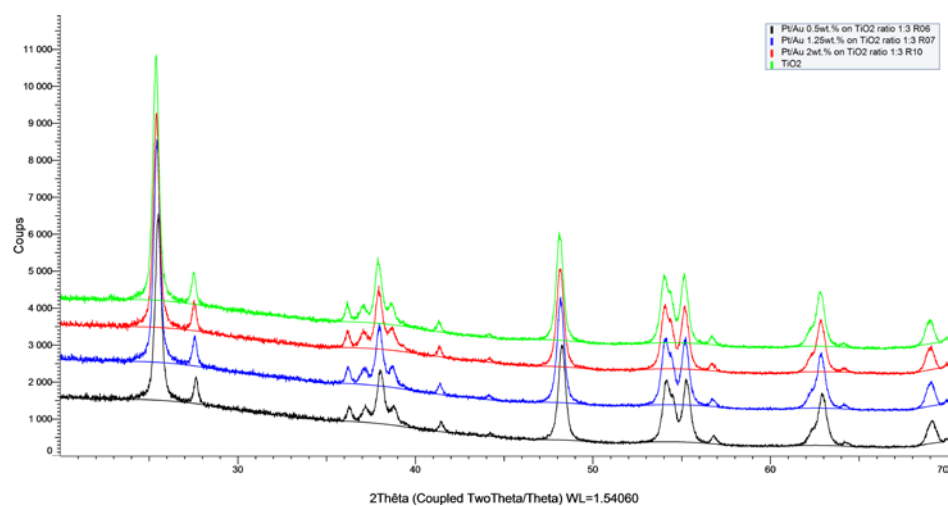


Figure S2. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pt-Au/TiO<sub>2</sub>, ratio 1:3.

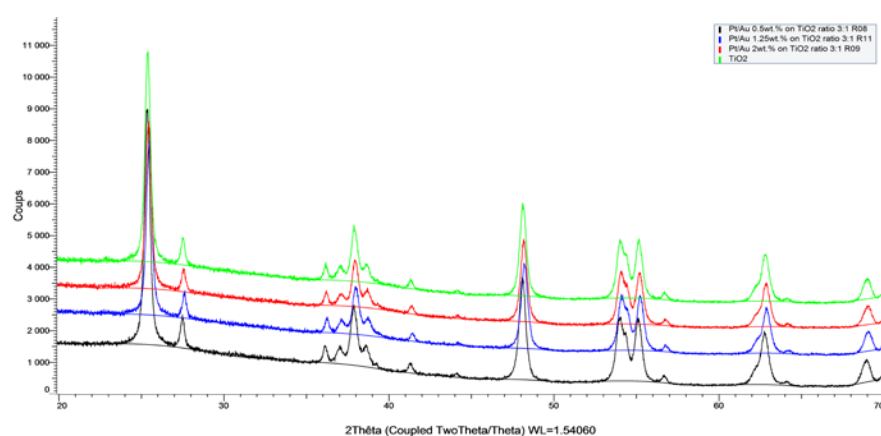


Figure S3. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pt-Au/TiO<sub>2</sub>, ratio 3:1.

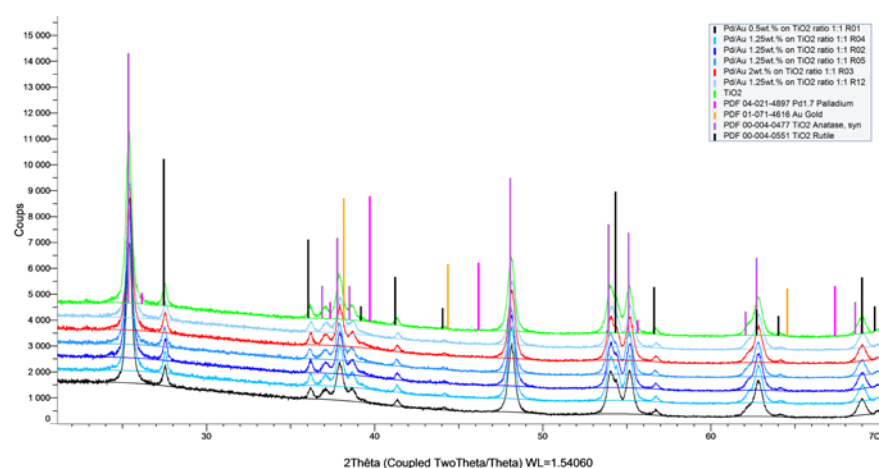


Figure S4. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pd-Au/TiO<sub>2</sub>, ratio 1:1.

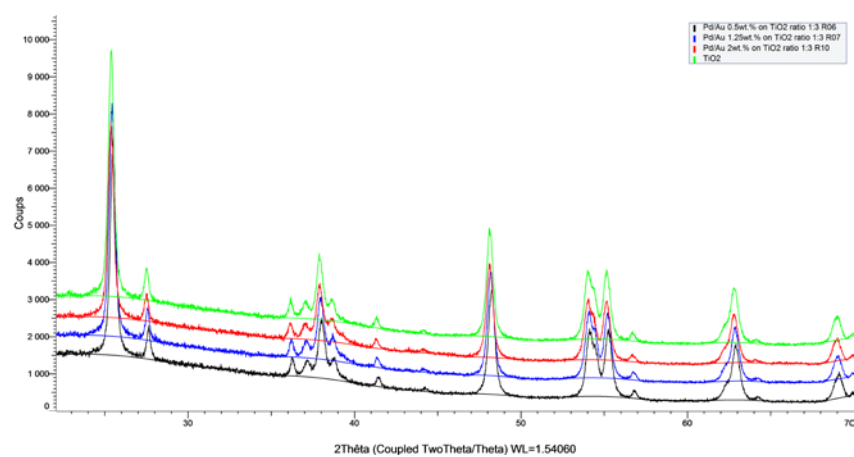


Figure S5. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pd-Au/TiO<sub>2</sub>, ratio 1:3.

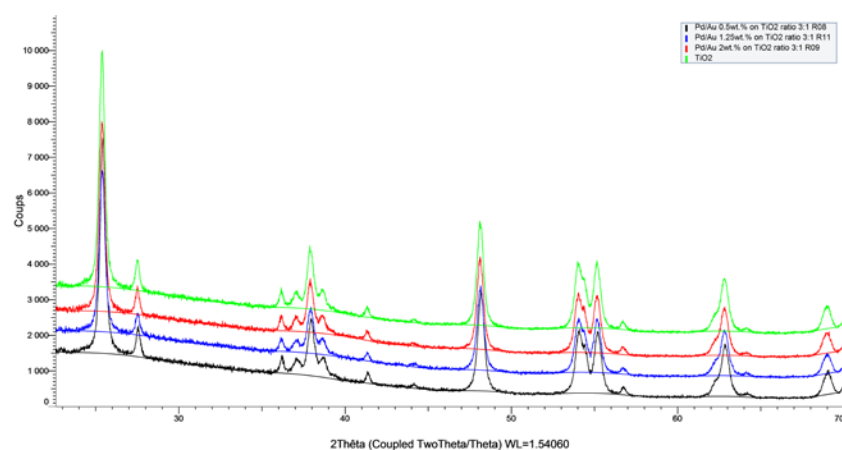


Figure S6. X-ray diffractograms of 0.5, 1.25, and 2wt.% of Pd-Au/TiO<sub>2</sub>, ratio 3:1.

**Table S2.** XRF and ICP analyses results obtained for Au-Pt/TiO<sub>2</sub> catalysts.

		Mean Value wt. %						
		XRF				ICP		
Pt-Au/TiO <sub>2</sub> Expected values	Expected molar Ratio Pt:Au	Pt	Au	Au+Pt	Pt:Au molar ratio	Pt	Au	Au+Pt
0.5	1:1	0.14	0.28	0.42	1 : 1.98	0.16	0.24	0.40
1.25	1:1	0.38	0.69	1.07	1 : 1.80	0.42	0.62	1.04
2	1:1	0.38	0.68	1.06	1 : 1.77	0.75	1.02	1.77
0.5	1:3	0.38	0.67	1.05	1 : 1.75	0.12	0.37	0.49
1.25	1:3	0.71	1.04	1.75	1 : 1.45	0.29	0.90	1.18
2	1:3	0.09	0.42	0.51	1 : 4.62	0.43	1.36	1.79
0.5	3:1	0.27	1.02	1.29	1 : 3.74	0.19	0.13	0.32
1.25	3:1	0.42	1.54	1.96	1 : 3.63	0.50	0.26	0.77
2	3:1	0.17	0.14	0.31	1.23 : 1	1.19	0.50	1.69
2%Pt/TiO <sub>2</sub>		0.949	0.005					

**Table S3.** XRF and ICP analyses results obtained for Au-Pd/TiO<sub>2</sub> catalysts.

		Mean Value wt. %						
		XRF				ICP		
Pd-Au/TiO <sub>2</sub> Expected values	Expected molar Ratio Pd:Au	Pd	Au	Au+Pd	Pd:Au molar ratio	Pd	Au	Au+Pd
0.5	1:1	0.45	0.38	0.84	1 : 0.46	0.18	0.31	0.49
1.25	1:1	1.27	0.87	2.14	1 : 0.37	0.48	0.89	1.37
2	1:1	1.37	1.37	2.75	1 : 0.54	0.68	1.29	1.97
0.5	1:3	1.00	0.46	1.45	1 : 0.25	0.09	0.40	0.49
1.25	1:3	1.03	1.12	2.14	1 : 0.59	0.22	1.15	1.37
2	1:3	0.69	1.69	2.38	1 : 1.33	0.29	1.59	1.88
0.5	3:1	1.12	0.21	1.33	9.71 : 1	0.30	0.17	0.47
1.25	3:1	1.04	0.52	1.57	3.69 : 1	0.72	0.45	1.17
2	3:1	1.42	0.82	2.24	3.21 : 1	1.21	0.78	1.99