**Next-Generation Water-Soluble Homogeneous Catalysts for Conversion of Glycerol to Lactic Acid**

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**Discussion**

1. What is/are the goal(s) of the study in this article?
2. Why is the catalyzed conversion of glycerol to lactic acid useful?
3. Which types of ligands were used in the design of previously reported catalysts, shown in **Scheme 1**?
4. What potential problems did the authors identify as limiting the catalytic activity of homogeneous catalysts for the conversion of glycerol?
5. How did the authors propose to address each problem?
6. Compounds **8**, **9** and **12** are compared in **Chart 3**.
	1. How do the three compounds differ?
	2. What do the carbonyl stretching frequencies for compounds **8**, **9** and **12** suggest about the electronic effect of the ligands? Explain.
	3. Use the Covalent Bond Classification (CBC) method to give the [MLlXxZz]Q± notation, electron count and valence number for compounds **8**, **9** and **12.**
7. Define turnover number (TON) and turnover frequency (TOF). Why are they important in representing a catalyst activity?
8. Use **Chart 1** and **Figure 3** to compare the structure and activity of compounds (**1**-**3**) and (**4**-**9**).What did the authors conclude about the activity of ruthenium vs. iridium catalysts in this series?
9. Use **Chart 1** and **Figure 3** to compare the structure and activity of compounds **4** and **5.**
	1. Use the Covalent Bond Classification (CBC) method to give the [MLlXxZz]Q± notation, electron count and valence number for compounds **4** and **5**..
	2. Which compound has a higher activity ?
	3. What reason do the authors propose for the difference in activity between compounds **4** and **5**?
	4. How do the authors test their hypothesis?
10. Use **Chart 1** and **Figures 3,4** to compare the structure and activity of compounds **7** and **9**.
	1. Which compound has a higher activity?
	2. Compare and contrast the structure of compounds **7** and **9**.
	3. Use the Covalent Bond Classification (CBC) method to give the [MLlXxZz]Q± notation, electron count and valence number for compounds **7** and **9**.
11. Use **Charts 1,2** and **Figure 3** to compare the structure and activity of compounds **5** and **10.**
	1. Use the Covalent Bond Classification (CBC) method to give the [MLlXxZz]Q± notation, electron count and valence number for compounds **5** and **10**.
	2. Which compound has a higher activity?
	3. What do the authors propose to explain the difference in catalytic activity?
12. Why did the authors choose microwave heating over conventional heating?
13. Use **Figure 6** to examine the relation between stir rate and TON. How do the authors justify the effect of stir rate on TON?
14. Name the reaction steps in the catalytic cycle proposed by the authors in **Figure 7**. Use the Covalent Bond Classification (CBC) method to give the [MLlXxZz]Q± notation, electron count and valence number for each intermediate.

