**A Stable Monomeric SiO2 Complex with Donor-Acceptor Ligands: Foundational Implications of Lewis-Acid base interactions in Stabilizing SiO2**

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<http://onlinelibrary.wiley.com/doi/10.1002/anie.201611851/abstract>

**Implementation notes:**

Students should have access to the paper and have read the first and second paragraphs of the paper. Students should also refer to scheme 2 and table 2. In addition, the authors, unfortunately, use two different methods for representing the ligands (**La** = L1, **Lb** = L2 or **Lc** = L3), which could be pointed out to students in advance to avoid confusion or could serve as a teaching point (question 2).

**Questions**

1. Draw Lewis structures of **Lb** (C5H5N which is a ring) and **La** (C5H4N(N(CH3)2)) found in Scheme 1. Include H-atoms. An optional extension of this question would be to ask students which ligand they would expect to be a better electron donor based on their knowledge of functional groups.
2. Are the ligand labels **La** (Scheme 1) and L1 (Table 2) consistent? How did you arrive at your answer? (*Note:* **Lb** is L2 and **Lc** is L3)
3. Referring to the pictures in Table 2 the symbol **L** is connected to the Si using an arrow. Describe what you think the arrow means about this interaction. Would you describe the **L** as Lewis Acid (electron acceptor) or a Lewis Base (electron donor)?
4. Based on your structure of **La** and **Lb** in question 1, indicate the part of the ligand acting as a Lewis acid or base.
5. For SiO2, which atom is the most electropositive and would be most likely to accept additional electrons?
6. Look at Table 2 in the paper. In DFT calculations, absolute energies cannot be determined accurately, however relative energies may be calculated. Column A includes ΔG values for SiO2 which are the calibration point and are set to equal zero. Column B represents the energy change resulting from the addition of **L** to SiO2 resulting in a Si(**L**)O2 complex.
   1. Calculate the energy differences between SiO2 and Si(**L**)O2 for **L1**, **L2**, and **L3**. Based on your answer, is the addition of a ligand to SiO2 energetically favorable or not?
   2. Does addition of **L1**, **L2** or **L3** offer the most stable Si(**L**)O2 complex?
   3. Which ligand is the most electron donating?
   4. How are stability and electron donating ability related?
   5. An optional extension question would be to ask students if this data corroborates or contradicts their prediction comparison of **L1** and **L2** in Q1.
7. In column C, the addition of a donor-acceptor ligand (**D-A**)is considered. The D of that ligand is behaving the same as the previously discussed **L** ligands. Describe the interaction between the oxygen of the SiO2 and the **A** portion of the **D-A**.
8. Examine the ΔG values in column C.
   1. Does the addition of **D-A** (column C) stabilize SiO2 relative to free SiO2 (column A)?
   2. Compared to the addition of **L** (column B), does the addition of **D-A** stabilize SiO2 more or less?
9. Examine the ΔG values in column D.
   1. Does the addition of **D-A** and **L** (column D) stabilize SiO2 relative to free SiO2 (column A)?
   2. Compared to the addition of **L** (column B), does the addition of **D-A** and **L** stabilize SiO2 more or less?
   3. Compared to the addition of **D-A** (column C), does the addition of **D-A** and **L** stabilize SiO2 more or less?
10. SiO2 is unstable by itself and cannot be isolated but the researchers were able to synthesize a compound that contained SiO2 that is stable. What conclusions can you draw about how to stabilize a molecule like SiO2 with an electropositive Si and electronegative O based on your answers to Q8 and Q9? Suggest another molecule that could act as **L**.