Created by S. Chantal E. Stieber (sestieber@cpp.edu), Brandon Quillian (brandon.quillian@armstrong.edu), Chip Nataro (nataroc@lafayette.edu), Gary Guillet (gary.guillet@armstrong.edu) and Maria Carroll (mcarro17@providence.edu) posted on VIPEr (www.ionicviper.org) on June 3, 2017. 

**A Stable Monomeric $SiO_2$ Complex with Donor-Acceptor Ligands: Foundational Application of VSEPR for Understanding Crystallographic Data**

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

You should have access to the paper and read the first, second, and fourth (beginning with "The X-ray structure…") paragraphs on the first page and the second full paragraph (beginning with "The X-ray diffraction analysis…") on the second page. Please also reference scheme 1 and figure 1.

**Questions**

1. In complex **2**, Si is coordinated to four atoms. What are the electronic ($AX_mE_n$; X = group, E = lone pair) and molecular geometries?

2. For the geometry from the previous question, what should the idealized angles around silicon be?

3. In complex **2**, there are two oxygen atoms bridging the silicon centers. What are the electronic and molecular geometries?

4. For the geometry from the previous question, what should the idealized angles around oxygen be?

5. Complex **3a** is best thought of as $SiO_2$ stabilized by two additional ligands. Draw the Lewis dot structure and predict the geometry and bond angles for $SiO_2$.

6. Refer to the single crystal X-ray diffraction data for compounds **2** and **3a** shown in Figure 1 of the article. Answer the following questions:
   a. What are the reported O-Si-O, N-Si-O and N-Si-N bond angles surrounding the silicon centers in each of these compounds?

| | **2** | **3a** |
|---|---|---|
| O-Si-O | | |
| O-Si-N | | |
| N-Si-N | | |

   b. Are the reported bond angles for the silicon centers in agreement with your bond angle prediction? Why or why not?

7. What are the reported bond angles for the bridging oxygen atoms in compound **2**? Are they in agreement with your bond angle predictions from question 4? Why or why not?

   Si1-O1-Si2 =
   O1-Si1-O3 =

8. List the reported Si-O bond distances for compound **2**. Are all Si-O bonds equivalent? Why or why not? Refer also to the structure shown in scheme 1.

| | **2** |
|---|---|
| Si1-O1 | |
| Si1-O2 | |
| Si1-O3 | |
| Si2-O1 | |
| Si2-O3 | |
| Si2-O4 | |

9. List the reported Si-O bond distances for compound **3a**. How do these compare to those from compound **2**?

| | **3a** |
|---|---|
| Si1-O1 | |
| S1-O2 | |

10. Examine the reported O2-P and Si1-O2 bond distances for compounds **2** and **3a**. How do these compare, and why?

| | **2** | **3a** |
|---|---|---|
| O2-P1 | | |
| Si1-O2 | | |