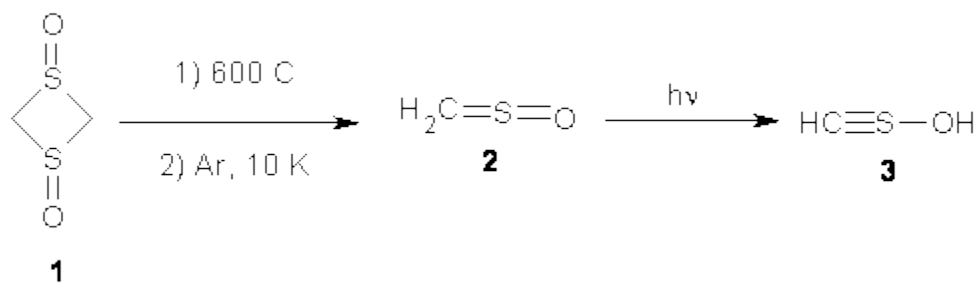
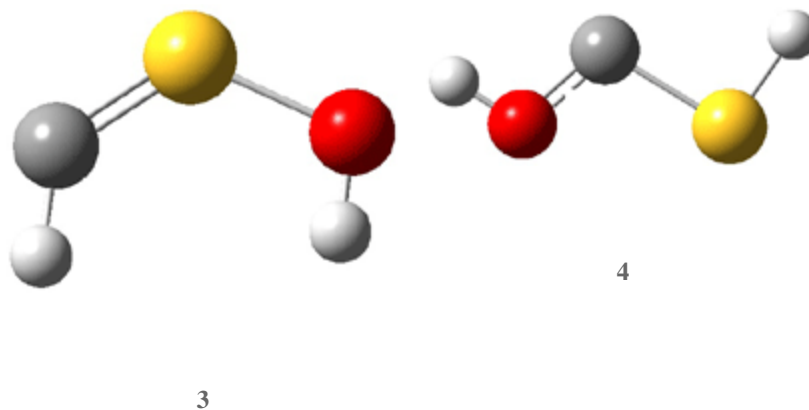


# THE C-S TRIPLE BOND

Does the Carbon-Sulfur triple bond exist? There's probably little doubt it does in the CS molecule. But now Schreiner and Mloston have offered up the H-C≡S-OH species as a possibility.<sup>1</sup> Obtained by flash photolysis of **1**, giving **2**, and upon irradiation at 254 nm, H-C≡S-OH **3** is the observed species and not the expected carbene HO-C-SH **4**. **3** is confirmed by excellent agreement between the observed and computationally predicted IR spectra.



The CCSD(T)/cc-pVTZ structures of **3** and **4** are shown in Figure 1. It is interesting that the carbene is not observed, even though it is 26.6 kcal mol<sup>-1</sup> more stable than **3**.



**Figure 1.** CCSD(T)/cc-PVTZ optimized structures of **3** and **4**.<sup>1</sup>

So is there a triple bond? The short C-S distance (1.547 Å) is very similar to that in CS (1.545 Å). NBO analysis indicates a triple bond. But the MOs indicate significant lone pair build-up on both C and S, consistent with the strongly non-linear angles about these two atoms. The authors conclude that **3** is a “structure with a rather strong CS double bond or a weak triple bond”.

Source: <http://comporgchem.com/blog/?p=510>