STRUCTURE OF DIHYDROXYCARBENE

Dihdroxycarbene was the subject of a post a few years ago relating to how this carbene does not undergo tunneling,[1] while related hydroxycarbene do undergo a tunneling rearrangement.

Now we have a gas-phase microwave determination of the *trans,cis* isomer of dihydroxycarbene.[2]The computed CCSD(T)/cc-pCVQZ structure is shown in Figure 1. What is truly remarkable here is the amazing agreement between the experimental and computed structure – as seen in Table 1.The bond distance are in agreement within 0.001 Å and the bond angles agree within 0.3°! Just further evidence of the quality one can expect from high-level computations. And computing this structure was certainly far easier than the experiments!

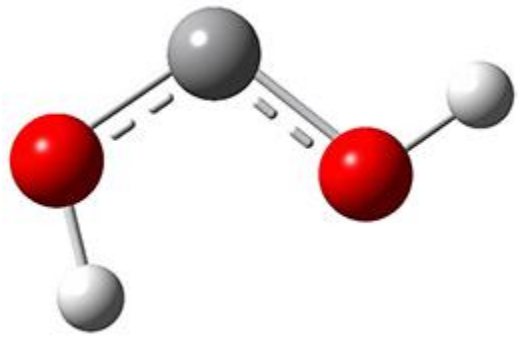

Figure 1. CCSD(T)/cc-pCVQZ optimized geometry of dihydroxycarbene.

Table 1. Experimental and computed (CCSD(T)/cc-pCVQZ) geometric parameters of dihydroxycarbene.[a]

	Expt.	Comp.
C-O	1.335	1.336
C-O	1.309	1.309
$O\text{-}H_{trans}$	0.961	0.960
$O\text{-}H_{cis}$	0.976	0.975
O-C-O	107.30	107.25
$C\text{-}O\text{-}H_{trans}$	106.8	106.8
$C\text{-}O\text{-}H_{cis}$	110.7	110.4

[a]Distances in Å and angles in deg.

Source: http://comporgchem.com/blog/?p=3130