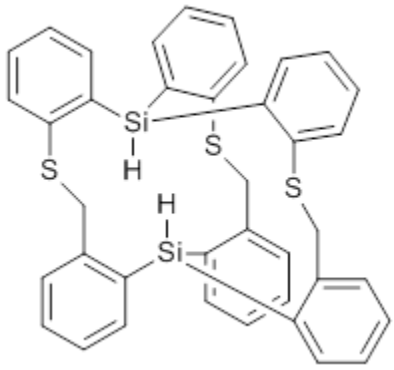
EXTREMELY SHORT NON-BONDING H···H DISTANCE

What is the closest non-bonding H···H distance within a single molecule? The world record had been 1.617 Å in a pentacyclodecane.[1] This record now appears to be broken by the preparation of the disilane **1**.[2] The ^{1}H NMR and IR suggest the interior hydrogens are very close. The x-ray structure of **1** indicates a very short Si-Si distance of 4.433 Å, a distance that must accommodate two S-H bonds, typically about 1.48 Å and the H···H non-bonded distance, which might be as short then as 1.47 Å! The crystal is unfortunately not large enough for a neutron diffraction study, which would enable precise location of the hydrogens.



However, computations can help here, and they suggest a H···H separation of only 1.57 Å: this is the distance obtained with B3PW91/6-311+G(2d,p), M062x/6-311+G(2d,p) and MP2/6-31G(d). The M062x/6-311+G(2d,p) structure is shown in Figure 1.

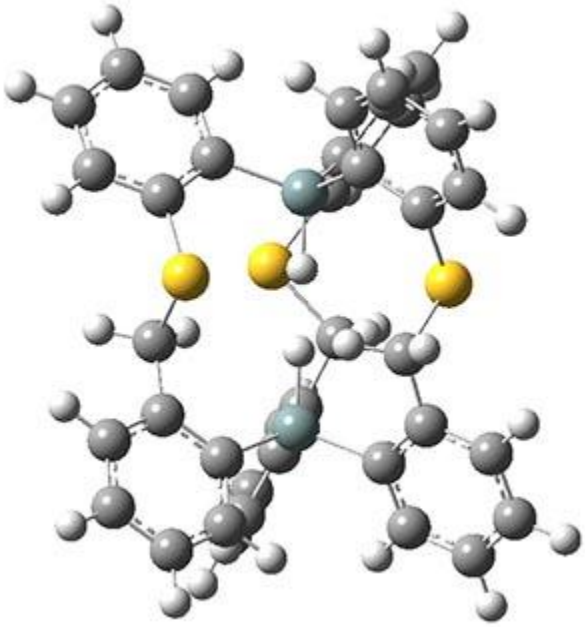


Figure 1. The M062x/6-311+G(2d,p) optimized structure of **1**.

Source: http://comporgchem.com/blog/?p=2853