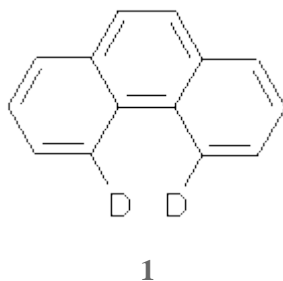


# NO H···H BONDING IN PHENANTHRENE DESPITE A BOND PATH

I blogged on Bickelhaupt's examination of the stability of kinked *vs.* linear polycyclic aromatics<sup>1</sup> in this post. Bickelhaupt argued against any H···H stabilization across the bay region, a stabilization that Matta and Bader<sup>2</sup> argued is present based on the fact that there is a bond path linking the two hydrogens.

Grimme and Erker have now added to this story.<sup>3</sup> They prepared the dideuterated phenanthrene **1** and obtained its IR and Raman spectra. The splitting of the symmetric ( $a_1$ ) and asymmetric ( $b_1$ ) vibrational frequencies is very small 9-12  $\text{cm}^{-1}$ . The computed splitting are in the same range, with very small variation with the computational methodology employed. The small splitting argues against any significant interaction between the two hydrogen (deuterium) atoms.

Further, the sign of the coupling between the two vibrations indicates a *repulsive* interaction between the two atoms. These authors argue that the vibrational splitting is almost entirely due to conventional weak van der Waals interactions, and that there is no “bond” between the two atoms, despite the fact that a bond path connects them. This bond path results simply from two (electron density) basins forced to butt against each other by the geometry of the molecule as a whole.



Source: <http://comporgchem.com/blog/?p=8>