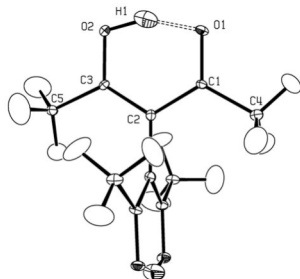


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Neutron Diffraction and X-ray Charge Density Studies of Tetraacetylene. P. Piccoli^a, E. Zhurova^b, J. Eckert^c, A. Pinkerton^b, T. Koetzle^a, A. Schultz^a, D. Hadzi^d, ^aIPNS, ANL, Argonne, IL 60439; ^bDept. of Chemistry, Univ. of Toledo, Toledo, OH 43606; ^cMaterials Research Laboratory, Univ. of California, Santa Barbara, CA 93106; ^dNational Inst. of Chemistry, Ljubljana, Slovenia.



Single crystal neutron diffraction data have been collected on a sample of tetraacetylene (TAE) at five temperatures between 20 and 298 K in order to characterize the temperature-dependent behavior of the short, strong, intramolecular hydrogen bond. Upon decreasing the temperature from 298 K to 20 K, the O2-H1 distance decreases from 1.17(1) to 1.081(2) Å while the O1...H1 distance increases from 1.33(1) to 1.386(6) Å. The convergence of the C-O bond lengths to identical values (1.285(4) Å) at 298 K, from inequivalent distances at low temperature, illustrates the dynamic equilibrium between the keto- and enol tautomers of this compound and is consistent with a resonance-assisted hydrogen bond. The O...O distance (2.432 ± 0.006 Å) varies little with temperature. Sub van der Waals

intermolecular C-H...O contacts may be responsible for this ordering at low temperature. Preliminary experimental charge density results from low temperature x-ray diffraction will also be presented.

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