Poster Presentation

MS035.P12

Tuning of hydrogen bonding network in functional material by deuteration

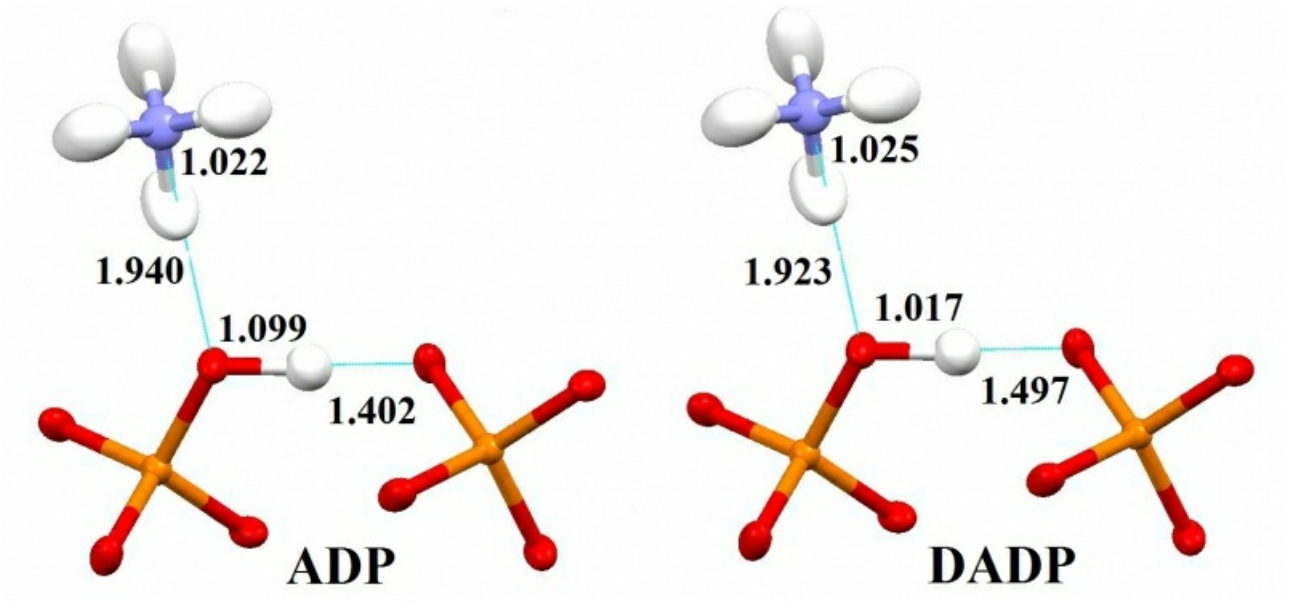
Rajul Ranjan Choudhury[1], Chitra Radhakrishnan[1]
[1]*Bhabha Atomic Research Center, Mumbai, India*
E-mail: rajul@barc.gov.in

Functional materials are those materials which possess particular native properties and functions of their own, for instance materials exhibiting ferroelectricity, piezoelectricity, magnetism or energy storage functions. An ability to tune the important properties of these functional materials can provide us with desired flexibility in device building and hence it is important to look for methods to do the same. One way of altering the properties of hydrogenous materials is to replace the hydrogens of the material by its stable isotope deuterium, this process is called deuteration. Since the electron clouds of its component atoms define the shape of a molecule, deuterated compounds have shapes and sizes that are very similar to their all-hydrogen analogues but there can be an observable change in their physical properties because deuteration can significantly alter the interactions like the hydrogen bond interactions which play a defining role in determine the physical properties of the crystals.

We shall be presenting the comparison between the structures of the hydrogenous as well as deuterated ammonium dihydrogen phosphates (ADP and DADP) obtained from single crystal neutron diffraction investigation conducted at Dhruva reactor in Trombay Mumbai. Although the neutron structure for ADP was solved long back but no single crystal neutron diffraction study of its deuterated analogue has been reported. ADP is known for a long time for its excellent electro-optic and non-linear optic (NLO) properties but recently the interest in these materials has been revived due to rising demand of a material with high fourth harmonic generation (FHG) efficiency required for the inertial confinement fusion (ICF) facilities [1]. Compared with deuterated potassium dihydrogen phosphate (DKDP) which is the most commonly used crystals for ICF facilities ADP crystal has a larger NLO coefficient, a higher laser damage threshold, a shorter UV transmission cut-off, a faster growth speed and a much lower production cost hence ADP is believed to be a powerful competitor against the DKDP and potassium dihydrogen phosphate (KDP) crystals that are extensively used today.

ADP crystals have two types of hydrogen bonds (figure-1) first is the double well O-H-O hydrogen bonds between phosphate ions and second is the N-H—O hydrogen bonds between the ammonium ions and phosphate ions. Both these hydrogen bonds undergo subtle changes on deuteration (figure-1). As a result almost all the important physical properties [2] of the crystals like the phase transition temperature, conductivity, refractive index, electro-optic coefficients etc are altered. Both primary as well as secondary isotope effects are analysed using a simple effective two diabatic state Hamiltonian [3] for a hydrogen bond between a donor D and an acceptor A.

1) Shaohua Ji, Fang Wang, Lili Zhu, Xinguang Xu, Zhengping Wang & Xun Sun (20133), scientific reports 3 : 1605 DOI: 10.1038/srep01605
2) Lili Zhu, Baoan Liu, Lisong Zhang, Qinghua Zhang, Zhengping Wang, and Xun Sun, (2015), Chinese Optics Letters, 13, 041601-041601
3) Ross H. McKenzie, (2012) , Chemical Physics Letters, 535 ,196–200



Keywords: neutron diffraction, hydrogen bonding, isotope effect