

Nonlinear Optical Potential of Engineered Sodium D-Isoascorbate Monohydrate Single Crystals: A Comprehensive Characterization Study

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Supporting article

Section S1:

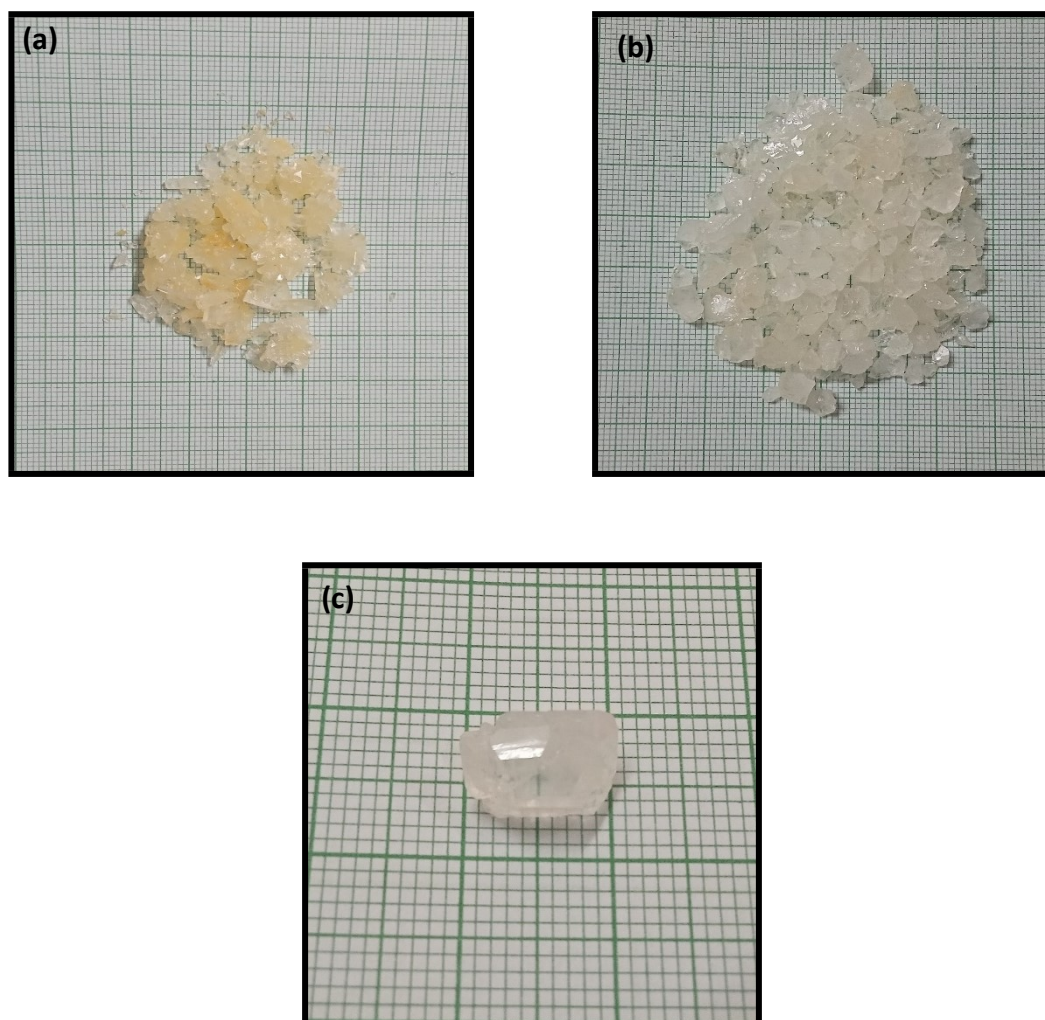


Figure S1: (a) Primary crystallisation process was carried out using precursors materials (D-isoascorbic acid and sodium carbonate). The process was completed within 2 weeks, yielding

lightly yellow-tinted, transparent crystals that were very small in size. This coloration may be due to the presence of minor impurities or suboptimal crystal formation. (b) crystals grown from 2nd recrystallization approach. This process was implemented by employing seed crystals obtained from 1st crystallization process (seed recrystallization process), which enhances the uniformity of the crystal growth by providing nucleation sites, reducing spontaneous heterogeneous nucleation to an extent. The crystals were harvested after 12 days, which appears visually clear as compared to image (a), suggesting improved impurity and fewer defects. (c) a sample image of crystal grown from slow cooling technique over 21 days to promote controlled and orderly crystal formation. This method reduces the inclusion of solvent molecules and impurities within the crystal lattice, leading to superior crystallographic quality. as a result, they a superior structural integrity surpassing both the primary and secondary crystallization process.

Section S2:

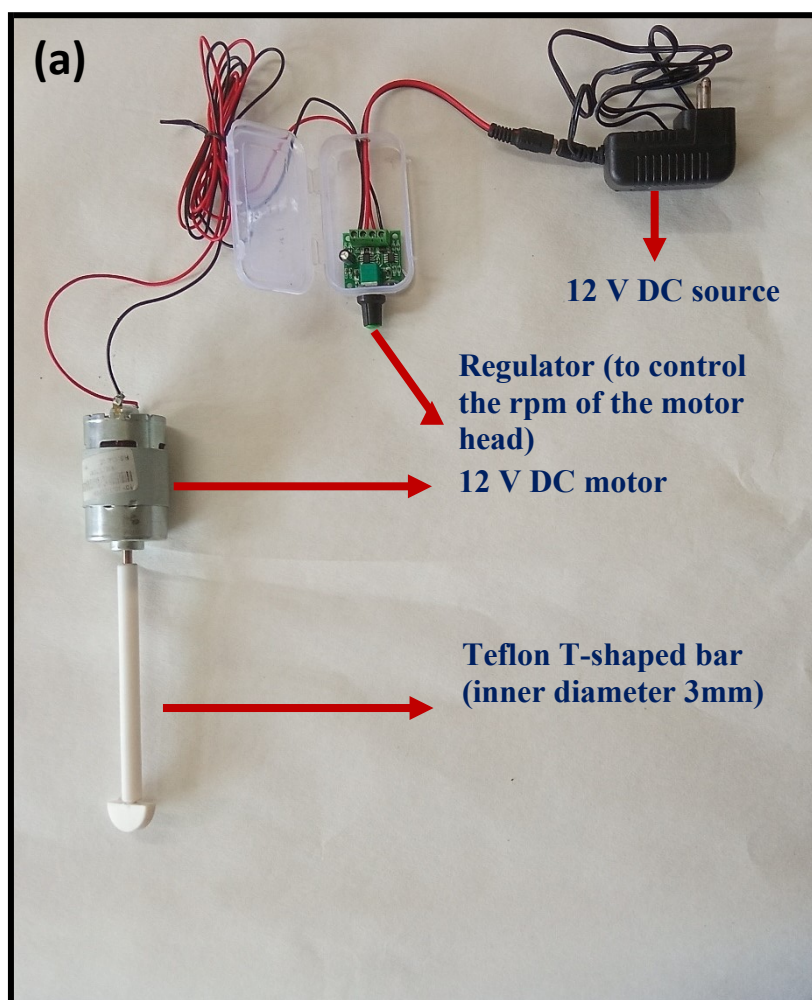


Figure S2: custom-made vertical stirrer to measure the solubility of as-grown NADISAM sample (an alternative approach to an immerse stirrer)

Section S3: Breif discussion of CDM model:

CDM is an approximation method introduced by Renne and Nijboer in 1960^{34,35}. Macroscopically this model considers a group of molecules as a collection of dipoles. The polarization of each dipole is influenced by the external electric field as well as the field generated by neighbouring dipoles. Microscopically, each dipole is an electron which bounds to the nucleus through harmonic restoring force (classical harmonic oscillator) us by a harmonic restoring force. Intrinsically, these oscillators do not possess any dipole moment. However, in the presence of an external electric field, the electron and nucleus move away from each other, inducing a dipole moment, which contributes to the polarization of the material

Section S4: sample preparation for Photoconductivity measurement.

A well-polished thin NDIAM crystal (2 mm) is coated with silver paste on two corners of the face whose area is $7.85 \times 10^{-1} \text{ cm}^2$ and dried. The crystal is then placed between the copper electrodes of the cryostat where the pressure is maintained at 10^{-6} mbar. The electrodes are then connected to the external voltage.

Section S5:

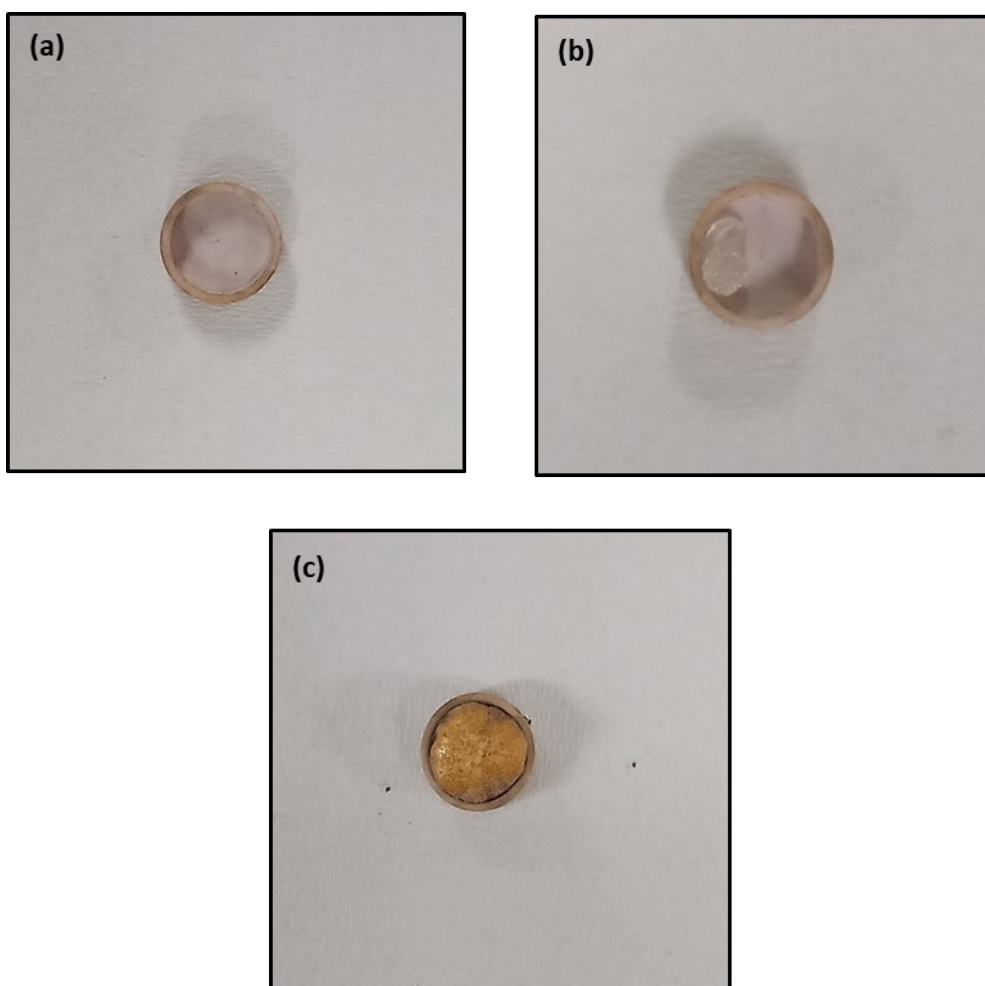


Figure S3. (a) TGDTA alumina pan before the experiment, (b) pan with 3.02 mg of NADISAM crystal before the experiment (c) pan with NADISAM crystal after 160°C results in decomposition of the material

Section S5:

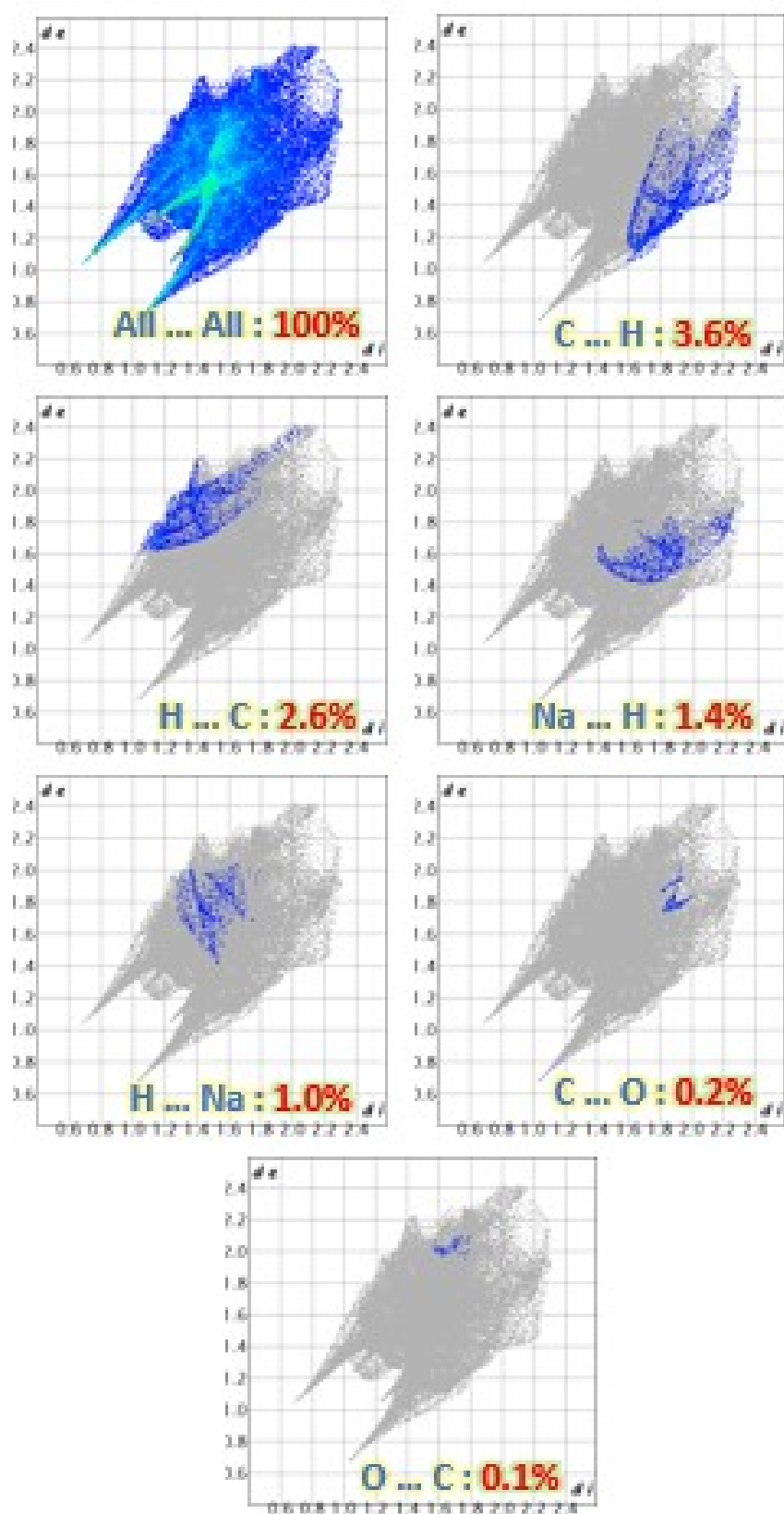


Figure S4. Fingerprint plot for all – all contributions and all minor interactions.

Section S6:

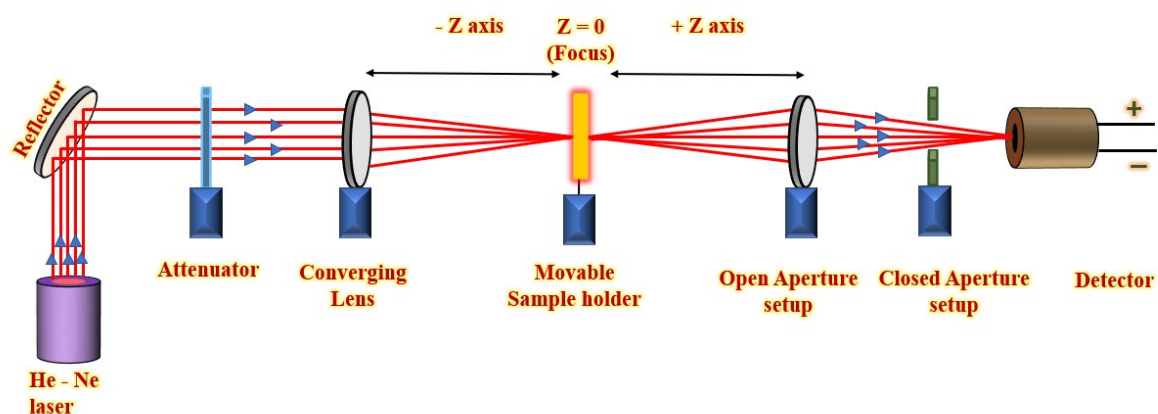
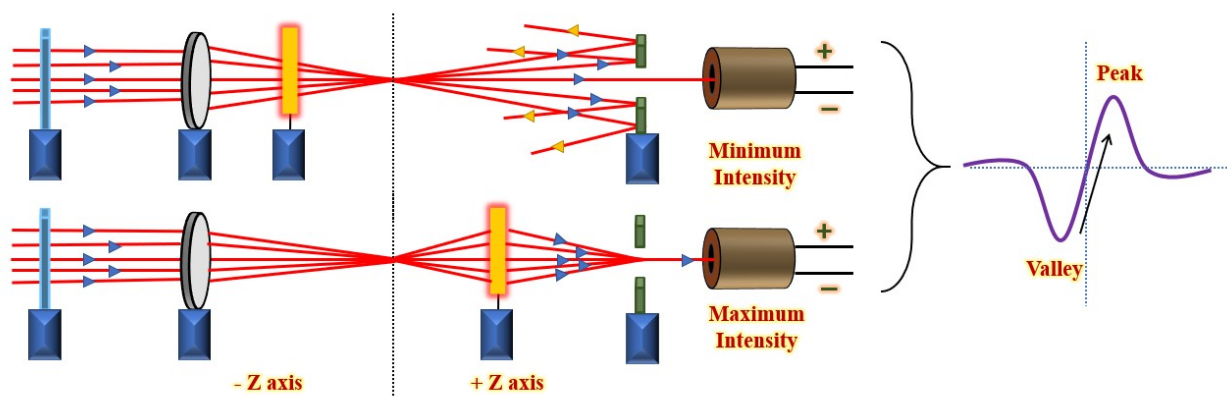
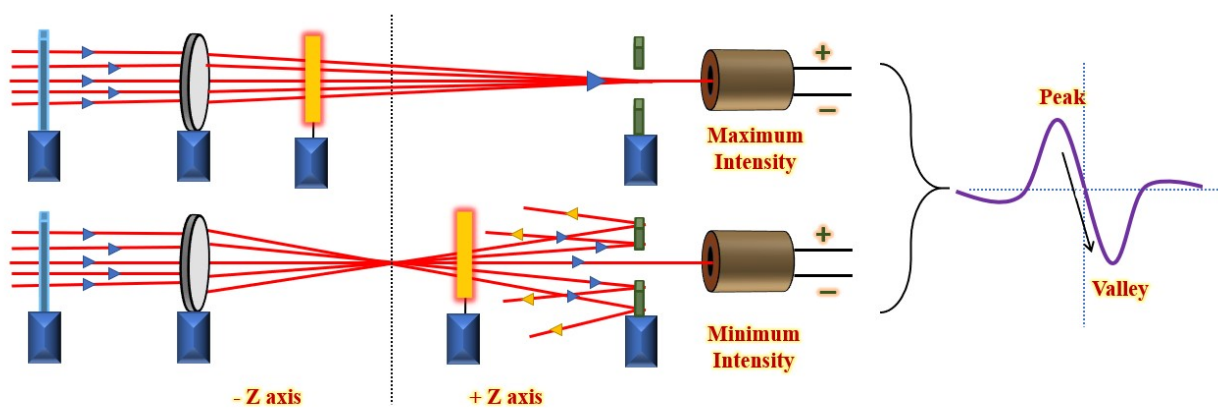


Figure S5. Experimental setup of Z scan analysis in open and closed aperture modes.



Self focussing nature of sample in closed aperture mode



Self de-focussing nature of sample in closed aperture mode

Figure S6. Mechanisms involved in closed aperture mode

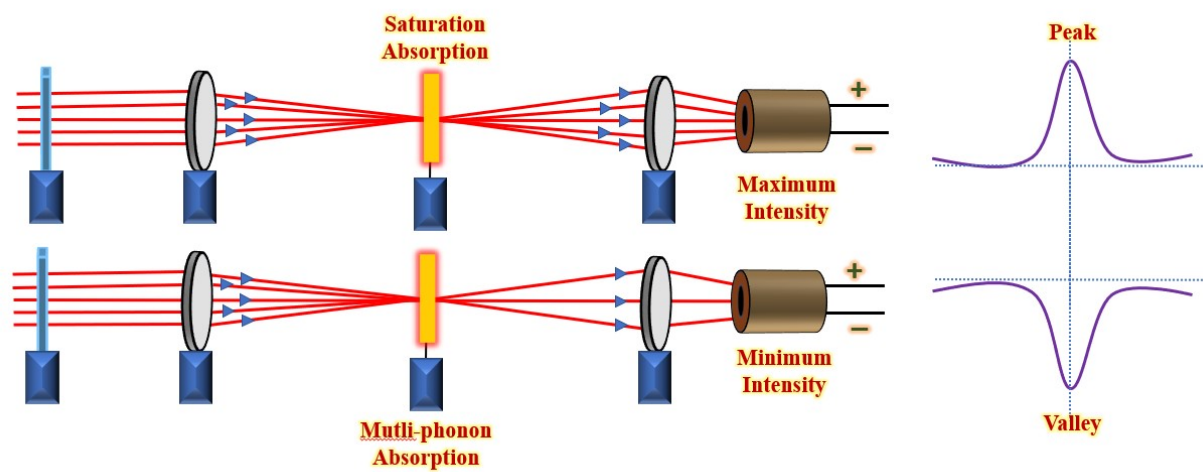


Figure S7. Mechanisms involved in open aperture mode.