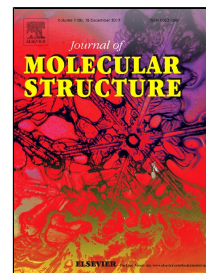


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Supramolecular network through N-H...O, O-H...O and C-H...O hydrogen bonding interaction and density functional theory studies of 4-methylanilinium-3-carboxy-4-hydroxybenzenesulphonate crystal



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Highlights

- 4MABS salt was synthesized and grown as single crystals
- The title salt involves extensive N-H...O, O-H...O and C-H...O hydrogen bonding interactions.
- The grown crystal is thermally stable up to 235 °C.
- The first hyperpolarizability (β) is found to be 5.01 times that of urea.
- The Vickers microhardness studies confirm the soft nature of the grown crystal.

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