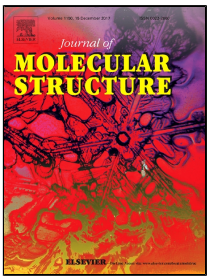
Accepted Manuscript



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

M. Rajkumar, P. Muthuraja, M. Dhandapani, A. Chandramohan

PII:	S0022-2860(17)31344-3
DOI:	10.1016/j.molstruc.2017.10.013
Reference:	MOLSTR 24384
To appear in:	*Journal of Molecular Structure*
Received Date:	11 August 2017
Revised Date:	03 October 2017
Accepted Date:	04 October 2017

Please cite this article as: M. Rajkumar, P. Muthuraja, M. Dhandapani, A. Chandramohan, 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, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.10.013

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 ºC.
- 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.