Comparing Charge Densities of Opioids: Morphine, Codeine and Dextrometorphane

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Opioids are not only of interest from their biological activity but also because of their unusual chemical structure. They consists of an oligocyclic strained cage structure with different types of rings and bonds. Matta [1] presented a method of reconstruction larger molecules from submolecular fragments based on theoretical calculations. To compare these results with experimental findings, we examined the charge densities of the title compounds obtained from a high resolution X-ray experiment at 25 K and CCD area detection. The datasets were refined with the XD program package [2]. A full topological analysis was performed including a submolecular partitioning making use of the zero flux surfaces of the electron density gradient vector field according to the "atoms in molecule"-theory of Bader [3]. To evaluate the atomic volumes and charges the program TOPXD [4] was used.

In order to examine the transferabillity of smaller fragments the topology of submolecular parts of the three molecules were compared with each other and with those of the Matta study.

[1] Matta C.F., J. *Phys. Chem.*, 2001, **A 105**, 11088. [2] Koritsanszky T. *et al.*, *XD*, Freie Universitaet Berlin. User Manual, 2001. [3] Bader R.F.W., *Atoms in Molecules*, Clarendon Press, Oxford, 1994. [4] Volkov A., Gatti C., Abramov Y., Coppens P., *Acta Cryst.*, 2000, **A56**, 332.

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