[MS13-P02] Charge density study of resveratrol(*trans*-3,4′,5-trihydroxystilbene)

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This work deals with the study of experimental electronic structure of resveratrol and with a comparison to theoretical calculations. Experimental X-ray data measurement of resveratrol was performed on an Oxford Diffraction Gemini R diffractometer equipped with a Ruby CCD detector and a graphite monochromator, using Mo-Kα radiation at 100(2) K. The final refinement of crystal structure data using SHELXL - 97 gave a R - factor of 0.0490 for 4004 diffractions. The topological analysis was performed using XD package. A complete atom - centered multipole refinement was carried out with the nonspherical atomic electron density given by the equation [1]:

$$\rho_{at}(r) = P_c\rho_{core}(r) + P_v\kappa^3\rho_{valence}(\kappa r) + \\ + \sum_{l=1}^{l_{max}} \kappa'^3 R_l(\kappa' r) \sum_{m=0}^{l} P_{lm\pm} d_{lm\pm}(\theta, \varphi).$$

Theoretical calculations were done using TONTO [2], CRYSTAL06 [3] and GAUSSIAN03 [4] software focused on the hydrogen bonding between two molecules of resveratrol. Comparison of experimental and theoretical electron, deformation densities and laplacian maps will be presented. The intermolecular OH bond lengths in the whole pack which consist of six molecules of our compound is considered.

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[1] Coppens, P., X-ray Charge Densities & Chemical Bonding, *Oxford University Press.*, 1997.

[2] TONTO, Jayatilaka, D. and Grimwood, D.J., Computational Science - ICCS, 2003, 2660, 142-151.

[3] CRYSTAL06 User's Manual, Dovesi, R. *et. al.,* University of Torino, Torino, 2006.

[4] GAUSSIAN03, Revision C.02, Frisch, M. J. *et al.,* Gaussian, Inc., Wallingford CT, 2004.

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