# SYNTHESIS, CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF IONIC ADDUCT OF 2,4-DIAMINO-6-PHENYL-1,3,5-TRIAZINE WITH MALONIC ACID

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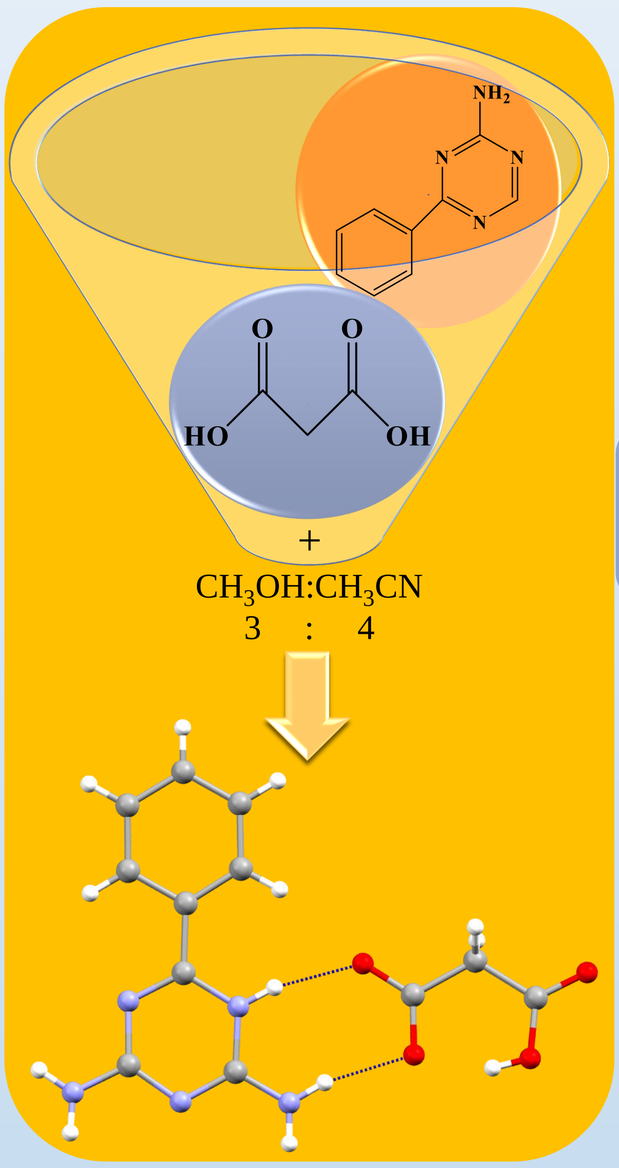
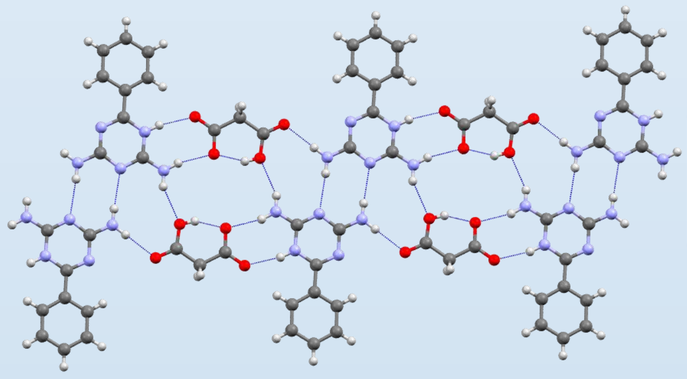
## INTRODUCTION

2,4-Diamino-6-phenyl-1,3,5-triazine (dpt) is a popular molecule widely used both in coordination and supramolecular chemistry due to the availability of nitrogen-rich organic triazine core acting as a good donor and acceptor in supramolecular synthesis to design materials with desired physicochemical properties. Co-crystallization of dpt with various organic and inorganic acids resulted in multidimensional supramolecular architectures [1, 2]

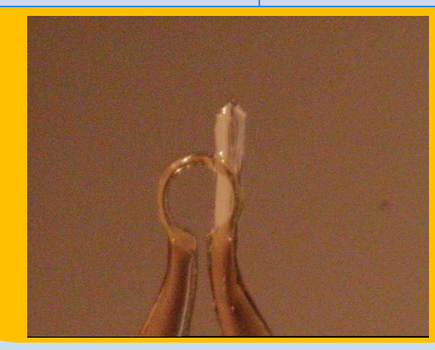
## SYNTHESIS




## X-ray

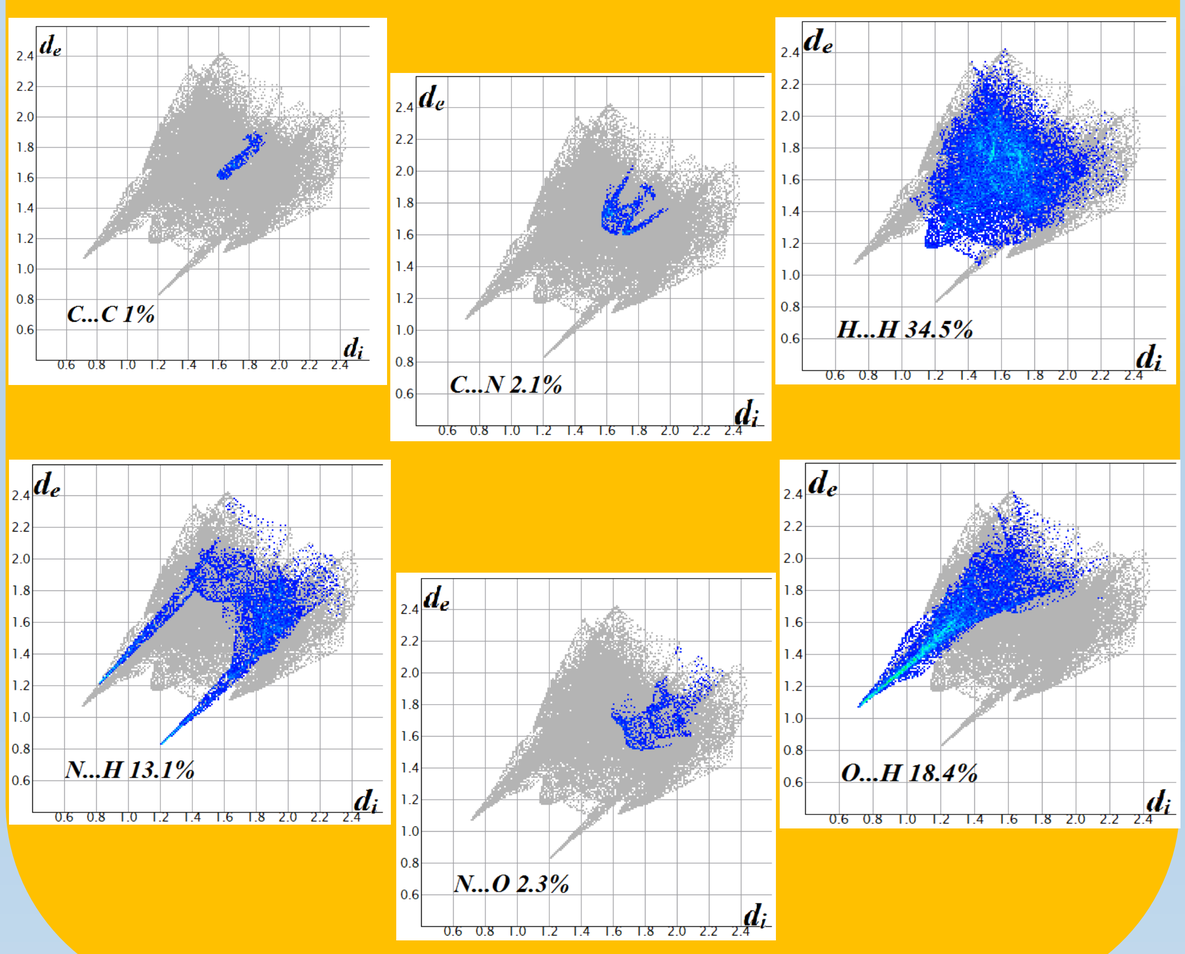


| | |
|---|---|
| **Empirical formula** | $C_{12}H_{13}N_5O_4$ |
| **T, K** | 293(2) |
| **Formula weight** | 291.27 |
| **Crystal system** | monoclinic |
| **Space group** | $P2_1/c$ |
| **Volume, E$^3$** | 1255.7(3) |
| **a/Å** | 8.4392(13) |
| **b/Å** | 5.1001(6) |
| **c/Å** | 29.207(5) |
| **α** | 90 |
| **β** | 92.719(14) |
| **γ** | 90 |



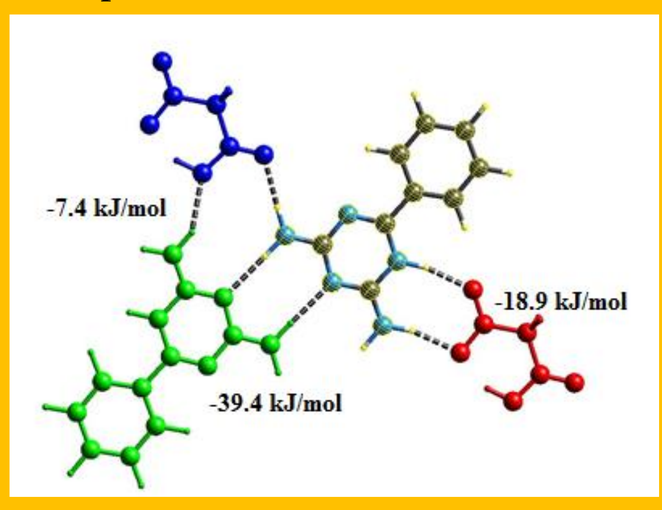
## HIRSHFELD SURFACE ANALYSIS

Hirshfeld surface analysis revealed that the H···H (34.5%), O···H (18.4%) and N···H (13.1%) interactions make the highest contributions to the Hirshfeld surface.




## ENERGY EVALUATION

The intermolecular energy evaluation calculated according to the energy model CE-B3LYP with 6-311G (d,p) basis set revealed that the N-H···N hydrogen bonds from homosynthon are more effective, having a higher energy value (-39.4 kJ/mol) compared to the N-H···O hydrogen bonds in heterosynthons (-18.9 kJ/mol and -7.4 kJ/mol), thus confirming significance of such interactions for stabilization of supramolecular architecture.




| | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|---|---|---|---|---|---|---|---|
| | 6.18 | B3LYP/6-31G(d,p) | -62.5 | -13.1 | -16.2 | 114.7 | -18.9 |
| | 8.98 | B3LYP/6-31G(d,p) | -54.5 | -13.1 | -18.4 | 70.9 | -39.4 |
| | 7.28 | B3LYP/6-31G(d,p) | -19.5 | -3.5 | -7.9 | 36.8 | -7.4 |

## CONCLUSION

Synthesis and characterization of this structure of basic dpt and flexible malonic acid are reported. The X-ray studies show that this structure represent an organic salt. In the result of the Hirshfeld analysis it was observed that the N-H···N hydrogen bonds from homosynthon are more effective, having a higher energy value -39.4 kJ/mol.

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