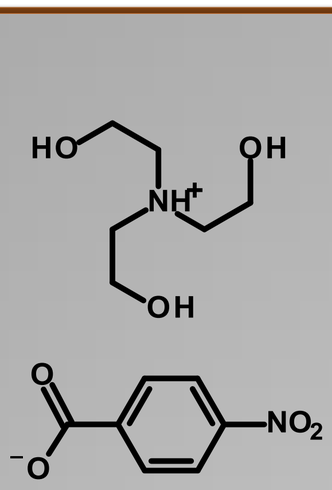
# INSIGHTS INTO CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF Cu(II) TRIETHANOLAMINE 4-NITROBENZOATE

**Anastasia GOROBET[1], Manuela E. CRISAN[2], Paulina N. BOUROSH[1], Lilia CROITOR[1]**

*[1]Institute of Applied Physics, Academy str., 5 MD2028, Chisinau, R. Moldova; nasteagorobet@gmail.com*

*[2]"Coriolan Drăgulescu" Institute of Chemistry, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*

Metal complexes formation using mixed organic ligands such as alkanolamines and benzoates is of current interest for assembling different types of coordination architectures with modified functional characteristics and new useful properties compared to starting ligands. The literature data show that the reaction conditions, the nature of the metal ions and the ligands are the main factors which dictate the type of complex.




**(HTEA)(4NB)**

+

**Ca(II)** → **$[Ca(TEA)_2](4NB)_2$**

**Ni(II)** → **$[Ni(4NB)(TEA)(H_2O)](4NB)$**

**Ni(II)** → **$[Ni(4NB)(TEA)(H_2O)](4NB)\cdot H_2O$**

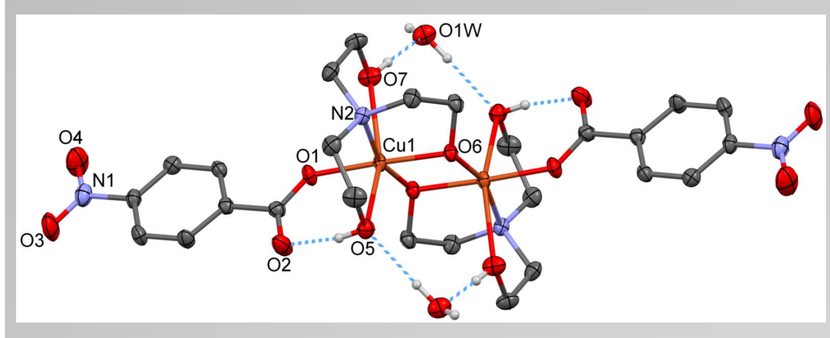
**Ni(II)** → **$[Ni(TEA)_2](4NB)_2$**

**Zn(II)** → **X**

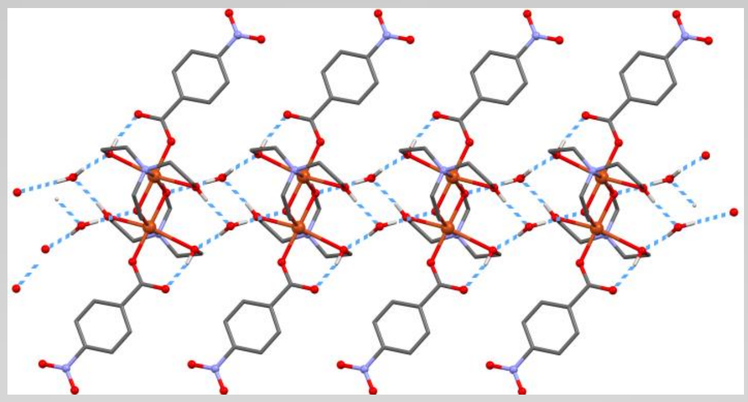
**Cu(II)** → **$[Cu_2(TEA)_2(4NB)_2]\cdot 2H_2O$** **(1)**

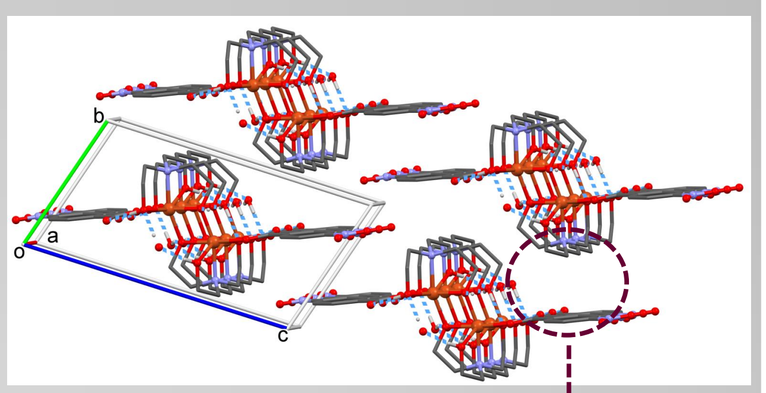
Recently, we successfully synthesized and structural characterized single crystals of new organic salt (HTEA)(4NB) [1] and its different types of Ca(II) [2] and Ni(II) [1] complexes obtained from the same Me(II)-organic salt system under various experimental conditions.

Over the time, dinuclear Cu(II) amino alcohol complexes have received particular attention, as building blocks in metallo supramolecular chemistry, as model of copper enzymes and precursors of molecular magnetic and catalytic materials. This study investigates the role of (HTEA)(4NB) salt in the structure formation of new metal complexes, focusing on dialkoxo bridged Cu(II) complex (**1**).




**$Cu_2(TEA)_2(4NB)_2].2H_2O$**



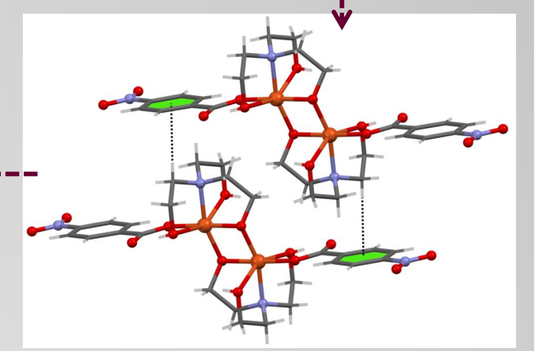



| | | | |
|---|---|---|---|
| **Formula** | $C_{26}H_{36}Cu_2N_4O_{16}$ | **b/Å** | 8.1977(5) |
| **T, K** | 293(2) | **c/Å** | 14.4815(10) |
| **FW** | 787.67 | **α/°** | 74.458(6) |
| **CS** | Triclinic | **β/°** | 86.428(6) |
| **SG** | P-1 (№ 2) | **γ/°** | 68.895(7) |
| **a/Å** | 7.4881(7) | **V/Å³** | 798.42(11) |

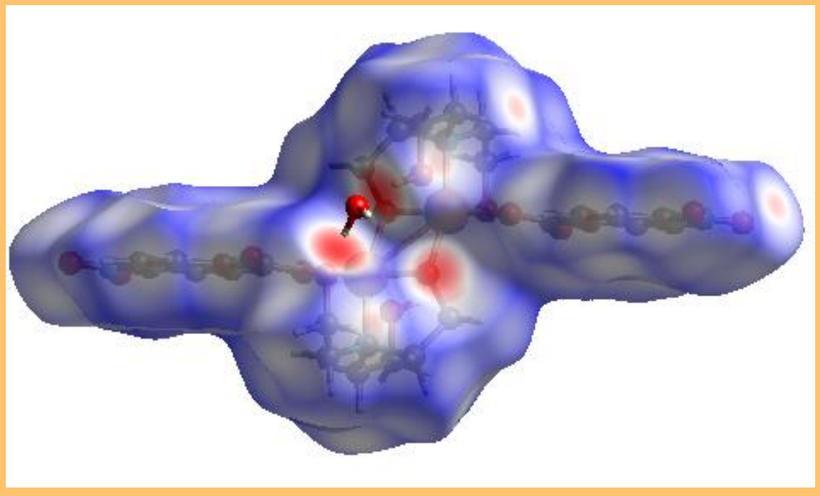
| | N | Symop | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | x, y, z | 8.89 | B3LYP/6-31G(d,p) | -9.9 | -5.2 | -60.3 | 33.1 | -46.4 |

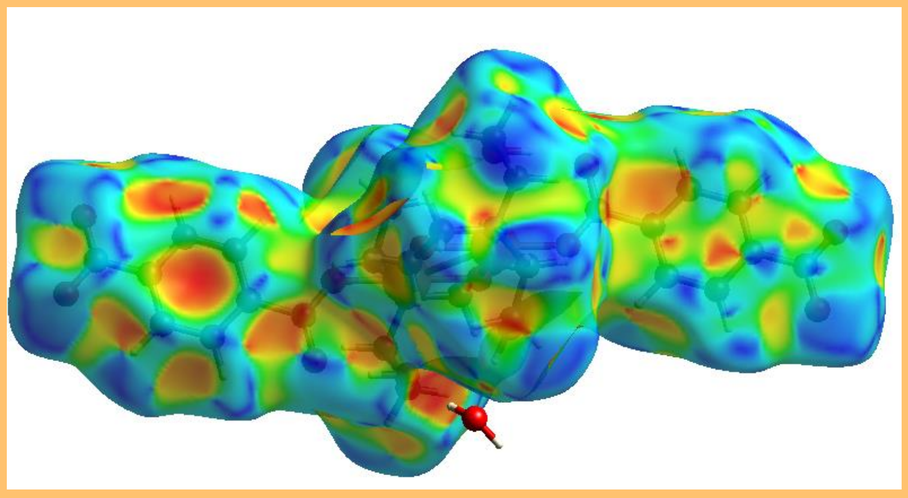
Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

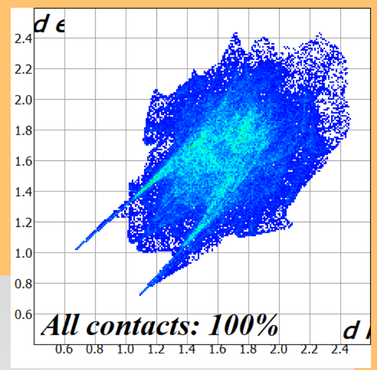
| Energy Model | k_ele | k_pol | k_disp | k_rep |
|---|---|---|---|---|
| CE-HF ... HF/3-21G electron densities | 1.019 | 0.651 | 0.901 | 0.811 |
| CE-B3LYP ... B3LYP/6-31G(d,p) electron densities | 1.057 | 0.740 | 0.871 | 0.618 |

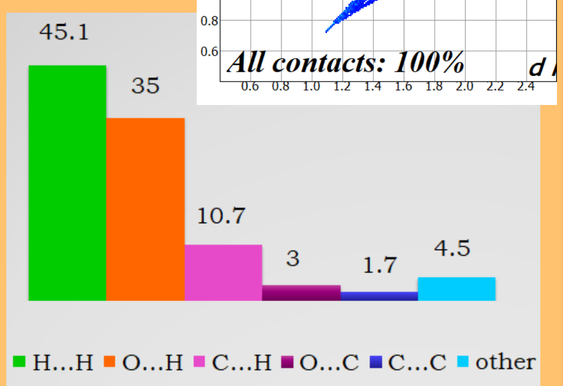


The structural investigation indicates that non-covalent intermolecular interactions, such as O–H···O and C–H···π, contribute to the packaging of the components in the crystal, while the Hirshfeld surface and 2D fingerprint graphs quantify these interactions and show their priority.








**CONCLUSIONS:** This study presents the building block role of (HTEA)(4NB) salt in the creation of various supramolecular architectures highlighting the new metal complexes formed by triethanolamine tetradentate ligand, known in some studies as atrane, which have applicative importance in agriculture and medicine.

***Acknowledgements***. *This work was partially supported by Project ANCD 20.80009.5007.15 of the Institute of Applied Physics and Program 2, Project 2.1 of the ''Coriolan Dragulescu'' Institute of Chemistry.*

[1] A. GOROBET, M. E. CRISAN, P. N. BOUROSH, A. V. SIMINEL, L. CROITOR // Supramolecular architectures and photoluminescent properties of triethanolammonium 4-nitrobenzoate salt and its Ni(II) complexes // Polyhedron, 193, 2021, 114893.
[2] A. GOROBET, M. CRISAN, M. PETRIC, P. BOUROSH, L. CROITOR // Structural study of Ca(II) coordination compound with triethanolamine and 4-nitrobenzoic acid // Rev. Roum. Chim., 2018, 63(12), 1183-1187.