shows exceptional thermal stability up to  $200^{\circ}$ C whereas **2** which is fully dehydrated at  $100^{\circ}$ C, begins to collapse after  $110^{\circ}$ C.

 Yaghi O., Li Q., MRS Bulletin 2009, 34, 682. [2] Naik A. D., Dîrtu M. M., Léonard A., Tinant B., Marchand-Brynaert, Su B. L., Garcia Y., Cryst. Growth Des. 2010, 10.1021/cg901473. [3] Naik A. D., Marchand-Brynaert J., Garcia Y., Synthesis 2008, 149.

# Keywords: MOF, crystal engineering, supramolecular chemistry

### FA4-MS31-P17

Zn<sub>2</sub>(O<sub>2</sub>CCF<sub>3</sub>)<sub>4</sub> and Zn<sub>7</sub>O<sub>2</sub>(O<sub>2</sub>CCF<sub>3</sub>)<sub>10</sub> – Syntheses and Crystal Structures. <u>Nina van Gellecom<sup>a</sup></u>, Georgi Genchev<sup>a</sup>, Walter Frank<sup>a</sup>, <sup>a</sup>*Institut für Anorganische und Strukturchemie II, Heinrich-Heine Universität Düsseldorf, Germany* E-mail: wfrank@uni-duesseldorf.de

The first examples of zinc trifluoracetates were reported in 1939 by F. Swarts [1]. These salts were found to be suitable precursors for the preparation of ZnO:F, which is of interest for the semiconductor research [2]. So far, only microcrystalline samples or solvates of zinc trifluoracetates have been described. Here we report on the syntheses and the crystal structures of the parent  $Zn_2(O_2CCF_3)_4$  (1) and of  $Zn_7O_2(O_2CCF_3)_{10}$  (2). Single-crystals of 1 have been obtained by the thermolysis of  $In(O_2CCF_3)_3$  in the presence of elemental zinc at 240 °C under static vacuum. 1 crystallizes in the monoclinic space group  $P2_1/c$  with lattice parameters of a =11.558(2) Å, b = 12.561(3) Å, c = 16.602(5) Å, and  $\beta =$ 134.121(17) ° with Z = 4. The structure is composed of two crystallographically independent Zn atoms that are linked by three trifluoroacetate groups. These fragments are connected by a further trifluoroacetate anion to form chains along [010]. Single-crystals of 2 have been prepared by the thermolysis of  $Ce(O_2CCF_3)_3$  in the presence of zinc powder under reduced pressure at 320 °C. 2 crystallizes in the triclinic space group  $P\overline{1}$  with lattice parameters of a = 10.754(3) Å, b = 13.543(5) Å, c = 17.634(5) Å,  $\alpha = 68.323(5)$  °,  $\beta = 89.772(5)$  ° and  $\gamma =$ 66.634(4) ° and with Z = 2. In the crystal of 2 the Zn<sub>7</sub>O<sub>2</sub> fragments, which are composed of two edge-sharing Zn<sub>4</sub>O tetrahedrons, are coordinated by ten trifluoroacetate groups. These fragments are linked by a bridging trifluoroacetate group to form chains along [001].

[1] Swarts F., Bull. Soc. Chim. Belg., 1939, 48, 176. [2] Klingshirn C., ChemPhysChem, 2007, 8, 782.

Keywords: zinc compounds, single-crystal X-ray diffraction, thermal behaviour

#### FA4-MS31-P18

### Novel 2D Assembly of Triptycene Cation Radicals vs. Traditional 1D Motifs Sergey V. Lindeman, Khushabu Thakur, Rajendra Rathore Department of Chemistry, Marquette University, Wisconsin, USA E-mail: sergey.lindeman@mu.edu

A series of triptycene derivatives with varying number of *o*dimethoxy substituents along with their corresponding cation radical salts has been synthesized. The methoxy-substituted benzene rings possess a lower oxidation potential whereas the



lengths of their  $C_{Ar}$ -O bonds provide a very sensitive indicator of the positive charge associated with the corresponding arene ring (i.e. 5.3 pm bond contraction per unit charge). The triptycene molecules were designed as a 3-

dimensional  $\pi$ -delocalized alternative to traditional planar 2dimensional ion-radical substrates. Using highly precise lowtemperature (100 K) X-ray structural data, the intra-molecular electronic interaction/delocalization was identified both in the neutral molecules and in the corresponding cation radicals. Specifically, C<sub>Ar</sub>-O bonds in the neutral triptycenes are progressively elongated by up to 1.0 pm with increasing electron donicity of the molecules whereas C<sub>Ar</sub>-O bonds in the corresponding cation radicals are additionally shortened by 2.0 pm (per unit charge) for interacting dimethoxy-substituted benzene rings. Importantly, both the neutral molecules and their cation-radical salts have a very uniform/conserved association mode of the dimethoxy-substituted arene rings in



crystals. They form close anti-parallel couples that are strengthened by multiple C- $H \cdots \pi$  hydrogen bonds and dipole-dipole interactions. These forces are further strengthened in the crystals of the cation radicals being assisted by favorable  $\pi$ - $\pi$ 

interactions. The regular association of triptycene rings produces 2-dimensional layers with continuous electronic  $\pi$ - $\pi$  delocalization throughout the plane of the layers via combination of intra- and inter-molecular charge resonance. This packing mode is principally different from the traditional



1-dimensional stacking of the planar aromatic ion radicals and hence opens new avenues in supramolecular design of the nextgeneration electronic materials for photovoltaic

applications.

Keywords: supramolecular self-assembly, cation radical salts, charge resonance

### FA4-MS31-P19

## Synthetic Polymers in Biological Environment. Jindřich Hašek, Jan Dohnálek, Tereza Skálová, Jarmila Dušková, Andrea Štěpánková, Petr Kolenko Institute of Macromolecular Chemistry, Academy of Science, 16206 Praha 6, Czech Republic E-mail: hasek at imc.cas.cz

Many practical applications where synthetic polymers are in a direct contact with bio-macromolecules are known. Positive and also some negative consequences of polymer activity in