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#### FA4-MS26-P25

**Low-melting molecular complexes of chloroform and dichloromethane.** Dmitry S.Yufit, Judith A.K.Howard, Department of Chemistry, Durham University, South Rd., Durham, DH1 3LE, UK  
E-mail: [d.s.yufit@dur.ac.uk](mailto:d.s.yufit@dur.ac.uk)

In continuation of our studies of low-melting co-crystals [1], both components of which are liquid under ambient conditions, the crystals of new molecular complexes of chloroform (I) and dichloromethane(II) have been grown *in situ* and structurally characterized. The structures of new co-crystals of II with cyclohexanone, 1,4-dioxane and butanone-2 are compared with corresponding complexes of I and with the structures of pure components of these co-crystals. In spite of seeming simplicity of the components, the structures display a variety of types and motifs of intermolecular interactions. Indeed, if the (Cl)C-H...O contacts are present in all studied structures, different spatial arrangements of these contacts combined with a delicate balance of weaker interactions of C-H...Cl, C-H...O and even of O...Cl types make the structures of each of these compounds unique, curious and challenging for prediction. Examples of unforeseen products of co-crystallization experiments will also be discussed.

[1] Yufit D.S., Howard J.A.K., *CrystEngComm*, 2010, 12, 737-741

**Keywords:** low-temperature crystallization, molecular complexes, intermolecular interactions

#### FA4-MS26-P26

**Absolute Structure of Two Derivatives of a Longipinene from *Stevia lucida*.** Graciela Díaz de Delgado<sup>a</sup>, Pablo A. Chacón<sup>b</sup>, Juan M. Amaro-Luis<sup>b</sup>, Hyunsoo Park<sup>c</sup>, José Miguel Delgado<sup>a</sup>, <sup>a</sup>Laboratorio de Cristalografía and <sup>b</sup>Laboratorio de Productos Naturales, Universidad de Los Andes, Mérida, Venezuela, <sup>c</sup>IUMSC, Indiana University, USA.  
E-mail: [migueld@ula.ve](mailto:migueld@ula.ve)

7 $\beta$ ,9 $\alpha$ -Dihydroxy-longipin-2-en-1-one (**1**), obtained by basic hydrolysis of a mixture of diesters of longipin-2-ene-1-one, afforded a 7 $\beta$ -hydroxy-9-one (compound **2**) via Collins oxidation and a 7,9-dione (compound **3**) via Jones oxidation. Compound **2** is orthorhombic,  $P2_12_12_1$ , with  $a=6.7905(2)$ ,  $b=11.4566(3)$ ,  $c=17.4319(5)$  Å,  $V=1356.13(7)$  Å<sup>3</sup>,  $Z=4$ . The refinement converged to  $R=0.0301$ ,  $wR=0.0790$ ,  $S=1.043$ . Compound **3** is also orthorhombic,  $P2_12_12_1$ , with  $a=6.4241(1)$ ,  $b=10.5101(2)$ ,  $c=19.1813(4)$  Å,  $V=1295.08(4)$  Å<sup>3</sup>,  $Z=4$ . The refinement converged to  $R=0.0290$ ,  $wR=0.0743$ ,  $S=1.057$ . In compound **2**, the hydroxyl group participates in a R(9) hydrogen bond with the ketone O at C1 of a molecule with symmetry operation  $2-x, -1/2+y, 1/2-z$ . They produce zig-zag chains along  $b$  which interact with similar chains through hydrogen bonds between an H from the methyl group at C10

and the ketone O2 at C9. Additionally, there is one intramolecular hydrogen bond between the methyl group at C10 and the ketone O2 at C9 with graph set symbol S(5). In the absence of the hydroxyl at C7, the hydrogen bond patterns and packing of compound **3** is different. Pairs of molecules related by  $-1+x, y, z$  are connected by a hydrogen bond between an O atom and the H's of two methyl groups, resulting in a R<sub>2</sub><sup>1</sup>(8) graph set. They form chains along the  $a$ -axis which interact via van der Waals forces.

**Keywords:** Natural Products, Hydrogen Bonding, Absolute Structure