dimeric stannate {[Li][(RO)<sub>3</sub>Sn]}<sub>2</sub> (2) [3] behaves as a  $\sigma$ -donor with the very weak  $\pi$ -acceptor ability. Data obtained show that compounds 1 and 2 are of value as nucleophiles with respect to transition metals.

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## MS19 P09

**3-(4-halojenoanilino)phthalides** Orhan Büyükgüngör<sup>a</sup> and Mustafa Odabaşoğlu<sup>b</sup>, <sup>a</sup>Department of Physics, Ondokuz Mayis University, TR-55139, Samsun, Turkey, <sup>b</sup>Department of Chemistry, Ondokuz Mayis University, TR-55139, Samsun, Turkey. E-mail: orhanb@omu.edu.tr

## Keywords: phthalide, isobenzofuranon, benzolacton

Phthalides (isobenzofuranones) are five-membered lactones found in plants and are known to show diverse biological activities as hormones, pheromones and antibiotics. These compounds possess several important properties, such as fungicidal, ctericidal and herbicidal, analgesic and hypotensive and vasorelaxant activities. In addition, phthalide derivatives are useful in the treatment of circulatory and heart-related diseases. They are also found to be associated with pesticideal activities. Considering the potential interest of such phthalide-3-phosphonates in synthetic organic chemistry, and as agrochemical and pharmaceutical agents, we decided to investigate the solid-state structures of 3-substituted phthalides by X-ray diffraction methods and present here the

3-(4-halojenoanilino)phthalides of the compounds (I-IV).

Crystals of  $C_{14}H_{10}FNO_2$ , (I) show paired N-H...O hydrogen bonds that link the molecules into  $R_2^2(12)$  dimmers; the hydrogen-bonded dimmers are linked into chains by an aromatic  $\pi$ - $\pi$  stacking interaction [1]. The structure of  $C_{14}H_{10}CINO_2$ , (II), is stabilized by N-H...O, C-H... $\pi$  and  $\pi$ - $\pi$  interactions [2]. Crystals of  $C_{14}H_{10}BrNO_2$ ,

(III), contain N-H...O hydrogen bond interactions that generate C(6) chains; these chains are linked by C-H...O hydrogen bonds, generating an  $R_4^{\ 3}(21)$  ring motif [3]. The structure of  $C_{14}H_{10}INO_2$ , (IV), whose asymmetric unit contains three independent molecules, are stabilized by three N-H...O, three C-H...O and one N-H...I intermolecular hydrogen bonds, the N-H...O and C-H...O hydrogen bonds generating an edge-fussed  $R_2^{\ 2}(11)$  ring motif which appears as a molecular ladder in the structure [4]. The phthalide parts of all four molecules are planar and the dihedral angles between the phthalide group and the benzene ring are 74.10 (9)°, 75.58 (15)°, 62.2 (2)° and mean 80.5 (4)° for I, II, III and IV, respectively.

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## MS19 P10

Largesupramolecularassembliesofp-sulfonatocalix[4]areneCliveL. Oliver,LeonardJ.Barbour,DepartmentofChemistry,UniversityofStellenbosch,South AfricaE-mail:oli@sun.ac.za

## Keywords: supramolecular, self-assembly, architecture

The supramolecular enclosure of chemical space is ubiquitous in biological systems and serves as inspiration for mimicry of their architecture with synthetic systems. In this regard, the self-assembly of *p*-sulfonatocalix[4]arene, which usually occurs in an "up-down" (bi-layer) fashion, have been induced to occur in an "up-up" arrangement on the addition of lanthanide cations [1,2]. This results in two unique structures with either an icosahedral or a cuboctahedral arrangement of calixarene anions, the former mimicking the geometry of the cowpea chloritic mottle virus.



Here we report the discovery of a further two structures [1 and 2] with spherical arrangements of p-sulfonatocalix[4]arene anions that are not consistent with the geometry of Platonic or Archimedean solids. Crystal data for 1 are a=51.248(4), b=53.333(4), c=28.223(2)Å, space group  $P2_12_12$  whilst that for 2 are a=b=59.262(1), c=49.342(1)Å, space group I-4. The arrangements of the calixarene anions are unique in both structures with 2 consisting of an unprecedented two different spherical arrangements.

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