

polymeric chain through [010]. In addition, the silver(I) ions in 3 are four- and five-coordinated in individual polymeric chains. In 4, the inter-molecular N-H...O hydrogen bonds form one-dimensional polymeric chains through the *a* axis. These linear chains are inter-connected to each other by N-H...O hydrogen bonds. The molecular packing is also supported by  $\pi$ - $\pi$  interactions, leading to a sheet structure parallel to *bc* plane. Complex 5 is a coordination polymer, in which the monomeric [Ag(dmpen)(sac)]<sub>n</sub> units are linked by Ag...Ag interactions and the dmpen ligand acts as a bridge between the silver(I) ions, forming a two-dimensional network parallel to the plane (100). For all of the compounds, antimicrobial activity was studied against selected wild type and clinical microorganisms in vitro by using Minimum inhibitory concentration (MIC) and the disc diffusion method. MIC values of complexes 1-5 were determined in range 13.5-55  $\mu$ g/ml. These MIC values were approximately the same as those of standard medicinal antibiotics. Therefore, these complexes could be a new candidate for the treatment of microbial diseases.

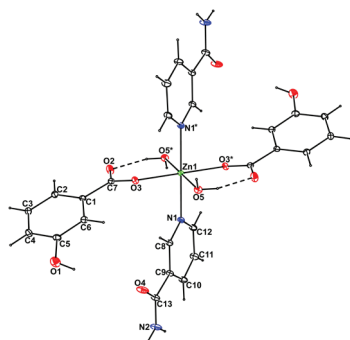
**Keywords:** saccharinate complexes; silver(I) complexes; antimicrobial properties

#### FA4-MS05-P07

**Diaquabis(3-Hydroxybenzoato- $\kappa$ O)Bis(Nicotinamide- $\kappa$ N)Zinc(II).** Onur Şahin<sup>a</sup>, Orhan Büyükgüngör<sup>a</sup>, Dursun Ali Köse<sup>b</sup>, Hacı Necefoğlu<sup>c</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. <sup>b</sup>Department of Chemistry, Hacettepe University, 06800, Ankara, Turkey. <sup>c</sup>Department of Chemistry, Kafkas University, 06100, Kars, Turkey.

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The title compound, [Zn(C<sub>7</sub>H<sub>5</sub>O<sub>3</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>], is a two-dimensional hydrogen-bonded supramolecular complex. The Zn<sup>II</sup> ion resides on the centre of symmetry and is in an octahedral coordination environment comprising two pyridyl N atoms, two carboxylate O atoms and two O atoms from water molecules. Intermolecular N-H...O and O-H...O hydrogen bonds produce R<sub>1</sub><sup>1</sup>(6), R<sub>2</sub><sup>2</sup>(7), R<sub>2</sub><sup>2</sup>(8), R<sub>2</sub><sup>2</sup>(16), R<sub>2</sub><sup>2</sup>(20), R<sub>2</sub><sup>2</sup>(22) and R<sub>3</sub><sup>3</sup>(30) rings which lead to a one-dimensional polymeric chains. An extensive two-dimensional network of N-H...O, O-H...O, C-H...O hydrogen bonds, and C-H... $\pi$  interactions are responsible for crystal stabilization.



**Keywords:** zinc complex; crystal structure analysis; hydrogen bond

#### FA4-MS05-P08

**Bis[ $\mu$ -(acesulfamato-N,O)(acesulfamato-N,O)bis(2-methylpyridine)cadmium(II)].** Zarife Sibel Şahin<sup>a</sup>, Hasan İçbudak<sup>b</sup>, Şamil Işık<sup>a</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. <sup>b</sup>Department of Chemistry, Ondokuz Mayıs University, 55139, Samsun, Turkey.

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The title compound, (C<sub>40</sub>H<sub>44</sub>Cd<sub>2</sub>N<sub>8</sub>O<sub>16</sub>S<sub>4</sub>), is a three-dimensional hydrogen-bonded supramolecular complex, which crystallizes in the monoclinic space group C2/c with unit-cell parameters *a*=14.9475(12)Å, *b*=16.5004(11)Å, *c*=21.4067(15)Å and *Z* = 4. Within the dinuclear complex, two Cd(II) ions are bridged by two carboxylate O atoms. Each Cd(II) ion is coordinated by two N and three O atoms of the acesulfamato ligands and two N atoms of the 2-methylpyridine ligands, resulting in a distorted pentagonal bipyramidal coordination. Intermolecular C-H...O hydrogen bonds produce R<sub>1</sub><sup>1</sup>(8) and R<sub>2</sub><sup>2</sup>(20) rings which lead to a two-dimensional polymeric chains. An extensive three-dimensional network of C-H...O hydrogen bonds, and  $\pi$ ... $\pi$  interactions are responsible for crystal stabilization.

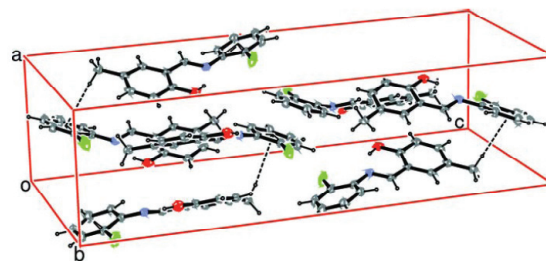
**Keywords:** cadmium complex; crystal structure analysis; hydrogen bond

#### FA4-MS05-P09

**(E)-2-[(2-Chlorophenyl)iminomethyl]-4-Methylphenol.** Özlem Deveci<sup>a</sup>, Şamil Işık<sup>a</sup>, Ferda Erşahin<sup>b</sup>, Erbil Ağar<sup>b</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, Samsun. <sup>b</sup>Department of Chemistry, Arts and Sciences Faculty, Ondokuz Mayıs University, Samsun.

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The molecule of the title compound, C<sub>14</sub>H<sub>12</sub>ClNO, adopts the enol-imine tautomeric form, with an intramolecular O—H...N hydrogen bond. In the molecule, the two benzene rings are twisted with respect to each other by 30.6(2)<sup>o</sup>. The crystal structure is stabilized by intermolecular C—H... $\pi$  interactions.



**Figure 1.** A perspective view of the molecular packing of compound. Dashed lines indicate hydrogen bonds and C-H... $\pi$  interactions.

In STOE IPDS-II diffractometer system, diffraction data

of  $C_{14}H_{12}ClNO$ , was collected with using MoK $\alpha$  radiation in 296 K. Compound was crystallised on orthorhombic system, space group Pbc $a$   $a = 7.5121$  (7) Å,  $b = 11.9190$  (15) Å,  $c = 27.500$  (3) Å,  $V = 2462.3$  (5) Å<sup>3</sup>,  $Z = 8$ .

Data collection and cell refinement: Stoe X-Area. To solve and refine the structure we used the programs SHELXS-97 and SHELXL-97, respectively. Molecular graphics: ORTEP3 for Windows.

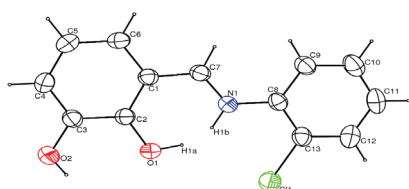
**Keywords:** schiff base; enol-imine; anti-tumour

#### FA4-MS05-P10

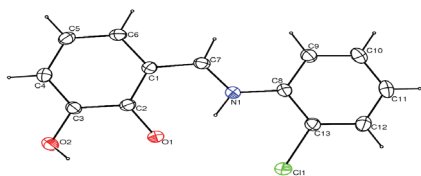
**The Structure of (Z)-6-[(2-chlorophenylamino)methylene]-2-hydroxycyclohexa-2,4-dienone at Two Different Temperatures.** Ersin Temel<sup>a</sup>, Çiğdem Albayrak<sup>b</sup>, Mustafa Odabaşoğlu<sup>c</sup>, Orhan Büyükgüngör<sup>a</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. <sup>b</sup>Sinop Faculty of Education, Sinop University, Sinop, Turkey, <sup>c</sup>Denizli Technical Vocational School, Pamukkale University, Denizli, Turkey.

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The crystal structure of the title compound, a Schiff base, was determined at 296 K and 100 K. The position of hydrogen atom characterizing the Schiff base type could not be certainly determined at 296 K. However, it can be said that the OH form is more dominant than NH form, with the percentages of 58 and 42, respectively. On the other hand, at 100 K it is found that the H atom is bonded to N atom. The packing is mainly stabilized by inter-molecular hydrogen bonds of O-H...O type. These hydrogen bonds give rise to R<sub>2</sub><sup>2</sup>(10) dimeric rings in the extended structure. The packing is also supported by  $\pi$ ... $\pi$  interactions between benzene rings.



(a) 296 K



(b) 100 K

Fig. Perspective views of title compound with the atom numbering scheme: (a) at 296 K and (b) at 100 K.

**Keywords:** X-ray crystallography; schiff base

#### FA4-MS05-P11

**Crystal Structure and Quantum Mechanical Calculations of (E)-4-methoxy-2-[(o-tolylimino)methyl] phenol.** Arzu Özek<sup>a</sup>, Orhan Büyükgüngör<sup>a</sup>, Çiğdem Albayrak<sup>b</sup>, Mustafa Odabaşoğlu<sup>c</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey. <sup>b</sup>Faculty of Education, Sinop University, Sinop, Turkey. <sup>c</sup>Denizli Technical Vocational School, Pamukkale University, Denizli, Turkey.

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Schiff base ligands are very important compounds in the chemical industry and medicine. In general, O-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and ketoamine (or quinoid) forms. Depending on the tautomers, two types of intramolecular hydrogen bonds are possible: O—H...N in benzenoid and N—H...O in quinoid tautomers. The H atom in title compound (I) is located on atom O1, thus the phenol-imine tautomer is favored over the keto-amine form, as indicated by the C2—O1, C8—N1, C1—C8 and C1—C2 bond lengths. A similar work was also observed in our previous work [1]. In the crystal structure, weak intermolecular C—H...O hydrogen bonds results in the formation of C(5) chains along the  $c$  axis, in which they may be effective in the stabilization of the structure.

The experimental geometry of title compound (I) obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations (semi-empirical, ab-initio Hartree-Fock HF and density-functional theory DFT/B3LYP). Ab-initio HF, DFT and semi-empirical (AM1 and PM3) calculations and full-geometry optimizations were performed by means of GAUSSIAN 03W package [2]. We observe an acceptable general agreement between them. Although the DFT molecular orbital theory was considered as the most accurate method for geometry optimization for free and complex ligands [3], the HF method led to better results in regard to the bond lengths and angles.

[1] Özek, A., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2008). J. Chem. Crystallogr. in print. [2] Friesner, R. A. (2005). PNAS 102, 6648. [3] Frisch, M. J. et al. (2004). GAUSSIAN03 Revision E.01. Gaussian, Inc., Wallingford CT 06492, USA.

**Keywords:** single-crystal X-ray diffraction; quantum mechanics

#### FA4-MS05-P12

**Two Monoclinic Polymorphs of Bis(4-cyanobenzylidene)Butanediamine: The Crystal Structure and Hirshfeld Surface Studies.** Reza Kia<sup>a</sup>, Hoong-Kun Fun<sup>a</sup>. <sup>a</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800, Penang, Malaysia.

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Polymorphism, the existence of more than one crystal