

To compare the strengths of these interactions and to investigate their geometrical preferences, the approach suggested by Lommerse et al. [1], using the normalized distance  $R_{HX}$  and the spatially normalized distance vs. angle ( $R_{HX}^3$  vs.  $1 - \cos[180 - (D-H \cdots X)]$ ) plot, was applied.

The study implies: (1) Even if the N-H(s) were deprotonated / substituted, O-H(s) and C-H(s) in the molecules could serve as hydrogen bond donors. O-H(s) are normally better donors than N-H(s), while C-H(s) build weaker interactions. (2) No notable differences were found among F, Cl and Br in both examined criteria. (3) In general, the capability as hydrogen bond acceptor is  $X^- > X-M > X-C$ , which is complied with results of others [2]. (4) Important counter anions in coordination chemistry, such as  $BF_4^-$ ,  $PF_6^-$  and  $SbF_6^-$ , exhibit comparable hydrogen bond acceptor capabilities like transition metal-halides. (5) Special attention is drawn to  $MX_4^{2-}$  type counter anions (templates). The several cases recorded show exclusively the formation of much stronger hydrogen bonds compared to normal metal-halides. Their possible roles in complex synthesis and nucleation are still unclear, further studies with theoretical methods would follow. (6) Although  $CH_2Cl_2$  /  $CHCl_3$  are often used and are observed in structures, X-C is seldom involved in hydrogen bonding. In the rare cases at most very weak interactions were built. While on the other hand the increased acidity of the C-H(s) makes them possible hydrogen bond donors.

[1] J.P.M. Lommerse, A.J. Stone, R. Taylor, F.H. Allen, *J. Am. Chem. Soc.* **1996**, *118*, 3108-3116. [2] L. Brammer, E.A. Bruton, P. Sherwood, *Cryst. Growth Des.* **2001**, *1*, 277-290.

**Keywords:** hydrogen bond, halogens, N-heterocycles

## MS73.P11

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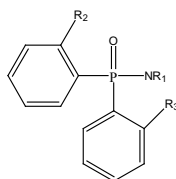
### Structural investigation of phenol-phosphonic amides

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The synthesis and use of phosphine ligands in homogeneous catalysed reactions is a field of research that is gaining more interest [1]. There is currently a special focus [2] on the synthesis of unsymmetrical ligands, for various reasons, including asymmetric catalytic transformations [3]. The stereoelectronic nature of the ligand plays a significant role in the outcome of the reaction<sup>2</sup> and, as a result, we have investigated a potentially new route to ortho-substituted arylphosphine ligands.

Several of these ligands are crystalline which enables their investigation by means of X-ray crystallography. A series of phenol-phosphonic amides was investigated as shown in Scheme 1. An interesting feature exhibited by all of these structures is that of phenol-phosphine oxide intramolecular hydrogen bonding. Packing motifs, hydrogen bonding and geometrical features of the structures were compared in this study.

Calculation of Tolman cone angles and solid angles were determined to illustrate the steric behaviour of these phosphine ligands [4]. Electrostatic potential properties such as  $V_{min}$  and  $d_{cp}$  were calculated in order to quantify the electronic effect of these ligands. The calculations were performed in Gaussian with Density functional theory (DFT) incorporating the B3LYP functional and 6-31G(d,p) basis set [5].



$R_1 = Et, Pr, Bu, R_2 = H, OH, R_3 = H, OH, PPh_2$

Scheme 1: Phenol phosphonic amides

[1] P.W.N.M. Leeuwen, P.C.J. van Kamer, J.N.H. Reek, P. Dierkes, *Chem. Rev.* **2000**, *100*, 2741-2770. [2] W. Tang, X. Zhang, *Chem. Rev.* **2003**, *103*, 3029-3069. [3] S. Jeulin, S.D. de Paule, V. Ratovelomanana-Vidal, J.P. Genêt, N. Champion, P. Dellis, *Angew. Chem. Int. Ed.* **2004**, *43*, 320-325. [4] C.A. Tolman, *Chem. Rev.* **1977**, *77*, 313-348. [5] C.H. Suresh, N. Koga, *Inorg. Chem.* **2002**, *41*, 1573-1578.

**Keywords:** phosphonic-amides, hydrogen-bonding, DFT

## MS73.P12

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### How many molecules can you crystallize in one experiment? the role of hydrogen bonding in chalcone-flavanone isomerization.

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Chalcones, flavones and flavanones are naturally occurring compounds from plants and they have a wide range of biological activities. We are interested in studying the molecular structures using X-ray diffraction of these compounds so that a relationship between the chemical structure and the biological activities may be seen. The crystallization of  $C_{16}H_{14}O_5$ , 3-methoxy-4,2',5'-trihydroxyxchalcone from a mixture of ethanol-water produced *three* different types of crystals which were visually distinct. We report the results of these 3 crystal structure determinations that show, respectively, the chalcone and the flavanone isomers and a third structure showing the conformational disorder resulting from the molecular rearrangement due to the intramolecular isomerization reaction between the flavanone and the chalcone molecular structure! The role that intermolecular interactions such as hydrogen bonding and stacking play in the self assembly and biological activity of these structures is investigated.

**Keywords:** chalcone, flavanone, molecular rearrangement

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### The hydrogen bond in supramolecular network

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In recent years, supramolecular arrangement and intermolecular interactions have played an important role in crystal engineering. A detailed analysis of hydrogen bonds in some molecules can classify this as *I- very strong*, *II- strong* and *III-weak* [1]. An easy way to visualize the intermolecular interactions is to apply a graphical analysis of the patterns that represent these interactions [*motif*  $G_d^a(r)$ ] [2] in crystals. In this paper we analyze the crystals of the organic substance enrofloxacin and other inorganic substances such as copper acetate, ferrous sulfate, etc. Of X-ray data, tables are constructed of lengths and hydrogen bond angles. Finally we illustrate how to classify the bond and its possible application in Crystal Engineering and / or the design of molecular devices. Below is a brief summary of this work.

Data collection X-ray diffractometer was carried out with a Gemini with Atlas area detector and two sources of radiation  $\lambda_{Mo} = 0.7103$  and  $\lambda_{Cu} = 1.5418 \text{ \AA}$  to 130 K.

The asymmetric unit of enrofloxacin corresponds to the moiety