

B61, 46-57.

Keywords: hydrogen bonding, cocrystals, intermolecular packing

## P06.10.52

*Acta Cryst.* (2008). A64, C398

### Crystal structure of (4*Z*)-2-phenyl-4-(3,4,5-trimethoxybenzylidene)-1,3-oxazol-5(4*H*)-one

Mukeshkumar M. Jotani<sup>1</sup>, Bharat B. Baldaniya<sup>2</sup>

<sup>1</sup>Bhartiya Vidya Bhavan's Seth R. A. College of Science, Physics, Vidya Gauri Neelkanth Marg, Khanpur., AHMEDABAD, GUJARAT, 380 001, India, <sup>2</sup>M. G. Science Institute, Navrangpura, Ahmedabad, Gujarat, 380 009, India, E-mail: mmjotani@rediffmail.com

1,3-oxazole is a very useful intermediate synthetic organic material for the synthesis of imidazole that possess a wide spectrum of biological activities such as herbicides, antibacterial, antifungal, etc. In addition, the oxazole itself is also found to possess antibacterial and antifungal activities. In view of this, the crystal structure of title compound has been determined. The yellow colored, block shaped crystals of size  $0.3 \times 0.3 \times 0.2 \text{ mm}^3$  were grown by slow evaporation from the benzene solution. The compound crystallizes in triclinic system having space group *P*-1. The crystal data are:  $a = 7.3732(8) \text{ \AA}$ ,  $b = 15.7823(17) \text{ \AA}$ ,  $c = 8.1325(8) \text{ \AA}$ ,  $\alpha = 62.085(7)^\circ$ ,  $\beta = 82.506(7)^\circ$ ,  $\gamma = 91.954(6)^\circ$ ,  $Z = 2$ ,  $\mu = 0.100 \text{ mm}^{-1}$ ,  $D_x = 1.367 \text{ Mg-m}^{-3}$ . Intensity data on BRUKER AXS KAPPA APEX2 CCD diffractometer are collected in  $\omega$  and  $\phi$  scan with  $\theta$  ranging from  $2.53$  to  $25.0^\circ$  and 2885 unique reflections are recorded. The structure is solved by SIR92 program and refined by SHELXL-97 program to final R-value of 0.0597 for 2114 reflections with  $I > 2\sigma(I)$ . In the structure, all the three rings are planar within themselves, and the benzene ring and benzylidene moiety making a dihedral angle of  $11.23(15)$  and  $3.19(14)^\circ$  respectively. An intermolecular C-H...O interaction forms a dimer that exhibit  $R^2_2(14)$  graph-set motif. In addition crystal structure is stabilized by C-H... $\pi$  and  $\pi$ - $\pi$  stacking interactions.

Keywords: single-crystal X-ray diffraction, organic crystals, hydrogen bonding

## P06.10.53

*Acta Cryst.* (2008). A64, C398

### Two proton transfer compounds from benzene-1,2,4,5-tetracarboxylic acid and 1,10-phenanthroline

Mahboubeh A. Sharif<sup>1</sup>, Hossein Aghabozorg<sup>2</sup>, Mohammad Heidari<sup>2</sup>, Leila Roshan Lari<sup>2</sup>, Najmeh Firoozi<sup>2</sup>, Mohammad Ghadermarzi<sup>3</sup>

<sup>1</sup>Department of Chemistry, Islamic Azad University, Qom Branch, Chemistry, No. 129, Razaghi Avenue, Saeidi Square, Qom, Qom, 3719618853, Iran, <sup>2</sup>Department of Chemistry, Tarbiat Moalem University, Tehran, Iran, <sup>3</sup>Department of Chemistry, Faculty of Sciences, University of Kurdistan, Sanandaj, Iran, E-mail: sharif44m@yahoo.com

Recently, there has been considerable interest in proton transfer systems and their structures. Two proton transfer compounds (phenH)(btcH<sub>3</sub>) · H<sub>2</sub>O, **1**, and (phenH)<sub>2</sub>(btcH<sub>2</sub>) · btcH<sub>4</sub>, **2**, were obtained by the reaction of benzene-1,2,4,5-tetracarboxylic acid (btcH<sub>4</sub>) with 1,10-phenanthroline (phen) in 1:1 and 1:2 molar ratio, respectively. The characterizations were performed using IR, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy and single-crystal X-ray diffraction. The compound **1** is crystallized in triclinic system and *P*1<sup>-</sup> space group with following

cell parameters:  $a = 7.8529(5) \text{ \AA}$ ,  $b = 9.8333(6) \text{ \AA}$ ,  $c = 12.2847(7) \text{ \AA}$ ,  $\alpha = 94.5910(10)^\circ$ ,  $\beta = 91.3670(10)^\circ$ ,  $\gamma = 94.7300(10)^\circ$ ,  $Z = 2$ . The final *R* value of **1** is 0.0354 for 3627 total reflection. The compound **2** is crystallized in the space group *P*2<sub>1</sub>/*c* of the monoclinic system, and contains two molecules per unit cell. The structure has been refined to a final value for the crystallographic *R* factor of 0.0364 based on 4881 reflections. The unit cell parameters are:  $a = 11.9154(6) \text{ \AA}$ ,  $b = 13.5560(6) \text{ \AA}$ ,  $c = 12.2030(6) \text{ \AA}$  and  $\beta = 110.4880(10)^\circ$ . The ranges of the D-H...A angles and the H...A and D...A distances indicate the presence of strong hydrogen bonding in both compounds. Hydrogen bonds with D...A distances ranging from 2.4331(15) to 3.4766(19) Å, are observed in the crystal structure of **1** whereas, the range of D...A distances in **2** is between 2.4472(13) to 3.4287(18) Å. In both structures, **1** and **2**, anionic and cationic units have been arranged in the lattice in a parallel manner connect the various components into self-associated supramolecular structures and providing considerable  $\pi$ - $\pi$  stacking between (phenH)<sup>+</sup> rings. The centroid distances between the planes are 3.4779(9) and 3.8707(8) Å, respectively.

Keywords: crystal structures, hydrogen bonding, supramolecular assemblies

## P06.10.54

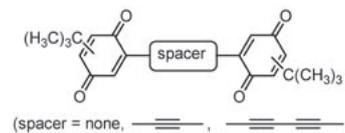
*Acta Cryst.* (2008). A64, C398

### X-ray structures of quinone dimers linked either directly or through acetylene spacers

Naoto Hayashi, Akifumi Kanda, Takahiro Ohnuma, Hiroyuki Higuchi

University of Toyama, Chemistry, Gofuku, Toyama, Toyama, 9308555, Japan, E-mail: nhayashi@sci.u-toyama.ac.jp

X-ray structures of two directly-linked quinone dimers have been investigated. Although the positions of tert-butyl substituents differed, their X-ray structures were significantly close. The carbonyl oxygen atoms underwent van der Waals contact in an intramolecular manner, and quinone moieties were distorted into the boat shape in common. As MO calculations indicated the quinone moiety became flexible when quinones were directly linked, the origins of the boat forms should be attributed to the intrinsic flexibility of the molecular skeleton as well as the packing demand. In contrast, quinone moieties of quinone dimers bearing acetylene and diacetylene spacers have been found to be planar. This may be arisen from no intramolecular contact of oxygen atoms by introduction of the acetylene spacers. Flexibility of the molecular skeleton of these molecules will also be discussed.



Keywords: inter- and intramolecular interactions, packing, isomers

## P06.10.55

*Acta Cryst.* (2008). A64, C398-399

### Homogeneous and heterogeneous mixed crystals composed of phenoxy radical and phenol

Keiko Ninomiya<sup>1</sup>, Naoto Hayashi<sup>2</sup>, Taku Kamoto<sup>2</sup>, Hiroyuki Higuchi<sup>2</sup>

<sup>1</sup>Kyoto University, Katsura, Kyoto, Kyoto, 6158530, Japan, <sup>2</sup>University of Toyama, Gofuku, Toyama, Toyama, 9308555, Japan, E-mail: kuwata@