

**(Z)-3-(4-Nitrophenyl)-2-phenyl-2-propenoic acid monohydrate****Sadiq-ur-Rehman,<sup>a</sup> Saqib Ali,<sup>b</sup>  
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**Key indicators**

Single-crystal X-ray study

T = 173 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.042

wR factor = 0.114

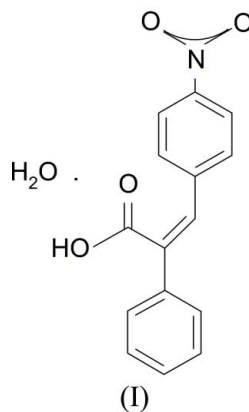
Data-to-parameter ratio = 9.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound,  $\text{C}_{15}\text{H}_{11}\text{NO}_4 \cdot \text{H}_2\text{O}$ , there are hydrogen-bonded clusters involving conventional and unconventional hydrogen bonds of the types  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{O}$ . Pairs of molecules lie parallel to each other in a head-to-tail fashion, exhibiting strong  $\pi-\pi$  overlapping.

**Comment**

Carboxylate ligands have been widely used in coordination chemistry and their complexes are generally known to be stable (Oldham *et al.*, 1987). Recently, much effort has been devoted to the self-assembly of organic and inorganic molecules in the solid state because it extends the range of new solids with desirable physical and chemical properties (Canty & van Koten, 1995). In this paper, we report the structure of such a compound, (I), that has been synthesized in our laboratory.



The structure of (I) (Fig. 1) is composed of strongly hydrogen-bonded clusters involving all O atoms of the acid and water of solvation (Fig. 2); details of the hydrogen-bonding geometry are given in Table 2.  $\text{O5}-\text{H51} \cdots \text{O4}$  is a strong bond with an  $\text{H} \cdots \text{O}$  distance of 2.19  $\text{\AA}$ , while the second H atom of the water of solvation is involved in two rather weaker hydrogen bonds ( $\text{H52} \cdots \text{O3}$  and  $\text{H52} \cdots \text{O1}$ ), with distances of 2.39 and 2.42  $\text{\AA}$ , respectively. In addition to the conventional hydrogen bonds, an unconventional interaction of the type  $\text{C}-\text{H} \cdots \text{O}$  is also present.

The molecular dimensions in (I) are in agreement with the dimensions reported for similar structures, *viz.* (Z)-methyl $\beta$ -p-nitrophenyl- $\alpha$ -phenyl acrylate, (E)-methyl $\beta$ -p-nitrophenyl- $\alpha$ -phenyl acrylate, and (E)-methyl $\beta$ -methyl- $\beta$ -p-nitrophenyl- $\alpha$ -phenyl acrylate (Tinant *et al.*, 1983), 3-(4-nitrophenyl)-2-phenylacrylic acid, its ammonium salt and 3-methoxyphenyl

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derivative (Kuleshova *et al.*, 2003) and an Sn complex of 3-(4-nitrophenyl)-2-phenylacrylic acid (Sadiq-ur-Rehman *et al.*, 2004).

The benzene rings are oriented at 55.12 (7)° with respect to each other while the mean plane of the carboxylate group (C1/C2/O1/O2) lies at an angle of 77.33 (10)° with respect to the mean plane of phenyl ring C10–C15. The nitro group is twisted at an angle of 11.02 (13)° from the mean plane of benzene ring C4–C9.

Pairs of molecules lie parallel to each other in a head-to-tail fashion such that the nitrophenyl ring overlaps the phenyl ring of a symmetry-related molecule (symmetry code:  $\frac{1}{2} + x, \frac{3}{2} - y, 2 - z$ ) and *vice versa*, thereby exhibiting strong  $\pi$ - $\pi$  overlapping; the separation between the least-squares planes of these rings is 3.39 Å.

### Experimental

A mixture of phenylacetic acid (0.15 mol), *p*-nitrobenzaldehyde (0.15 mol), anhydrous K<sub>2</sub>CO<sub>3</sub> (0.095 mol) and acetic anhydride (0.38 mol) was slowly raised to 353–373 K and maintained at this temperature range for 24 h. To the hot solution, H<sub>2</sub>O (200 ml) and 10% HCl (100 ml) were added. The mixture was stirred at room temperature for 2 h and filtered. The solid mass obtained was recrystallized from commercial ethanol. Yellow crystals of (I) suitable for crystallographic studies were obtained after three weeks.

#### Crystal data

C<sub>15</sub>H<sub>11</sub>NO<sub>4</sub>·H<sub>2</sub>O  
*M<sub>r</sub>* = 287.26  
 Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
*a* = 7.578 (2) Å  
*b* = 10.282 (2) Å  
*c* = 16.832 (4) Å  
*V* = 1311.5 (5) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.455 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.11 mm<sup>-1</sup>  
*T* = 173 (2) K  
 Prism, colorless  
 0.18 × 0.15 × 0.12 mm

#### Data collection

Nonius KappaCCD diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan  
 (SORTAV; Blessing, 1997)  
*T<sub>min</sub>* = 0.980, *T<sub>max</sub>* = 0.987

26803 measured reflections  
 1855 independent reflections  
 1280 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.116  
 $\theta_{\max}$  = 28.3°

#### Refinement

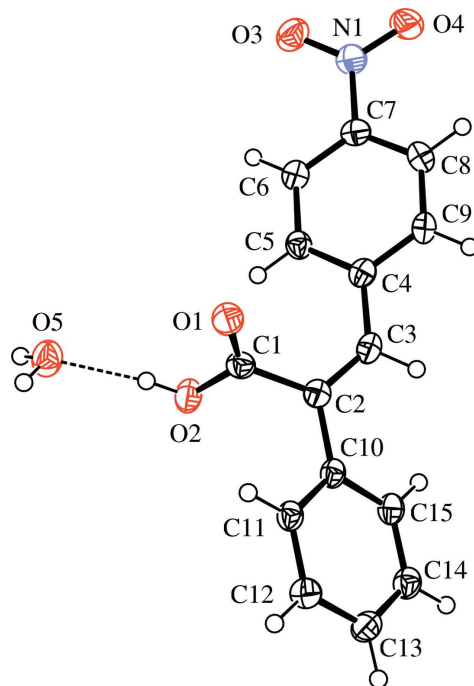
Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.042  
*wR* (*F*<sup>2</sup>) = 0.114  
*S* = 1.08  
 1855 reflections  
 198 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.248P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.29 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{Å}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.026 (4)

**Table 1**

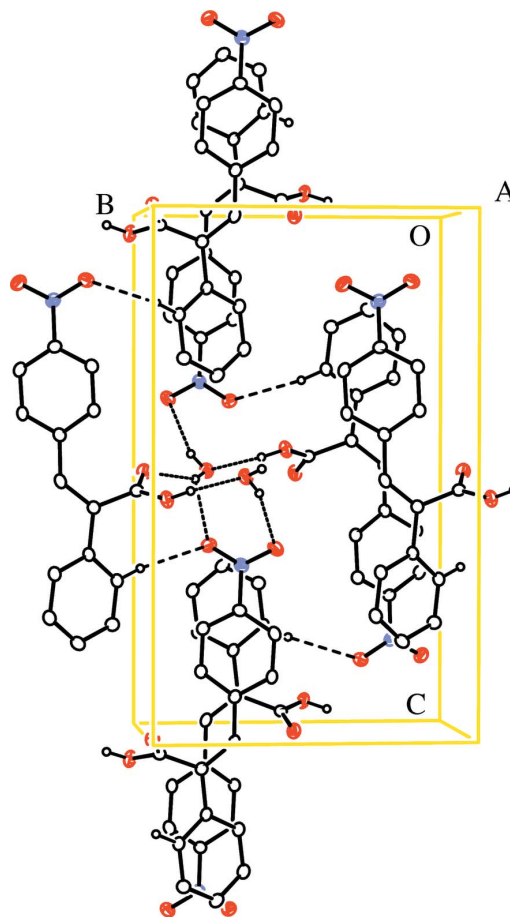
Selected geometric parameters (Å, °).

O1–C1	1.211 (3)	O4–N1	1.238 (3)
O2–C1	1.332 (4)	N1–C7	1.450 (4)
O3–N1	1.231 (3)		
O3–N1–O4	122.4 (3)	O4–N1–C7	119.0 (3)
O3–N1–C7	118.6 (3)		



**Figure 1**

ORTEP drawing (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 50% probability level. The dashed line indicates a hydrogen bond.



**Figure 2**

ORTEP drawing (Johnson, 1976) of the packing, showing the hydrogen bonding (dashed lines).

**Table 2**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 $\cdots$ O5	0.84	1.84	2.673 (3)	171
O5—H51 $\cdots$ O4 <sup>i</sup>	0.82	2.19	2.978 (3)	161
O5—H52 $\cdots$ O3 <sup>ii</sup>	0.82	2.39	2.935 (3)	125
O5—H52 $\cdots$ O1 <sup>iii</sup>	0.82	2.42	3.159 (3)	151
C11—H11 $\cdots$ O3 <sup>i</sup>	0.95	2.54	3.476 (4)	170

Symmetry codes: (i)  $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$ ; (ii)  $-x, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (iii)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z$ .

Due to lack of significant anomalous dispersion effects, Friedel pairs were merged. The H atoms were located in difference Fourier syntheses and were included in the refinement at geometrically idealized positions, with C—H = 0.95 Å and O—H = 0.84 Å. The O—H bonds for water were fixed at 0.82 Å. During the refinement,  $U_{iso}(H)$  values were set at 1.5 (hydroxyl) and 1.2 (the rest) times  $U_{eq}$  of the atoms to which they were bonded.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALE-PACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure:

*SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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