

**trans-1-Cyano-2-(2-methoxyphenyl)-
1-nitroethylene**Vladimir N. Nesterov,^{a,c*} Victor P. Kislyi,^b Tatiana V. Timofeeva,^a Mikhail Yu. Antipin^{a,c} and Victor V. Semenov^b^aDepartment of Physical Sciences, New Mexico Highlands University, Las Vegas, NM 87701, USA, ^bInstitute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prospekt, Moscow, Russian Federation, and ^cInstitute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov St, B-334 Moscow, Russian Federation

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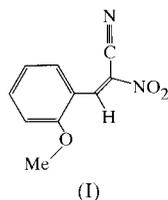
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The title compound, C₁₀H₈N₂O₃, has been prepared by condensation of 2-methoxybenzaldehyde and nitroacetonitrile in ethanol at room temperature. Its investigation has been undertaken as a part of search for new nonlinear optical compounds. The π -conjugated molecule is almost planar. Molecules in the crystal are packed in stacks with antiparallel molecular orientation and slightly alternating distances between mean molecular planes.

Comment

Organic non-linear optical (NLO) crystals are attracting the attention of chemists, physicists, optical and device scientists because of their superiority to the conventional inorganic crystals (see, for instance, Zyss, 1994). The present work is part of our project on synthesis, structure investigation and property evaluation of organic potential NLO compounds. Recently, we investigated a series of polarized molecules having a dicyanovinyl acceptor part and various donors



connected by π -conjugated chains of different length. There are derivatives of 2-aryl-1,1-dicyanovinyl and 4-aryl-1,1-dicyano-1,3-butadiene (Antipin *et al.*, 1997; Antipin, Clark *et al.*, 1998; Antipin, Timofeeva *et al.*, 1998; Timofeeva *et al.*, 2000; Nesterov *et al.*, 2000). Molecules of the title compound, (I), have another type of acceptor group.

The molecule of (I) is almost planar. The dihedral angle between *o*-methoxyphenyl and 1-cyanoethylene moieties is

1.90 (7)° and the dihedral angle between the 1-cyanoethylene moiety and the nitro group is 2.40 (6)°. The mean deviations from the least-squares plane passing through all non-H atoms in molecule (I) is 0.024 (3) Å. The 1-cyano-1-nitroethylene fragment in (I) is almost coplanar with the *o*-methoxyphenyl moiety despite the shortened intramolecular contact H6A...C9 of 2.472 Å (van der Waals radii sum is 2.87 Å; Rowland & Taylor, 1996). Planarity of this molecule indicates a significant level of π -conjugation in this system.

Bond lengths in molecule (I) do not differ significantly from those found in the other derivatives of 2-aryl-1,1-dicyanoethylene (Antipin, Clark *et al.*, 1998) and are close to the standard bond lengths (Allen *et al.*, 1987) in corresponding π -conjugated systems.

The H7A atom in (I) has a short non-bonded contact with the O atoms of methoxy and nitro groups: H7A...O1 2.236 Å and H7A...O2 2.309 Å (van der Waals radii sum is 2.68 Å; Rowland & Taylor, 1996).

The molecules in the crystal are packed in stacks along a, with antiparallel molecular orientation inside them. The interplanar distances in these stacks are slightly alternating, and are equal to 3.37 (7) and 3.41 (8) Å.

The title compound crystallizes in a centrosymmetric space group and therefore has no NLO properties (second harmonic generation) in the crystalline state.

Experimental

(I) was obtained by the reaction of 2-methoxybenzaldehyde (0.005 mol) with nitroacetonitrile (0.005 mol) in the presence of a catalytic amount of morpholine in 20 ml ethanol at room temperature (Mechkov & Demireva, 1985). Light-yellow crystals were obtained by isothermic evaporation from a solution in ethanol.

Crystal data

C ₁₀ H ₈ N ₂ O ₃	$D_x = 1.398 \text{ Mg m}^{-3}$
$M_r = 204.18$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 24 reflections
$a = 7.1952(13) \text{ \AA}$	$\theta = 10\text{--}11^\circ$
$b = 17.356(3) \text{ \AA}$	$\mu = 0.106 \text{ mm}^{-1}$
$c = 8.3298(16) \text{ \AA}$	$T = 298(2) \text{ K}$
$\beta = 111.148(14)^\circ$	Prism, light yellow
$V = 970.2(3) \text{ \AA}^3$	$0.45 \times 0.30 \times 0.25 \text{ mm}$
$Z = 4$	

Data collection

Siemens P3/PC diffractometer	$h = 0 \rightarrow 9$
$\theta/2\theta$ scans	$k = 0 \rightarrow 23$
2776 measured reflections	$l = -11 \rightarrow 10$
2592 independent reflections	2 standard reflections
1664 reflections with $I > 2\sigma(I)$	every 98 reflections
$R_{\text{int}} = 0.021$	intensity decay: 5%
$\theta_{\text{max}} = 29.06^\circ$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.0957P]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.140$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.112$	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
2592 reflections	$\Delta\rho_{\text{min}} = -0.193 \text{ e \AA}^{-3}$
137 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.049 (6)

Table 1

Selected geometric parameters (Å, °).

O1—C2	1.3483 (18)	N2—C9	1.138 (2)
O1—C10	1.442 (2)	C1—C7	1.437 (2)
O2—N1	1.2106 (18)	C7—C8	1.3328 (19)
O3—N1	1.2242 (17)	C8—C9	1.421 (2)
N1—C8	1.4701 (19)		
C2—O1—C10	118.95 (14)	C8—C7—C1	130.60 (14)
O2—N1—O3	124.41 (14)	C7—C8—C9	129.19 (15)
O2—N1—C8	118.96 (13)	C7—C8—N1	118.76 (13)
O3—N1—C8	116.63 (14)	C9—C8—N1	112.05 (13)
C6—C1—C7	124.51 (13)	N2—C9—C8	179.5 (2)
C2—C1—C7	117.51 (13)		
C2—C1—C7—C8	-178.55 (16)	O3—N1—C8—C7	177.13 (15)
C1—C7—C8—C9	0.4 (3)	O2—N1—C8—C9	177.48 (16)
C1—C7—C8—N1	-178.99 (14)	O3—N1—C8—C9	-2.3 (2)
O2—N1—C8—C7	-3.0 (2)		

Data collection: *P3* (Siemens, 1989); cell refinement: *P3*; data reduction: *SHELXL97* (Sheldrick, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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