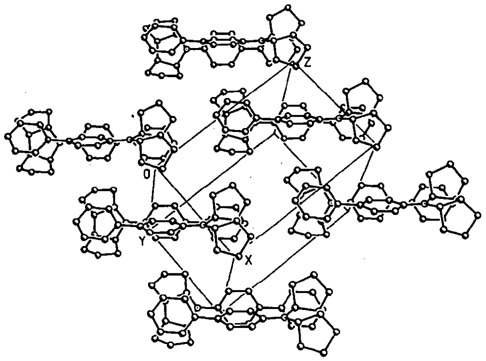

Fig. 3. Molecular packing.

mum and maximum peaks in the final ΔF map were $-0{\cdot}23$ and $0{\cdot}17$ e Å^{-3}, respectively, and the maximum $|\Delta/\sigma|$ was 0·024. The scattering factors for the non-H atoms were taken from Cromer & Mann (1968), with the anomalous-dispersion corrections taken from the work of Cromer & Liberman (1970). The scattering factors for the H atoms were obtained from Stewart, Davidson & Simpson (1965). Values used to calculate the linear absorption coefficient are from *International Tables for X-ray Crystallography* (1974). Figures generated using *SHELXTL-Plus* (Sheldrick, 1987). Positional and equivalent isotropic thermal parameters for the non-H atoms are listed in Table 1, while the bond lengths and angles for the non-H atoms are listed in Table 2.* The drawings of molecules (*A*) and (*B*) with the atom-labeling schemes are shown in Figs. 1 and 2, respectively, and the packing diagram is in Fig. 3.

Related literature. The aminobiphenyl substituted with the chiral tricyclic amine (Whitesell, Minton & Chen, 1988) was prepared as a chiral analog of biphenyl as a possible candidate for non-linear optical, second harmonic generation (Chemla & Zyss, 1987). Single-crystal X-ray analysis was undertaken to investigate the influence of the C_2 symmetric amine subunit on crystal packing.

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* Tables of anisotropic thermal parameters, H-atom positional parameters, bond lengths and angles involving H atoms, torsion angles and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52708 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of the Complex of Imidazole and Picric Acid*

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Abstract. $C_6H_2N_3O_7^-.C_3H_5N_2^+$, $M_r = 297{\cdot}2$, orthorhombic, *Pbca*, $a = 8{\cdot}944\,(2)$, $b = 13{\cdot}496\,(5)$, $c = 20{\cdot}195\,(7)$ Å, $V = 2438\,(1)$ Å^3, $Z = 8$, $D_x = 1{\cdot}61$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}7107$ Å, $\mu = 0{\cdot}133$ mm^{-1}, $F(000) = 1216$, $T = 293$ K, $R = 0{\cdot}061$ for 1369 observed reflections. The imidazole ring is protonated and makes a dihedral angle of 112·6 (1)° with the six-membered ring of the picric acid. The imidazole ring dimensions are in good agreement

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	U_{eq}(Å^2)
N(1)	0·0228 (3)	0·7894 (3)	0·2932 (2)	0·055 (1)
C(2)	0·0502 (4)	0·8439 (3)	0·2412 (2)	0·060 (1)
N(3)	0·1350 (4)	0·7912 (3)	0·2011 (2)	0·065 (1)
C(4)	0·1632 (5)	0·7021 (4)	0·2290 (2)	0·070 (2)
C(5)	0·0920 (4)	0·7008 (3)	0·2867 (2)	0·065 (2)
C(6)	0·1594 (3)	0·3994 (2)	0·0530 (2)	0·036 (1)
O(1)	0·1531 (3)	0·3712 (2)	0·1122 (1)	0·049 (1)
C(7)	0·0849 (4)	0·3532 (2)	−0·0021 (2)	0·040 (1)
C(8)	0·0998 (4)	0·3825 (3)	−0·0666 (2)	0·047 (1)
C(9)	0·1855 (4)	0·4650 (3)	−0·0808 (2)	0·048 (1)
C(10)	0·2565 (4)	0·5183 (3)	−0·0311 (2)	0·045 (1)
C(11)	0·2430 (4)	0·4848 (3)	0·0326 (2)	0·040 (1)
N(4)	−0·0129 (3)	0·2682 (2)	0·0097 (1)	0·053 (1)
O(2)	−0·0833 (3)	0·2649 (2)	0·0618 (1)	0·071 (1)
O(3)	−0·0230 (3)	0·2047 (2)	−0·0339 (2)	0·077 (1)
N(5)	0·1988 (4)	0·4976 (3)	−0·1492 (2)	0·067 (1)
O(4)	0·2835 (3)	0·5661 (3)	−0·1614 (1)	0·092 (1)
O(5)	0·1238 (4)	0·4549 (3)	−0·1913 (1)	0·095 (1)
N(6)	0·3162 (4)	0·5426 (3)	0·0844 (2)	0·054 (1)
O(6)	0·2970 (4)	0·6329 (2)	0·0833 (2)	0·082 (1)
O(7)	0·3887 (4)	0·5015 (2)	0·1265 (2)	0·092 (1)

Table 2. *Bond lengths* (Å) *and valence angles* (°) *with e.s.d.'s in parentheses*

N(1)—C(2)	1·305 (5)	N(1)—C(5)	1·353 (6)
C(2)—N(3)	1·318 (6)	N(3)—C(4)	1·351 (6)
C(4)—C(5)	1·327 (6)	C(6)—O(1)	1·258 (4)
C(6)—C(7)	1·438 (5)	C(6)—C(11)	1·433 (4)
C(7)—C(8)	1·368 (5)	C(7)—N(4)	1·462 (4)
C(8)—C(9)	1·383 (5)	C(9)—C(10)	1·390 (5)
C(9)—N(5)	1·454 (5)	C(10)—C(11)	1·370 (5)
C(11)—N(6)	1·460 (5)	N(4)—O(2)	1·227 (4)
N(4)—O(3)	1·231 (4)	N(5)—O(4)	1·220 (5)
N(5)—O(5)	1·226 (5)	N(6)—O(6)	1·231 (4)
N(6)—O(7)	1·204 (5)		
C(2)—N(1)—C(5)	109·4 (3)	N(1)—C(2)—N(3)	107·4 (4)
C(2)—N(3)—C(4)	109·3 (4)	N(3)—C(4)—C(5)	106·8 (4)
N(1)—C(5)—C(4)	107·1 (4)	O(1)—C(6)—C(7)	125·7 (3)
O(1)—C(6)—C(11)	122·6 (3)	C(7)—C(6)—C(11)	111·7 (3)
C(6)—C(7)—C(8)	124·5 (3)	C(6)—C(7)—N(4)	119·5 (3)
C(8)—C(7)—N(4)	116·0 (3)	C(7)—C(8)—C(9)	119·0 (3)
C(8)—C(9)—C(10)	121·3 (3)	C(8)—C(9)—N(5)	119·1 (3)
C(10)—C(9)—N(5)	119·5 (3)	C(9)—C(10)—C(11)	117·9 (3)
C(6)—C(11)—C(10)	125·5 (3)	C(6)—C(11)—N(6)	117·3 (3)
C(10)—C(11)—N(6)	117·2 (3)	C(7)—N(4)—O(2)	118·3 (3)
C(7)—N(4)—O(3)	118·3 (3)	O(2)—N(4)—O(3)	123·4 (3)
C(9)—N(5)—O(4)	118·1 (3)	C(9)—N(5)—O(5)	118·1 (4)
O(4)—N(5)—O(5)	123·8 (4)	C(11)—N(6)—O(6)	117·0 (3)
C(11)—N(6)—O(7)	120·0 (3)	O(6)—N(6)—O(7)	123·0 (3)

with respect to the parent molecule [Craven, McMullan, Bell, & Freeman (1977). *Acta Cryst.* **B33**, 2585–2589]. The six-membered ring is not exactly planar ($\chi^2 = 7·8$) with a maximum deviation of −0·024 (2) Å at C(7). The nitro groups are twisted out of the plane of the six-membered ring by varying amounts: the *ortho* nitro groups O(2)—N(4)—O(3) and O(6)—N(6)—O(7) are twisted by 148·0 (1) and 48·0 (1)°, respectively, while the *para* nitro group is twisted by 5·4 (1)°. The crystal structure is stabilized by two intermolecular hydrogen bonds: N(1)—H···O(1) $(-x, 0·5+y, 0·5-z)$ 2·710 (4), N(3)—H···O(1) $(0·5-x, 0·5+y, z)$ 2·825 (5) Å and eleven intermolecular C—H···O and N—H···O interactions < 3·42 Å.

Experimental. The title compound was prepared by mixing imidazole and picric acid in equimolecular amounts in hot chloroform, followed by slow evaporation of the resulting solution and this gave yellow crystals. Size of crystal 0·22 × 0·30 × 0·34 mm. Nicolet *R*3 four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Lattice parameters from 25 machine-centred reflections with $4·0 < 2\theta < 16·2°$. 2489 reflections with $3 < 2\theta < 50°$ for one octant, 1369 independent with $I > 3·0\sigma(I)$, index range $h\,0 \rightarrow 9$, $k\,0 \rightarrow 14$, $l\,0 \rightarrow 21$, $2\theta/\theta$-scan mode, variable scan speed. Two standard reflections (220, 230) monitored every 50 measurements; no significant variation. Lp correction. Data adjusted to an approximately absolute scale and an overall U value of 0·046 Å^2, absorption ignored and $R = 0·052$. Structure solved by direct methods and partial structure expansion by an iterative E–Fourier procedure using *SHELXTL*5 (Sheldrick, 1985). Least-squares refinement of all non-H atoms anisotropic; H atoms of CH were allowed to ride on bonded C with a fixed isotropic $U = 0·06$ Å^2. The H atoms bonded to N atoms were located on a difference Fourier map at an advanced stage of anisotropic refinement and their coordinates refined. $\sum w(\Delta F)^2$ minimized, $w = [\sigma^2(F_o) + 0·001(F_o)^2]^{-1}$, where σ is standard deviation of observed amplitudes, based on counting statistics. In the last cycle $(\Delta/\sigma)_{max} = 0·011$; $\Delta\rho$ from −0·21 to 0·22 e Å^{-3}, $S = 1·21$; final $R = 0·061$, $wR = 0·063$; scattering factors from *International Tables for X-ray Crystallography* (1974). All computations performed on a Nova 4S computer and plots drawn on Tektronix plotter with the *SHELXTL* system of programs.

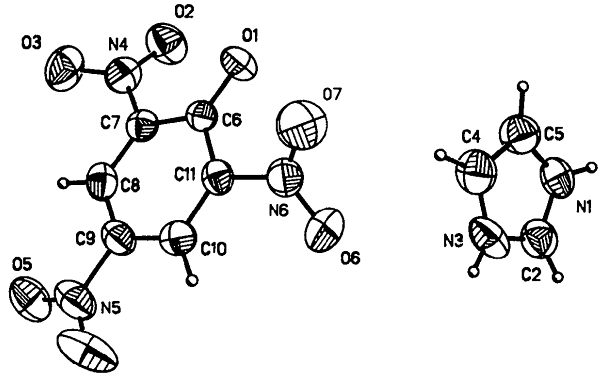

Fig. 1. The molecular structure of the title compound with the atomic numbering scheme.

Atomic coordinates are in Table 1.* A perspective molecular drawing and the atomic labelling scheme are displayed in Fig. 1. Bond distances and angles are listed in Table 2.

Related literature. The title compound was prepared in connection with our studies on the protonation sites of organic bases with several nitrogen functions (Soriano-García, Toscano & Espinosa, 1985; Soriano-García, Toscano & Schatz-Levine, 1987).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52594 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Ethyl 2-Acetyl-3-[5-(*p*-tolyl)-2-furyl]acrylate

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Abstract. $C_{18}H_{18}O_4$, $M_r = 298{\cdot}3$, orthorhombic, $Pbca$, $a = 7{\cdot}519\,(1)$, $b = 21{\cdot}926\,(6)$, $c = 19{\cdot}134\,(4)$ Å, $V = 3154{\cdot}5$ Å^3, $Z = 8$, $D_m = 1{\cdot}24$, $D_x = 1{\cdot}256$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}54178$ Å, $\mu = 0{\cdot}68$ mm^{-1}, $F(000) = 1264$, $T = 293$ K, final $R = 0{\cdot}052$ for 1890 unique observed reflections. There is extensive π delocalization involving the phenyl, furyl and acetylethylenic groups as shown by the pattern of bond lengths and the planarity of the system (the phenyl/furyl and acetylethylenic group/furyl dihedral angles are 1·3 and 1·0°, respectively) while the ethoxycarbonyl moiety is nearly perpendicular to the conjugated system (dihedral angle 91·5°). The molecules are held together by van der Waals forces only.

Experimental. Transparent prism-like crystal of dimensions 0·1 × 0·15 × 0·75 mm; D_m by flotation in bromoform/n-octane; systematic absences: $0kl$ for k odd, $h0l$ for l odd and $hk0$ for h odd; Syntex $P2_1$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation; room temperature; choice of unit-cell parameters verified by *UB* (Sivý, Sivý & Koreň, 1987), refinement on the basis of 15 reflections, $10 < \theta < 25°$; intensity data ($h = 0$ to 8, $k = 0$ to 25, $l = 0$ to 22) by $\theta/2\theta$ scans, $2\theta \leq 130°$; three standards measured every 100 reflections, no significant systematic fluctuation; 2682 unique reflections, 1890 with $I \geq 2\sigma(I)$ considered observed and included in the refinement; data reduction using *XP*21 (Pavelčík,

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