5	105.4[b]	101.9[c]	98.9[d]
6	110.2	108.9	105.5
7	113.2	111.4	108.0

References: (a) Kai, Knochel, Kwiatkowski, Dunitz, Oth, Seebach & Kalinowski (1982); (b) Lam, Huang & Hambley (1990); (c) Koh, Huang & Sim (1992); (d) this work; (e) Bernlöhr, Beckhaus, Lindner & Rüchardt (1984).

The three diphenyl bicycloalkyl compounds were synthesized by free radical dimerization using di-tert-butyl peroxide as initiator (Huang & Lim, 1967). The starting material, phenyl cycloalkane, was mixed with di-tert-butyl peroxide in the molar ratio 2:1 and heated for about 30 h at ~403 K under N_2. After cooling, both the volatile by-products and the starting materials were removed by distillation under reduced pressure. The residue was then purified chromatographically using silica gel (60–200 mesh, E. Merck). Over a period of several months, single crystals of (1) were grown in a mixture of water/n-hexane/acetonitrile; (2) and (3) were crystallized from ethanol and n-hexane, respectively, after chromatographic purification. All starting materials were commercially available except phenyl cycloheptane which was prepared by the method of Corson & Ipatieff (1943). The m.p.'s for (1), (2) and (3) were 410.5, 455 and 412 K, respectively [literature values 414–415, 455–457 and 415.5–416 K (Beckhaus, Schoch & Rüchardt, 1976)].

All three structures were solved by direct methods using XS (SHELXTL-Plus; Siemens, 1989) and refined by full-matrix least-squares analysis using XLS (Sheldrick, 1976, 1985). The data were reduced and Lorentz and polarization corrections applied using the programs mentioned. C atoms were refined anisotropically in all three structures whereas H atoms were placed at calculated positions with fixed isotropic thermal parameters.

Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55798 (33 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1030]

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Structure of N-(2,6-Dimethylphenyl)-5-methylisoxazole-3-carboxamide and Molecular-Orbital Study of C—H⋯O Bonded Dimers

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Abstract

The molecular structure of the title compound comprises two nearly orthogonal planar systems. The main feature of the crystalline structure is the existence of C—H⋯O interactions linking two molecules about the centers of inversion. From crystallographic data, charges and interaction enthalpy are calculated for the monomer and the dimer by means of the AM1 (Austin model 1) semi-empirical method. A substantial stabilization of the molecular structure through dimer formation is observed.

Comment

N-(2,6-Dimethylphenyl)-5-methylisoxazole-3-carbox-amide or D2624 (conventional pharmaceutical name) (Fig. 1) is a promising anticonvulsant drug (Lepage, Tombret, Cuvier, Marivain & Gillardin, 1992). Experimental bond lengths and bond angles are similar to those observed in related compounds (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The molecular structure is mainly composed of two planar systems, nearly orthogonal to one another [102 (1)°], which is a conformation seen in several anticonvulsant molecules (Codding, Duke, Aha, Palmer, McClurg & Szkaradzinska, 1990). In the crystal structure, short C—H···O contacts link two asymmetrical molecules forming dimers about the centers of inversion. These C—H···O interactions are characterized by an inter-molecular distance C(4)···O(7^i) of 3.290 (4) Å and an angle C(4)—H(4)···O(7^i) of 159 (4)°; the H(4) atom is almost situated in the plane O(7^i), C(6^i), C(3^i), where the oxygen sp^2 lobes are located (Fig. 2). The dimers display a herringbone arrangement as is common for planar aromatic hydrocarbons, *e.g.* naphthalene.

There are many examples of interactions between O atoms and C—H groups in the literature. These interactions involve aromatic, alkyne, alkene or even
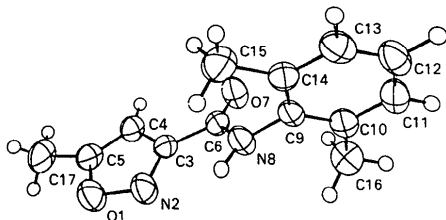

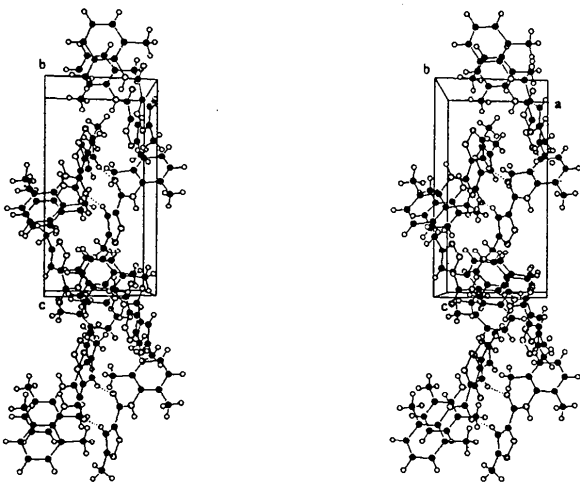Fig. 1. The D2624 molecule with the atom-numbering scheme.

Fig. 2. View of D2624 molecules in the unit cell. Dotted lines represent hydrogen bonds.

aliphatic C—H groups (Taylor & Kennard, 1982; Seiler, Weisman, Glendening, Weinhold, Johnson & Dunitz, 1987; Desiraju, 1989). The electrostatic nature of C—H···O interactions has been established by theoretical studies and it has been shown that they resemble conventional hydrogen bonds. Recently, this type of interaction was presented as a substitute to classical O—H···O and N—H···O hydrogen bonds in drug–receptor binding (Bertolasi, Ferretti, Gilli & Borea, 1990). Dimers linked by C—H···O interactions have also been observed in the crystal structure of *p,p'*-dinitrobenzanilide but no theoretical explanations were given (Hariharan & Srinivasan, 1990).

In order to state more precisely the conditions under which such a short contact could be estab-lished, we performed semi-empirical calculations on D2624 and related molecules, using the AM1 (Austin model 1) Hamiltonian method (Dewar, Zoebisch, Healy & Stewart, 1985). The AM1 method has been successfully used for the study of hydrogen bonds in nitroanilines (Vinson & Dannenberg, 1989), the water dimer (Dannenberg, 1988) and hexuloses (Woods, Szarek & Smith, 1990).

The stabilization of D2624 dimers was related to the charges calculated by the AM1 method. The rotational barriers around the C(3)—C(6) and N(8)—C(9) bonds were found from a search of other conformers. AM1-calculated geometry is globally correct. Bond lengths between non-H atoms were found to be within 0.05 Å of experimental values, except for the O(1)—N(2) bond, which is under-estimated by 0.09 Å, and the O(1)—C(5) bond, which is overestimated by 0.07 Å. MNDO (modified neglect of diatomic overlap) calculations performed on isoxazole revealed the same discrepancy (Olivella & Vilarrasa, 1981). An interesting feature of the calculated geometry is the presence of a short intra-molecular C—H···O interaction between O(7) and an H atom on the methyl group, C(15) or C(16). This intramolecular C—H···O interaction is not present in the crystal and might be related to the known deficiency of the AM1 method which favors bifur-cation in hydrogen bonding to oxygen centers (Merz, Hoffmann & Dewar, 1989; Coitino, Irving, Rama, Iglesias, Paulino & Ventura, 1990; Weaver, Khalil & Smith, 1991; Rzepa & Yi, 1991).

Rotational barriers around the C(6)—C(3) (Fig. 3a) and the C(9)—N(8) bonds (Fig. 3b) have been calculated by stepping the O(7)—C(6)—C(3)—N(2) and C(10)—C(9)—N(8)—C(6) dihedral angles in 10° intervals, and by minimizing energy without applying any constraints, except to the selected torsion angle. Computed torsion angles at minimum enthalpy were found to be 169 and 66° (173 and 77° in the crystal), respectively, and were found to be mutually indepen-dent. The relatively high rotational barriers, calcu-

lated to be 13.4 and 22.2 kJ mol^{-1}, respectively, suggest that the conformer present in solution is identical to the crystal conformer. The calculated rotational barrier around the C(9)—N(8) bond (Fig. 3b) deserves some attention. The computed enthalpy for a 90° torsion angle is higher by 3.8 kJ mol^{-1} than that at the 66° torsion-angle minimum. We explain this by the fact that there is no possibility of an intramolecular C—H···O interaction between O(7) and an H atom on the methyl group, C(15) or C(16), when the C(10)—C(9)—N(8)—C(6) torsion angle is 90°. However, this interaction is present in other calculated conformations.

AM1-calculated geometry for the dimer is reasonably close to the experimental structure with a mean C(4)···O(7^i) distance of 3.21 instead of 3.29 Å, an

O(7)···O(7^i) distance of 4.66 instead of 4.48 Å and a C(4)···C(4^i) distance of 3.97 instead of 4.41 Å. AM1-optimized geometry for the individual unit in the dimer is similar to the optimized geometry of the monomeric molecule. The computed distance H(4)···O(7^i) is 2.29 Å, which is much lower than the sum of the hydrogen and oxygen van der Waals radii.

Selected AM1 charges calculated for D2624, monomer and dimer, are given in Fig. 4. The charge on H(4) (+0.197) of D2624 is higher than that computed for the parent isoxazole (+0.174). It is close to the value calculated for the trinitrobenzene hydrogens (+0.217), which give C—H···O interactions (Taylor & Kennard, 1982). In the dimer, the calculated charge on H(4) is still higher (+0.213), in comparison to the monomer. Inversely, the calculated charge on O(7) is −0.339 in the monomer and −0.366 in the dimer. These variations are indicative of a C—H···O interaction.
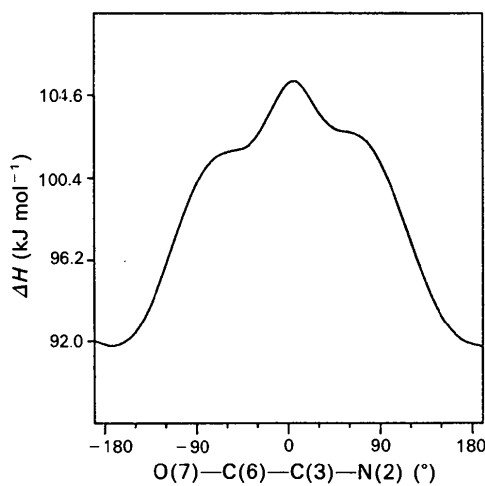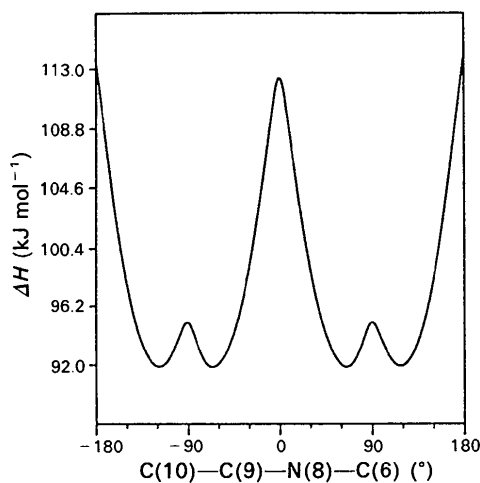
Fig. 3. Calculated enthalpy of formation (ΔH) for D2624 with (a) variation of O(7)—C(6)—C(3)—N(2) torsion angle and (b) variation of C(10)—C(9)—N(8)—C(6) torsion angle.
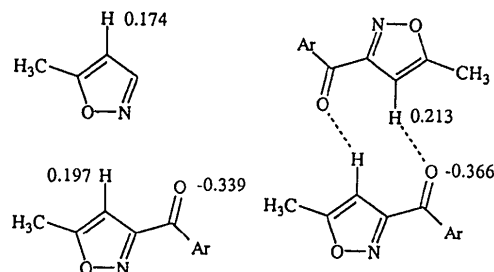

Fig. 4. AM1-calculated charge distribution for an isoxazole, a monomer of D2624 and a dimer of D2624.

Calculated heats of formation are 91.6 and 163.6 kJ mol^{-1} for the monomer and the dimer, respectively. Although the interaction enthalpy, −19.7 kJ mol^{-1}, is not wholly attributable to the two C—H···O interactions, it certainly reflects a substantial stabilization of the dimer by these C—H···O interactions.

Experimental

Crystal data

$C_{13}H_{14}N_2O_2$	Cell parameters from 25
$M_r = 230.27$	reflections
Monoclinic	$\theta = 11.3$–$12.9°$
$P2_1/a$	$\mu = 0.082$ mm^{-1}
$a = 8.107$ (1) Å	$T = 298$ K
$b = 9.482$ (2) Å	Prismatic
$c = 15.64$ (4) Å (unique axis)	$0.40 \times 0.25 \times 0.20$ mm
$\gamma = 97.73$ (2)°	Colorless
$V = 1191$ (2) Å^3	Crystal source: single crys-
$Z = 4$	tals were prepared by
$D_x = 1.284$ Mg m^{-3}	cooling of a saturated so-
Mo $K\alpha$ radiation	lution of D2624 in toluene
$\lambda = 0.7107$ Å	

Data collection

Enraf-Nonius CAD-4 diffractometer	$\theta_{max} = 25°$
$\omega/2\theta$ scans	$h = -9 \to 9$
	$k = 0 \to 11$
Absorption correction: none	$l = 0 \to 15$
	2 standard reflections
2011 measured reflections	monitored every 100
2011 independent reflections	reflections
1298 observed reflections	intensity variation: not
$[I > \sigma(I)]$	significant

Refinement

Refinement on F	$w = 1/\sigma(F)$
Final $R = 0.044$	$(\Delta/\sigma)_{max} < 0.001$
$wR = 0.042$	$\Delta\rho_{max} = 0.2$ e Å^{-3}
$S = 1.84$	$\Delta\rho_{min} = -0.2$ e Å^{-3}
1298 reflections	Atomic scattering factors
196 parameters	from *International Tables*
Only coordinates of H atoms refined	*for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters (Å^2)*

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
O(1)	0.8459 (3)	0.1429 (2)	0.2507 (1)	4.79
N(2)	0.7955 (4)	0.2252 (3)	0.1832 (2)	4.16
C(3)	0.8471 (4)	0.1684 (3)	0.1141 (2)	3.01
C(4)	0.9316 (4)	0.0510 (3)	0.1317 (2)	3.48
C(5)	0.9249 (4)	0.0391 (3)	0.2173 (2)	3.78
C(6)	0.8001 (4)	0.2192 (3)	0.0286 (2)	3.14
O(7)	0.8574 (3)	0.1775 (2)	−0.0366 (1)	4.79
N(8)	0.6848 (3)	0.3094 (3)	0.0318 (2)	3.65
C(9)	0.5900 (4)	0.3479 (3)	−0.0397 (2)	3.09
C(10)	0.6615 (4)	0.4457 (3)	−0.0997 (2)	3.40
C(11)	0.5596 (5)	0.4837 (4)	−0.1651 (2)	4.13
C(12)	0.3934 (5)	0.4258 (4)	−0.1698 (2)	4.38
C(13)	0.3262 (4)	0.3296 (4)	−0.1096 (2)	4.13
C(14)	0.4239 (4)	0.2884 (3)	−0.0434 (2)	3.46
C(15)	0.3499 (6)	0.1814 (4)	0.0214 (3)	5.20
C(16)	0.8404 (5)	0.5102 (4)	−0.0937 (3)	4.79
C(17)	0.9773 (6)	−0.0644 (5)	0.2793 (3)	5.55

Table 2. *Bond lengths (Å) and angles (°)*

O(1)—C(5)	1.351 (4)	N(8)—C(9)	1.432 (4)
O(1)—N(2)	1.407 (3)	C(9)—C(10)	1.389 (4)
N(2)—C(3)	1.302 (4)	C(9)—C(14)	1.390 (4)
C(3)—C(4)	1.411 (4)	C(10)—C(11)	1.393 (5)
C(3)—C(6)	1.488 (4)	C(10)—C(16)	1.499 (5)
C(4)—C(5)	1.344 (5)	C(11)—C(12)	1.387 (5)
C(4)···O(7^i)	3.290 (4)	C(12)—C(13)	1.371 (5)
C(5)—C(17)	1.483 (5)	C(13)—C(14)	1.392 (5)
C(6)—O(7)	1.210 (4)	C(14)—C(15)	1.501 (5)
C(6)—N(8)	1.350 (4)		
C(5)—O(1)—N(2)	108.4 (2)	C(6)—N(8)—C(9)	125.0 (3)
C(3)—N(2)—O(1)	105.1 (2)	C(10)—C(9)—C(14)	122.5 (3)
N(2)—C(3)—C(4)	112.4 (3)	C(10)—C(9)—N(8)	120.5 (3)
N(2)—C(3)—C(6)	120.1 (3)	C(14)—C(9)—N(8)	116.9 (3)
C(4)—C(3)—C(6)	127.1 (3)	C(9)—C(10)—C(11)	117.4 (3)
C(5)—C(4)—C(3)	104.0 (3)	C(9)—C(10)—C(16)	121.6 (3)
C(4)—H(4)···O(7^i)	159 (4)	C(11)—C(10)—C(16)	121.0 (3)
C(4)—C(5)—O(1)	110.0 (3)	C(12)—C(11)—C(10)	120.9 (3)
C(4)—C(5)—C(17)	134.1 (4)	C(13)—C(12)—C(11)	120.4 (3)
O(1)—C(5)—C(17)	115.8 (3)	C(12)—C(13)—C(14)	120.5 (3)
O(7)—C(6)—C(3)	121.7 (3)	C(9)—C(14)—C(13)	118.3 (3)
O(7)—C(6)—N(8)	124.6 (3)	C(9)—C(14)—C(15)	121.6 (3)
N(8)—C(6)—C(3)	113.6 (3)	C(13)—C(14)—C(15)	120.1 (3)

Hydrogen-bond symmetry code: (i) $2 - x, -y, -z$.

The structure was solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). H atoms were located from a difference Fourier map. Full-matrix refinements were carried out by a modified version of *ORXFLS* (Busing, 1971) on a CDC Cyber 990. Distances and angles were calculated with *ORFFE*3 (Busing, Martin, Levy, Brown, Johnson & Thiessen, 1971) and angles of the least-squares planes according to *BP7C* (Ito & Sugawara, 1983). The molecular structure and atomic numbering of D2624 were drawn by *ORTEP*II (Johnson, 1976). A view of all molecules, as packed in the unit cell, was obtained using *MOLDRAW* (Cense, 1989). AM1 calculations were performed on Silicon Graphics 4D/25, either with *AMPAC*-3.01 or *MOPAC*-4.00 (Stewart, 1983). Geometries were fully optimized, employing the keyword *PRECISE*, without applying any constraints except the fixed torsion angle during rotational-barrier calculations.

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3,3′-Dimethyl-4,4′-bipyridine and 5,5′-Dimethyl-4,4′-bipyrimidine

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Abstract

In both title compounds, the aromatic rings adopt a staggered conformation as a result of steric repulsions. In the bipyridine derivative, the closest contacts between methyl H atoms and pyridyl H atoms are H(31)···H(172) [IUPAC pyridine C5 H atom to C3′ methyl group; 2.83 (6) Å] and H(71)···H(131) [2.84 (5) Å] leading to an angle between the pyridyl least-squares planes of 81.1°. In the bipyrimidine compound, the contacts are between N(3) and methyl H(71) [2.84 (3) Å] and N(3) and methyl H(72) [2.77 (3) Å] with an angle between the pyrimidyl planes of 46.0°.

Comment

The structure determination of 3,3′-dimethyl-4,4′-bipyridine (1) and 5,5′-dimethyl-4,4′-bipyrimidine (2) was undertaken during the course of a study into the electron-transfer properties of these bridging ligands *versus* their conformational changes. Details of the syntheses will be published elsewhere (Gourdon, 1992). Crystals of (1) and (2) were obtained by vacuum sublimation at 353 and 343 K, respectively.

Although the angle between ring planes in (1) is much larger than in (2), the central C—C distance is nearly the same in both compounds [1.508 (6) in (1), 1.498 (4) Å in (2)], indicating single-bond character. Distortions of the ring geometries from hexagonal are comparable with those in other bipyridine compounds [from the Cambridge Structural Database (Allen, Kennard & Taylor, 1983)] and in 4,4′-bipyrimidine (Tapolsky, Robert & Launay, 1988).
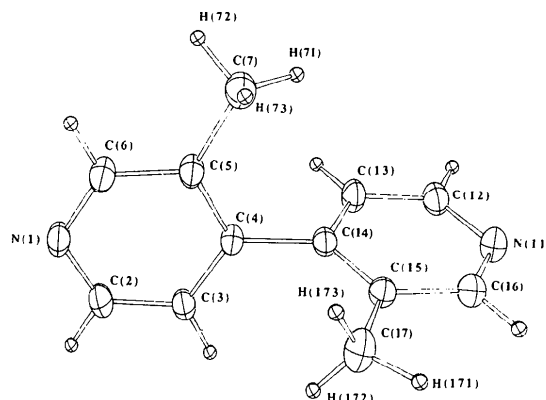

Fig. 1. View of (1) showing the atom-numbering scheme. Thermal ellipsoids are drawn at the 30% probability level except for those of H atoms which, for clarity, have an artificial U_{iso} of 0.0127 Å^2.
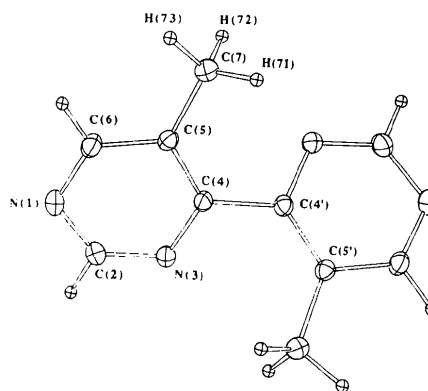

Fig. 2. View of (2) showing the atom-numbering scheme. The two halves of the molecule are related by the crystallographic two-fold axis. Thermal ellipsoids are drawn at the 30% probability level except for those of H atoms which, for clarity, have an artificial U_{iso} of 0.0127 Å^2.

Experimental

Compound (1)

Crystal data

$C_{12}H_{12}N_2$	Mo $K\alpha$ radiation
$M_r = 184.24$	$\lambda = 0.71069$ Å