STERICALLY CROWDED HETEROCYCLES. II. CONFORMATIONAL STRUCTURE OF 2-PHENYL-3-[(*Z*)-1,3-DIPHENYL-3-OXOPROPENYL]-IMIDAZO[1,2-*a*]PYRIDINE AND RELATED COMPOUNDS

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Received September 1, 1994
Accepted November 12, 1994

Dedicated to Professor Dr Fritz Sauter on the occasion of his 65th birthday.

Conformational behaviour of 2-phenyl-3-[(*Z*)-1,3-diphenyl-3-oxopropenyl]imidazo[1,2-*a*]pyridine *I* is studied using a molecular isoenergy map calculated by the PM3 method. A predicted potency of this approach is discussed with respect to the experimental solid state structures of related compounds *I* – *IV*. Complete X-ray structures of 7-methyl derivative *IV* and 11-phenyl derivative *V* are reported.

An interesting problem of inherent chirality of sterically crowded molecules seems to be associated with some restricted geometrical degrees of freedom in intramolecular movements. The idea of the enantiomerism due to restricted rotation between the aromatic ring and the olefinic carbon in appropriately substituted aryl olefins is considerably old[1] and its experimental verification had been achieved already in fourties by Adams and co-workers on the basis of resolution of a number of sterically crowded 3-aryl-3-chloroacrylic acids[2] and *N*-alkyl-*N*-arylsuccinamic acids[3]. The resolution of [2-(1-isopropylmethylpropenyl)phenyl]trimethylamnonium iodide was another example of the chirality evidence[4]. To our knowledge, no heterocyclic compound of this type has been reported yet. The easily accessible *I*-like ketones[5,6] offer now a suit-

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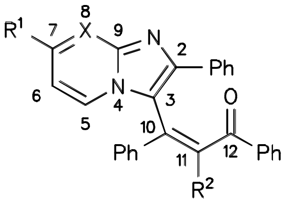
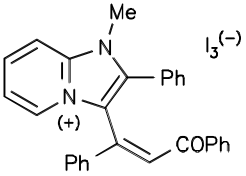
able experimental material for obtaining a deeper insight into conformational limitations of the chirality.

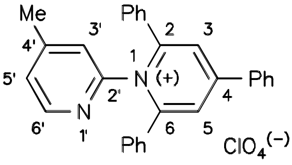
In this communication we wish to report semiempirical MO energy calculations of parent compound *I* with the aim to predict a number of corresponding conformers. The results are compared with the known[5,7] X-ray structures of related compounds *I* – *III*. A complete X-ray analysis of crystalline methyl derivative *IV* and phenyl derivative *V* has been performed to clear up additional substituent effects on the molecular geometry of appropriate conformers. The new compound *IV* was prepared by the ferricyanide oxidation[6] of substituted pyridinium perchlorate *VI*.



I, R^1 = R^2 = H; X = CH
II, R^1 = R^2 = H; X = N
IV, R^1 = Me; R^2 = H; X = CH
V, R^1 = H; R^2 = Ph; X = CH



III



VI

EXPERIMENTAL

The temperature data are uncorrected. Melting points were determined on a Boetius block. NMR spectra were taken on a VARIAN VXR-4OO instrument with TMS as internal standard at 297 K. The working frequency was 400 MHz for ^{1}H and 100 MHz for ^{13}C.

7-Methyl-2-phenyl-3-[(*Z*)-1,3-diphenyl-3-oxopropenyl]imidazo[1,2-*a*]pyridine (*IV*)

Suspension of salt *VI* (7 g, 14 mmol) in ethanol (350 ml) was refluxed and treated with solution of potassium ferricyanide (14 g, 43 mmol) and potassium hydroxide (3.5 g, 62 mmol) in water (70 ml). After 15 min boiling, the mixture was diluted with ice water (1 200 ml) and extracted with chloroform (5 × 80 ml). The collected organic extracts were washed with water (300 ml) and dried with sodium sulfate, the solvent was evaporated under reduced pressure and the red viscous residue was dissolved in hot ethanol (40 ml) and let to crystallize. After 3 days, the precipitated crystals were collected by suction, washed with ethanol (2 × 10 ml) and finally with diethyl ether (20 ml). Yield 4.5 g (77%) of yellow crystals of enone *IV*, m.p. 168 – 170 °C (ethanol). For $C_{29}H_{22}N_2O$ (414.5) calculated: 84.03% C, 5.35% H, 6.76% N; found: 84.29% C, 5.47% H, 6.62% N. ^{1}H NMR spectrum ($CDCl_3$): 2.352 s, 3 H (Me); 6.675 dd, 1 H, *J* = 7.1 and 1.3 (H-6); 7.132 dd, 1 H, *J* = 7.5 and 1.3 (*p*-Ph2); 7.214 dd, 2 H, *J* = 7.5 and 7.1 (*m*-Ph2); 7.33 – 7.40 mt, 5 H (*m*-Ph10, *p*-Ph10 and *m*-Ph12); 7.431 ddq, 1 H, *J* = 0.9, 1.7 and 1.0 (H-8); 7.49 – 7.54 mt, 3 H (*o*-Ph10 and *p*-Ph12); 7.697 dd, 2 H, *J* = 7.1 and 1.3 (*o*-Ph2); 7.726 dd, 1 H, *J* = 7.1 and 0.9 (H-5); 7.860 dd, 2 H (*o*-Ph12); 7.963 s, 1 H (H-11). ^{13}C NMR spectrum ($CDCl_3$): 20.71 (Me), 114.85 CH (C-6), 115.03 CH (C-8), 117.26 C (C-3), 124.10 CH (C-5), 127.03 2 CH (*o*-Ph2), 127.25 CH (*p*-Ph2), 127.91 2 CH (*o*-Ph12), 128.05 2 CH (*m*-Ph2), 128.31 2 CH (*m*-Ph10), 128.95 2 CH (*m*-Ph12), 130.21 CH (*p*-Ph10), 132.69 CH (*p*-Ph12), 133.80 C (*i*-Ph2), 135.81 C (C-7), 137.55 C (*i*-Ph10), 137.63 C (*i*-Ph12), 141.21 C (C-10), 142.97 C (C-2), 145.06 C (C-9), 189.52 C (CO). IR spectrum ($CHCl_3$): 1 598 and 1 648 cm (C=C–C=O).

2-Phenyl-3-[(*Z*)-1,2,3-triphenyl-3-oxopropenyl]imidazo[1,2-*a*]pyridine (*V*)

Enone *V* was isolated after the ferricyanide oxidation of 1-(pyridin-2-yl)-2,3,4,6-tetraphenylpyridinium perchlorate[8]. Crystals for the X-ray analysis (m.p. 199 – 201 °C) were obtained by a slow recrystallization from an ethanol–ether mixture.

1-(4-Methylpyridin-2-yl)-2,4,6-triphenylpyridinium perchlorate (*VI*)

2,4,6-Triphenylpyrylium perchlorate (8 g, 21 mmol), 2-amino-4-methylpyridine (2.7 g, 25 mmol) and ethanol (350 ml) were refluxed and stirred for 9 h. The mixture was then let to crystallize by cooling to room temperature. The precipitated crystals were washed with ethanol, ether and dried. Yield 8.6 g (88%) of colourless crystals, m.p. 259 – 261 °C. For $C_{29}H_{23}ClN_2O_4$ (499.0) calculated: 69.81% C, 4.65% H, 5.61% N; found: 69.63% C, 4.71% H, 5.45% N. ^{1}H NMR spectrum ($(CD_3)_2SO$): 2.113 s, 3 H (Me); 7.177 dd , 1 H, *J* = 5.1 and 1.5 (H-5′); 7.36 – 7.48 mt, 11 H (*o*- and *m*-Ph2, *o*- and *m*-Ph6 and H-3′); 7.672 d, 2 H, *J* = 7 (*m*-Ph4); 7.720 dd, 1 H, *J* = 7 and 7 (*p*-Ph4); 8.170 d, 1 H, *J* = 5.1 (H-6′); 8.366 dt, *J* = 7 and 1 (*o*-Ph4); 8.697 s, 2 H (H-3 and H-5). ^{13}C NMR spectrum: 20.27 (Me), 125.11 CH (C-3′), 125.37 2 CH (C-3 and C-5), 126.40 CH (C-5′), 128.27 4 CH (*m*-Ph2 and *m*-Ph6), 129.05 2 CH (*o*-Ph4), 129.69 4 CH (*o*-Ph2 and *o*-Ph6), 129.70 2 CH (*m*-Ph4), 130.32 2 CH (*p*-Ph2 and *p*-Ph6), 132.40 2 C (*i*-Ph2 and *i*-Ph6), 132.74 CH (*p*-Ph4), 133.39 C (*i*-Ph4), 148.23 CH (C-6′), 150.59 C (C-4′), 151.03 C (C-2′), 155.49 2 C (C-2 and C-6), 156.50 C (C-4).

X-Ray Analyses of Compounds *IV* and *V*

Compound IV: Monoclinic space group $P2_1/n$, a = 10.910(2), b = 13.247(3), c = 15.918(2) Å, β = 95.59(1)°, V = 2 289.6(7) Å^3, Z = 4, D_{calc} = 1.202 g cm^{-3}, μ(MoKα) = 0.07 mm^{-1}, F(000) = 872.

Compound V: Monoclinic space group $P2_1$, a = 9.932(2), b = 8.880(2), c = 14.512(3) Å, β = 98.12(2), V = 1 267.1(4) Å^3, Z = 2, D_{calc} = 1.249 g cm^{-3}, μ(MoKα) = 0.07 mm^{-1}, F(000) = 500.

Both structures were solved by direct methods and anisotropically refined by full-matrix least-squares. The hydrogen atoms were placed in positions found from ideal geometry with $U_{iso} = U_{eq}$ of the attached atoms. Data collection and structure refinement parameters are listed in Table I. Final coordinates and thermal parameters are given in Table II. Figs 1 and 2 show drawings of molecules *IV* and *V*.

Calculations

The molecular energies of enone *I* were calculated by the standard PM3 method[9]. The molecular isoenergy map was obtained from 273 energy values by a cartographic procedure (Surfer, Golden Software Inc., 1987).

RESULTS AND DISCUSSION

Mechanistic models of *I*-like molecules show their conformational behaviour to be approximated by a consideration of simultaneous rotations around the C3–C10 and C11–C12 bonds expressed by the corresponding torsion angles Φ_1(N4–C3–C10–C11) and Φ_2(C10–C11–C12–O1), respectively. Four conformation types may be a priori derived from the hypothetical planar structures *s,s-I, s,a-I, a,s-I* and *a,a-I* according to the

TABLE I
Data collection and structure refinement parameters

Parameter	*IV*	*V*
Crystal dimensions, mm	$0.2 \times 0.6 \times 0.8$	$0.35 \times 0.75 \times 0.2$
Diffractometer and radiation used	Enraf–Nonius CAD4, λ(MoKα) = 0.71073 Å	
Scan technique	$\omega/2\theta$	
Temperature	293 K	
No. and θ range of reflections for lattice parameter refinement	20; 16 – 18°	20; 16 – 18°
Range of *h*, *k* and *l*	$-12 \rightarrow 12$, $0 \rightarrow 15$ $-18 \rightarrow 18$	$-11 \rightarrow 11$, $0 \rightarrow 10$ $-17 \rightarrow 17$
Standard reflections monitored in interval; intensity fluctuation	120 min; –0.5%	120 min; –0.4%
Total number of reflections measured; 2θ range	6 616; 0 – 50°	4 449; 0 – 50°
Value of R_{int}	0.036	0.032
No. of unique observed reflections	2 342	1 938
Criterion for observed reflections	$I \geq 1.96\,\sigma(I)$	
Function minimized	$\sum w\,(\lvert F_o \rvert - \lvert F_c \rvert)^2$	
Weighting scheme	$w = [\sigma^2(F_o)]^{-1}$	
Parameters refined	289	334
Value of *R*, ωR and *S*	0.079, 0.061, 1.28	0.051, 0.043, 1.04
Ratio of max. least-squares shift to e.s.d. in the last cycle	0.001	0.07
Max. and min. heights in final Δρ map	0.36, –0.31 e $Å^{-3}$	0.15, –0.23 e$Å^{-3}$
Source of atomic scattering factors	ref.[10]	
Programs used	CRYSTALS (ref.[11]), SDP (ref.[12]), SHELXS86 (ref.[13]), PARST (ref.[14])	
Computers used	PDP 11/73, PC AT 486	

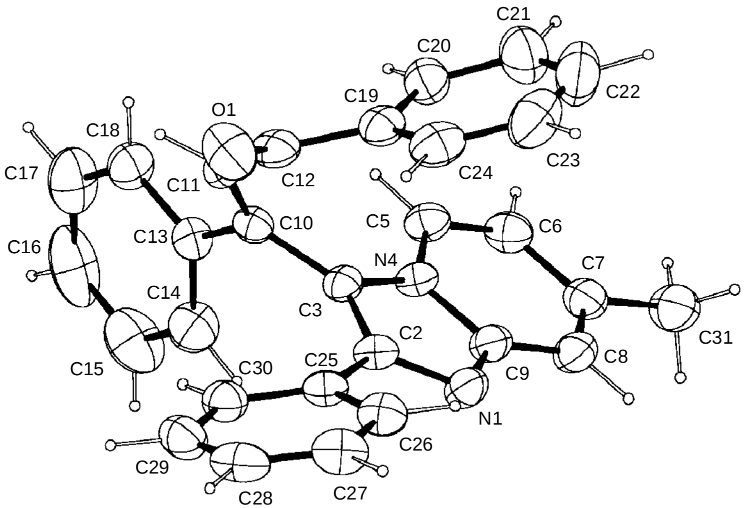


FIG. 1
X-Ray molecular structure of compound *IV*

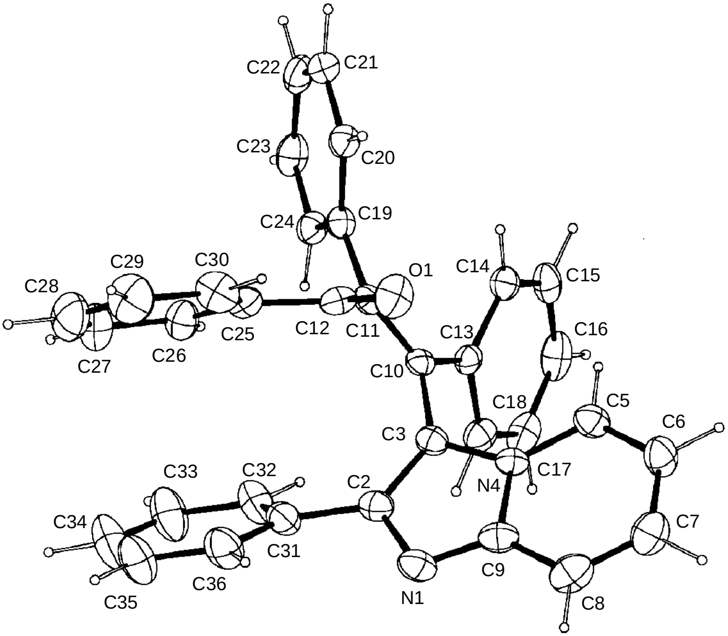


FIG. 2
X-Ray molecular structure of compound *V*

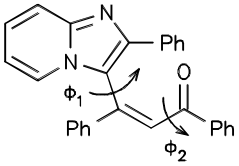
TABLE II
Final coordinates (. 10^4) and their equivalent isotropic thermal parameters (. 10^2) for non-hydrogen atoms. The isotropic equivalent parameter is defined as $U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \boldsymbol{a}_i \boldsymbol{a}_j$

Atom	*x*	*y*	*z*	U_{eq}, Å^2
		Molecule *IV*		
O1	4718(4)	2878(3)	6190(2)	8.7(3)
N1	3488(4)	5301(3)	8596(3)	5.9(3)
N4	2052(3)	4090(3)	8536(2)	4.8(2)
C2	3337(4)	4905(3)	7801(3)	5.0(3)
C3	2469(4)	4141(3)	7740(3)	4.7(3)
C5	1227(4)	3456(4)	8866(3)	5.7(3)
C6	1005(4)	3565(4)	9677(3)	6.1(3)
C7	1620(5)	4313(4)	10220(3)	6.1(3)
C8	2470(5)	4907(4)	9880(3)	6.4(3)
C9	2710(5)	4805(4)	9039(3)	5.5(3)
C10	1986(4)	3480(3)	7046(3)	4.9(3)
C11	2734(5)	2923(4)	6613(3)	5.9(3)
C12	4090(5)	2827(4)	6783(3)	6.0(4)
C13	642(5)	3523(4)	6787(3)	5.7(4)
C14	–20(5)	4391(5)	6915(3)	7.9(4)
C15	–1269(6)	4439(6)	6654(4)	9.7(5)
C16	–1868(6)	3619(8)	6274(5)	9.4(7)
C17	–1207(7)	2772(6)	6146(4)	9.3(6)
C18	21(5)	2710(4)	6396(3)	7.2(4)
C19	4676(5)	2649(4)	7649(3)	6.0(4)
C20	4050(5)	2161(4)	8245(3)	7.2(4)
C21	4631(7)	1949(5)	9026(4)	10.1(5)
C22	5828(8)	2232(6)	9227(5)	10.8(5)
C23	6458(6)	2729(6)	8650(5)	9.5(6)
C24	5895(5)	2931(4)	7860(4)	7.6(7)
C25	4051(4)	5304(3)	7133(3)	5.2(5)
C26	5236(5)	5655(4)	7366(3)	6.4(6)
C27	5940(5)	6066(4)	6778(4)	7.5(7)
C28	5486(6)	6120(4)	5945(4)	7.2(4)
C29	4317(6)	5776(4)	5703(4)	7.3(5)
C30	3593(5)	5377(4)	6293(3)	6.4(5)
C31	1332(5)	4415(4)	11115(3)	8.1(4)
		Molecule *V*		
O1	3862(4)	3533(4)	2405(3)	5.7(2)
N1	1304(4)	5169(6)	4270(3)	5.1(2)

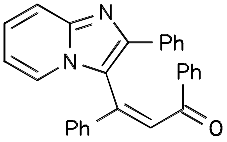
TABLE II
(*Continued*)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
N4	597(4)	3981(5)	2915(2)	3.8(2)
C2	1705(5)	5954(6)	3537(3)	4.4(3)
C3	1307(4)	5257(6)	2694(3)	3.8(2)
C5	−44(5)	2865(6)	2359(3)	4.8(3)
C6	−687(5)	1746(7)	2755(4)	5.7(3)
C7	−679(6)	1721(7)	3726(4)	6.3(3)
C8	−36(6)	2791(7)	4277(4)	5.8(3)
C9	644(5)	3980(7)	3881(3)	4.8(3)
C10	1533(4)	5589(5)	1734(3)	3.2(2)
C11	2799(4)	5556(5)	1520(3)	3.4(2)
C12	3932(5)	4874(6)	2197(3)	4.4(3)
C13	289(4)	5933(5)	1059(3)	3.5(3)
C14	147(5)	5454(6)	136(3)	4.2(3)
C15	−1008(5)	5816(6)	−472(3)	4.7(3)
C16	−2039(5)	6619(7)	−186(4)	5.2(3)
C17	−1940(5)	7055(6)	741(4)	5.0(3)
C18	−791(4)	6717(6)	1355(3)	4.4(3)
C19	3213(4)	6037(5)	626(3)	3.6(2)
C20	4071(4)	5164(6)	175(3)	4.2(3)
C21	4412(5)	5551(6)	−678(3)	4.9(3)
C22	3898(5)	6855(7)	−1110(3)	5.2(3)
C23	3075(5)	770(6)	−665(3)	4.8(3)
C24	2745(5)	7385(6)	189(3)	4.3(3)
C25	5132(5)	5774(6)	2573(3)	4.4(3)
C26	5146(5)	7349(7)	2464(4)	5.4(3)
C27	6242(6)	8182(7)	2871(4)	6.8(4)
C28	7331(7)	7490(1)	3388(5)	8.0(5)
C29	7338(6)	5945(9)	3502(5)	7.4(5)
C30	6245(5)	5103(7)	3095(3)	6.0(4)
C31	2413(5)	7428(6)	3697(4)	5.1(3)
C32	2097(6)	8620(7)	3091(4)	6.0(3)
C33	2765(6)	9999(7)	3255(5)	7.5(4)
C34	3740(7)	10172(9)	4006(5)	8.4(5)
C35	4051(7)	8996(9)	4622(5)	8.2(5)
C36	3386(6)	7619(8)	4469(4)	6.6(3)

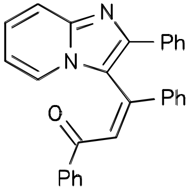
relative *syn*- or *anti*-orientations of the C=C bond to the heterocyclic system (Φ_1) and the carbonyl group C=O (Φ_2). It may be postulated that every partial *s*-conformation is characterized by the Φ_1 and Φ_2 torsion angles within the ranges (–90°,0°) or (0°,+90°) while the ranges (–180°,–90°) and (+90°,+180°) come into account for *a*-conformations only.



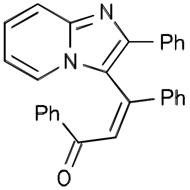
a,s–I



a,a–I



s,s–I



s,a–I

Conformation Analysis of Enone I

In accordance with the above mentioned criteria the conformational behaviour of molecule *I* has been investigated in the following way: The Φ_1 and Φ_2 values were systematically and stepwise changed and for a given (Φ_1,Φ_2) couple all other geometric degrees of freedom were optimized to obtain the lowest PM3 energies.

The calculated data enabled to depict the Φ_1–Φ_2 map shown in Fig. 3. The mirror right- and left-hand parts correspond to two enantiomers of enone *I*. Considering only the right-hand situation, two conformer pairs can be seen all having the Φ_1 values not too far from +90° (Table III) thus suggesting the molecule *I* consists of two almost orthogonal π-electron systems, e.g. the side chain linkage –(Ph)C=CCOPh and the 2-phenylimidazo[1,2-*a*]pyridine skeleton. The PM3 minima of two conformer couples *Ia, Ib* and *Ic, Id* (all belonging to the *a,a*-type) are separated by a low energy barrier about 7 kcal mol^{-1}. The molecular energy differences of the conformers *Ia* – *Id* are even smaller not exceeding 2.2 kcal mol^{-1}. On the other hand, racemization barriers are significantly higher (Table III) thus indicating a possibility of identification and maybe also resolution of corresponding enantiomers.

TABLE III
Energy and geometrical characteristics followed from the PM3 isoenergy map of molecule[a] *I*

Conformer	Φ_1, °	Φ_2, °	ΔH_f	ΔE_{rel}	ΔE_{rac}
Ia	±110.9	−132.2	115.7	0.0	19.3[b]
Ib	±90.9	−101.4	117.0	1.3	23.5
Ic	±94.1	+99.3	118.4	2.7	13.5
Id	±92.8	+116.5	117.9	2.2	18.1

[a] See Fig. 3, all energies in kcal mol^{-1}; [b] calculated rotation barrier of the PhCO group: 7.0 kcal mol^{-1}.

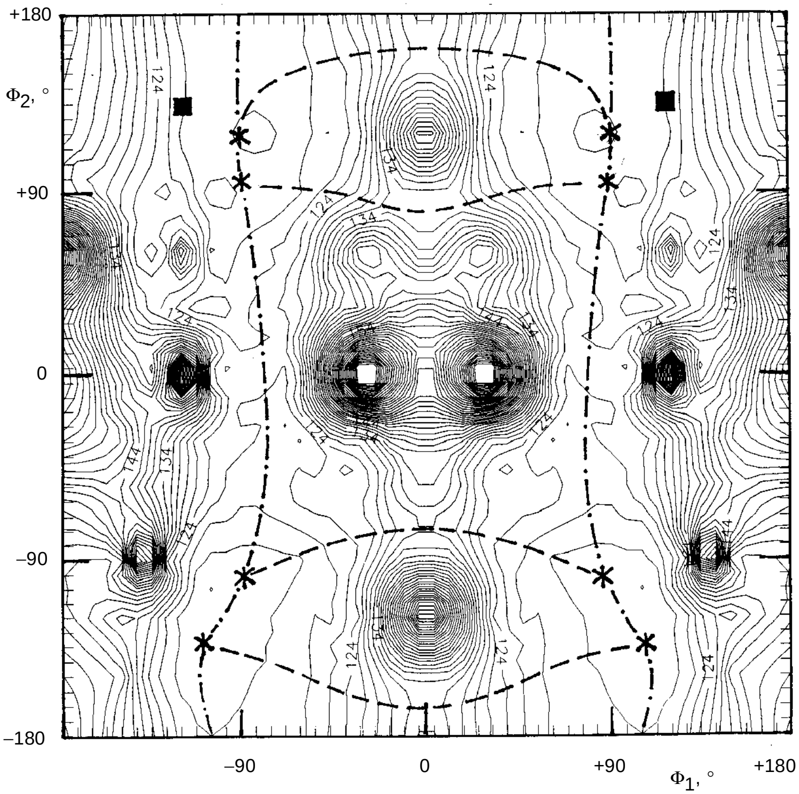


FIG. 3
Φ_1–Φ_2 isoenergy map calculated for molecule *I* by the PM3 method. Meanings of the symbols: * energy minima; ■ X-ray data; – – – racemization coordinate; – · – · – benzoyl group rotation coordinate

X-Ray Structure of Compounds I – V

According to the above mentioned Φ_1,Φ_2-criteria the hitherto X-ray analyzed[5,7] compounds *I – III* exhibit the *a,a* or *s,a* solid state conformers (Table IV). Hence, it may be concluded the different X groups in the both heterocyclic bases *I* and *II* do not cause any change of the *a,a* type of the solid state conformers. On the other hand, in periodide *III* the *s,a*-conformation within the cation has been interpreted as a consequence of the positive charge effect on the side linkage containing the carbonyl group[7].

To extend our knowledge of possible substituent effects on the solid state conformation of *I*-like molecules, the X-ray structures of 7-methyl derivative *IV* and 11-phenyl derivative *V* were investigated. As follows from Table IV, the introduction of the 7-methyl group perturbates the molecular skeleton so weakly that the *a,a*-conformational type recognized in solid state structure of the parent compound *I* is conserved. In

TABLE IV
Comparison of some torsion angles (in °) determined by the X-ray analysis

Compound	Φ_1[a]	Φ_2[b]	Conformer	Reference
I[a]	±123.4	±135.5	*a, a*	7
II[b]	±118.3	±130.4	*a, a*	5
III[a]	±66.0	∓22.1	*s, a*	7
IV	±126.9	±134.9	*a, a*	this work
V	±113.7	∓61.5	*a, s*	this work

[a] (N4–C3–C10–C11); [b] (C10–C11–C12–O1).

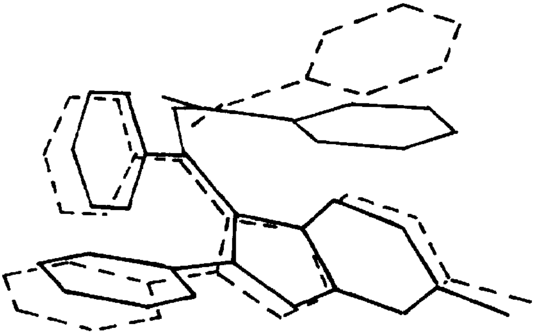


FIG. 4
Comparison of X-ray and PM3 calculated molecular shapes for compound *IV*. Dashed parts follow from the theoretical treatment

the case of compound *VI* the more bulky 11-phenyl group evidently forces the side chain PhCOC(Ph)=C(Ph) to adopt another energetically preferable shape. Consequently, the *a,s*-type of the solid state conformers was observed.

In Fig. 3 the structure of enone *I* found by X-ray analysis is indicated by the point (Φ_1 = 123.4°, Φ_2 = 135.5°) not far from calculated energy minimum of the predicted conformer *Id* (Φ_1 = 92.8°, Φ_2 = 116.5°). This reflects certain proximity of the energy map to that involving crystal matrix effects at least in the vicinity of the energy minima.

Comparison of molecular shapes of the enones *IV* and *V* obtained by the X-ray analysis and the PM3 optimization shows a general proximity of the experimental and theoretical phenomena. In the case of 7-methyl derivative *IV* (Fig. 4), certain divergencies are restricted only to the subspace of the terminal benzoyl group moving, similarly as in the parent compound *I* (ref.^{7}). On the other hand, the compound *V* containing four phenyl groups exhibits a perfect fit between the experiment and the theory (Fig. 5), thus suggesting a less important crystal field effects on the conformational behaviour of molecules with a higher restriction of inner rotations.

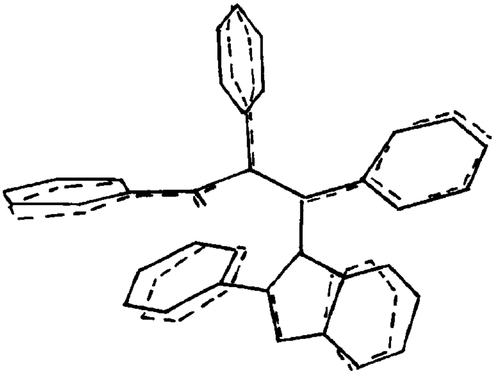


FIG. 5
Comparison of X-ray and PM3 calculated molecular shapes for compound *V*. Dashed parts follow from the theoretical treatment

Thanks to the non-centrosymmetric space group ($P2_1$) found for tetraphenyl derivative *V*, an interesting observation of one enantiomeric form only is seen in the molecular packing.

This work was supported within the project No. 203/93/0320 of the Grant Agency of the Czech Republic. The authors are indebted to the staff of Central Laboratories (Prague Institute of Chemical Technology) for the elemental analyses and measurement of IR spectra.

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