

moyenne des distances C—N, 113,3° pour celle des angles N—C—N et 107,5° pour celle des angles C—N—C. Autrement dit, le fait que la molécule d'hexaméthylènetétramine soit coordonnée à trois atomes d'argent ne modifie pas sa géométrie de façon significative.

Les feuillets sont unis les uns aux autres par des interactions de van der Waals. Les plus importantes de ces interactions sont rassemblées dans le Tableau 4.

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2-Methyl-5,6-diphenylanthra[2,1-*b*]pyrazole

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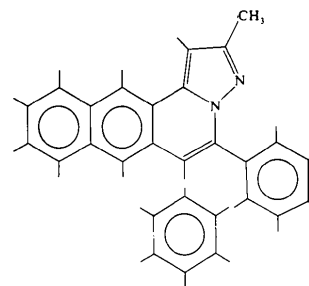
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Abstract

$C_{28}H_{20}N_2$, $M_r = 384.5$, is triclinic, with space group $P\bar{1}$ and $Z = 4$, $a = 12.572(3)$, $b = 14.832(3)$, $c = 12.122(2)$ Å, $\alpha = 111.64(1)$, $\beta = 92.56(2)$, $\gamma = 88.64(2)^\circ$, $V = 2098.7(7)$ Å³. The density, calculated from the unit-cell volume and contents, is 1.216 Mg m⁻³. The structural formula is:



(I)

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The structure was solved by direct methods (*MULTAN*) and refined by full-matrix least-squares procedures to a final crystallographic residual of 0.054 for 4005 observed reflections (Cu $K\alpha$ data). This study establishes that the major product of polyphosphoric acid cyclodehydration of 2-[3-methyl-5-(2-naphthyl)-1-pyrazolyl]-2-phenylacetophenone is 2-methyl-5,6-diphenylantra[2,1-*b*]pyrazole. It is con-

cluded that the synthesis of a diazasteroid, a possible product of this reaction, is sterically inhibited.

Introduction

Triclinic crystals of 2-methyl-5,6-diphenylantra[2,1-*b*]pyrazole were obtained from ethanol. The crystal

Table 1. *Positional and average isotropic thermal parameters with e.s.d.'s in parentheses*

The expression for the isotropic temperature factor is: $T = \exp(-B \sin^2 \theta / \lambda^2)$. $\langle B \rangle$ for the non-hydrogen atoms is defined as $\frac{1}{3} \sum_i B_{ii}$; the values for the H atoms are taken directly from the least-squares refinement.

	Molecule A				Molecule B			
	<i>x</i>	<i>y</i>	<i>z</i>	$\langle B \rangle$ (Å ²)	<i>x</i>	<i>y</i>	<i>z</i>	$\langle B \rangle$ (Å ²)
C(1)	0.3658 (2)	0.4000 (1)	0.3260 (2)	4.8 (1)	0.8914 (2)	0.1281 (1)	0.9136 (2)	4.8 (1)
C(2)	0.3801 (2)	0.3663 (1)	0.4140 (2)	4.7 (1)	0.8590 (2)	0.1149 (1)	1.0112 (2)	4.7 (1)
N(3)	0.4565 (1)	0.2932 (1)	0.4025 (1)	5.0 (1)	0.7807 (1)	0.0458 (1)	0.9967 (1)	4.8 (1)
C(4)	0.5216 (2)	0.2554 (1)	0.3077 (2)	4.9 (1)	0.7344 (2)	-0.0112 (1)	0.8897 (2)	5.1 (1)
C(5)	0.6182 (2)	0.2506 (2)	-0.0838 (2)	7.4 (1)	0.7292 (2)	-0.1123 (2)	0.4534 (2)	6.7 (1)
C(6)	0.5991 (3)	0.2811 (2)	-0.1752 (2)	9.3 (2)	0.7681 (2)	-0.1013 (2)	0.3554 (2)	7.9 (2)
C(7)	0.5157 (3)	0.3466 (2)	-0.1730 (2)	9.4 (2)	0.8385 (2)	-0.0266 (2)	0.3663 (2)	8.3 (2)
C(8)	0.4553 (2)	0.3833 (2)	-0.0762 (2)	7.7 (1)	0.8741 (2)	0.0344 (2)	0.4747 (2)	7.6 (1)
C(9)	0.5706 (2)	0.2543 (2)	0.1132 (2)	5.5 (1)	0.7290 (2)	-0.0592 (2)	0.6718 (2)	5.9 (1)
C(10)	0.4129 (2)	0.3925 (2)	0.1253 (2)	5.6 (1)	0.8800 (2)	0.0817 (2)	0.6931 (2)	5.9 (1)
C(1A)	0.4284 (2)	0.3621 (1)	0.2195 (2)	4.9 (1)	0.8470 (2)	0.0713 (1)	0.7956 (2)	4.9 (1)
C(4A)	0.5091 (2)	0.2907 (1)	0.2120 (2)	4.8 (1)	0.7691 (2)	-0.0009 (1)	0.7838 (2)	5.0 (1)
C(5A)	0.5553 (2)	0.2863 (2)	0.0183 (2)	5.5 (1)	0.7647 (2)	-0.0493 (2)	0.5691 (2)	5.7 (1)
C(8A)	0.4733 (2)	0.3555 (2)	0.0230 (2)	5.9 (1)	0.8401 (2)	0.0229 (2)	0.5798 (2)	6.1 (1)
N(11)	0.4727 (1)	0.2496 (1)	0.4838 (2)	5.7 (1)	0.7375 (1)	0.0304 (1)	1.0901 (1)	5.3 (1)
C(12)	0.5498 (2)	0.1837 (2)	0.4371 (2)	5.8 (1)	0.6638 (2)	-0.0369 (2)	1.0392 (2)	5.5 (1)
C(13)	0.5829 (2)	0.1861 (2)	0.3307 (2)	5.9 (1)	0.6595 (2)	-0.0656 (2)	0.9158 (2)	6.0 (1)
C(14)	0.5850 (2)	0.1165 (2)	0.4987 (2)	8.5 (2)	0.5970 (2)	-0.0712 (2)	1.1151 (2)	7.7 (1)
C(15)	0.2836 (2)	0.4761 (2)	0.3344 (2)	5.3 (1)	0.9745 (2)	0.2024 (2)	0.9277 (2)	5.4 (1)
C(16)	0.1813 (2)	0.4506 (2)	0.2910 (3)	7.7 (2)	0.9488 (2)	0.2868 (2)	0.9087 (2)	7.6 (1)
C(17)	0.1052 (2)	0.5219 (2)	0.2970 (3)	9.8 (2)	1.0262 (3)	0.3574 (2)	0.9253 (3)	9.4 (2)
C(18)	0.1322 (2)	0.6177 (2)	0.3430 (3)	8.7 (2)	1.1284 (2)	0.3407 (2)	0.9580 (3)	9.1 (2)
C(19)	0.2318 (3)	0.6438 (2)	0.3873 (3)	8.3 (2)	1.1556 (2)	0.2574 (2)	0.9750 (2)	8.1 (2)
C(20)	0.3081 (2)	0.5733 (2)	0.3835 (2)	7.2 (1)	1.0795 (2)	0.1882 (2)	0.9595 (2)	6.2 (1)
C(21)	0.3223 (2)	0.3989 (1)	0.5268 (2)	4.7 (1)	0.8989 (2)	0.1691 (1)	1.1347 (2)	4.8 (1)
C(22)	0.2372 (2)	0.3485 (2)	0.5410 (2)	7.2 (2)	0.8685 (2)	0.2641 (2)	1.1934 (2)	6.5 (1)
C(23)	0.1849 (2)	0.3769 (2)	0.6472 (3)	8.2 (2)	0.9064 (2)	0.3154 (2)	1.3079 (2)	7.5 (2)
C(24)	0.2193 (2)	0.4578 (2)	0.7394 (2)	6.7 (1)	0.9754 (2)	0.2722 (2)	1.3625 (2)	7.0 (2)
C(25)	0.3038 (2)	0.5079 (2)	0.7276 (2)	6.7 (1)	1.0066 (2)	0.1785 (2)	1.3061 (2)	7.3 (1)
C(26)	0.3553 (2)	0.4792 (2)	0.6222 (2)	6.1 (1)	0.9685 (2)	0.1263 (2)	1.1922 (2)	6.1 (1)
H(C5)	0.678 (2)	0.200 (2)	-0.086 (2)	9.7 (7)	0.674 (2)	-0.168 (2)	0.445 (2)	9.9 (7)
H(C6)	0.643 (2)	0.256 (2)	-0.242 (2)	9.5 (7)	0.738 (2)	-0.148 (2)	0.278 (2)	9.9 (7)
H(C7)	0.500 (2)	0.366 (1)	-0.242 (2)	8.4 (6)	0.862 (2)	-0.018 (1)	0.291 (2)	7.4 (6)
H(C8)	0.398 (2)	0.434 (1)	-0.067 (2)	6.6 (5)	0.926 (2)	0.091 (2)	0.491 (2)	7.1 (6)
H(C9)	0.628 (2)	0.205 (1)	0.112 (2)	7.1 (6)	0.682 (2)	-0.111 (1)	0.669 (2)	6.8 (5)
H(C10)	0.356 (1)	0.440 (1)	0.127 (1)	4.2 (4)	0.930 (1)	0.129 (1)	0.698 (2)	5.0 (5)
H(C13)	0.641 (1)	0.151 (1)	0.285 (2)	5.5 (5)	0.614 (2)	-0.114 (1)	0.860 (2)	7.0 (6)
H1(C14)	0.547 (2)	0.125 (2)	0.573 (2)	10.3 (7)	0.524 (2)	-0.064 (2)	1.099 (2)	9.8 (7)
H2(C14)	0.651 (2)	0.134 (2)	0.522 (2)	11.7 (8)	0.601 (2)	-0.139 (2)	1.093 (2)	10.0 (7)
H3(C14)	0.572 (3)	0.051 (2)	0.449 (3)	16.1 (9)	0.618 (2)	-0.044 (2)	1.199 (2)	9.8 (7)
H(C16)	0.162 (2)	0.381 (1)	0.265 (2)	7.7 (6)	0.868 (2)	0.305 (1)	0.895 (2)	7.9 (6)
H(C17)	0.044 (2)	0.499 (2)	0.263 (2)	9.9 (7)	1.002 (2)	0.418 (2)	0.916 (2)	9.9 (7)
H(C18)	0.080 (2)	0.669 (2)	0.350 (2)	8.4 (6)	1.180 (2)	0.395 (1)	0.975 (2)	8.1 (6)
H(C19)	0.254 (2)	0.716 (2)	0.431 (2)	11.7 (8)	1.232 (2)	0.251 (2)	1.007 (2)	10.9 (8)
H(C20)	0.381 (2)	0.594 (2)	0.414 (2)	9.8 (7)	1.095 (2)	0.126 (1)	0.973 (2)	8.1 (6)
H(C22)	0.214 (2)	0.288 (1)	0.476 (2)	7.0 (6)	0.821 (2)	0.293 (1)	1.155 (2)	6.2 (5)
H(C23)	0.132 (2)	0.333 (2)	0.662 (2)	10.0 (7)	0.885 (2)	0.382 (2)	1.344 (2)	10.5 (8)
H(C24)	0.191 (2)	0.480 (1)	0.816 (2)	7.6 (6)	1.005 (2)	0.309 (1)	1.440 (2)	5.9 (5)
H(C25)	0.329 (2)	0.559 (2)	0.793 (2)	10.1 (7)	1.054 (2)	0.144 (1)	1.342 (2)	7.7 (6)
H(C26)	0.412 (2)	0.517 (1)	0.606 (2)	8.2 (6)	0.984 (2)	0.052 (1)	1.151 (2)	7.1 (6)

used for data collection was a yellow, irregularly shaped, flat plate with dimensions $0.25 \times 0.25 \times 0.01$ mm. Three-dimensional data were collected on a Syntex automated diffractometer with monochromatic Cu $K\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$) using the θ - 2θ scan technique. Intensities were measured for 7841 unique reflections to a maximum $\sin \theta/\lambda = 0.61 \text{ \AA}^{-1}$. Values of $\sigma(I)$ were derived from counting statistics. There were 3836 reflections for which the measured intensity, I , was less than $2.33 \sigma(I)$ and these were considered to be below the threshold of measurement. Values of $\sigma(F)$ for the observed data were calculated from the formula $\sigma(F) = (F/2) \{ [\sigma^2(I)/I^2] + \delta^2 \}^{1/2}$ where δ is a measured instrumental uncertainty, 0.0258, determined from the variation in the intensities of periodically measured standard reflections. There was no fall-off of intensity as a function of time in these standard reflections. The data were converted to structure amplitudes by the application of Lorentz and polarization factors. No absorption correction was applied.

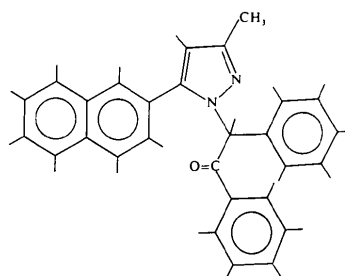
The structure was solved using a combination of direct methods and the Fourier technique. Using the program *MULTAN* (Germain, Main & Woolfson, 1971), many of the atoms of the two fragments could be recognized among the highest peaks of the first E map. However, the initial interpretation of this map was somewhat hindered because the chemical structure identified from this study was unexpected. A Fourier map phased from positions of atoms located from the first calculated E map revealed the locations of the missing atoms. The structure was refined by the method of full-matrix least squares; non-H atoms, after initial isotropic refinement, were refined anisotropically and H atoms, located from intermediate difference Fourier syntheses, were refined isotropically. The weights, w , for reflections were $\sigma^{-2}(F)$ with weights of zero for reflections below the threshold value. The function minimized in the least-squares process was $\sum w(|F_o| - |F_c|)^2$. The atomic scattering factors used for C and N atoms were those of Cromer & Mann (1968) and for H atoms those of Stewart, Davidson & Simpson (1965). A secondary-extinction correction (Zachariasen, 1963) was applied such that $F_{\text{corr}} = F_o [1 + \alpha \beta_{(2\theta)} \text{Lp} |F_o|^2]$ with $\alpha = 0.9 \times 10^{-7}$, determined graphically. The final R for observed data is 0.054 with a weighted R of 0.059; the final R on all data is 0.118. Final refined positional parameters with average isotropic thermal parameters are listed in Table 1 with e.s.d.'s.* A final difference Fourier map revealed the presence of no peaks greater than $0.2 \text{ e \AA}^{-3}$.

* Lists of structure factors, anisotropic thermal parameters and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35863 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

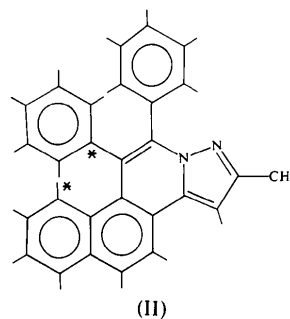
Computer programs used include *UCLALS4* (Gantzel, Sparks, Long & Trueblood, 1969) modified by Carrell (1975), the *CRYSTNET* package (Bernstein *et al.*, 1974) and other programs written in the ICR laboratory, including *VIEW* (Carrell, 1976) and *DOCK* (Badler, Stodola & Wood, 1979).

Discussion

The results of this study reveal that the major product of polyphosphoric acid cyclodehydration of 2-[3-methyl-5-(2-naphthyl)-1-pyrazolyl]-2-phenylacetophenone (Schweizer, Nelson & Stallings, 1980),



is 2-methyl-5,6-diphenylanthra[2,1-*b*]pyrazole (I) (see *Abstract*). It was hoped that this reaction would provide a facile route to the diazasteroid, 2-methyl-10,11-diphenylphenanthro[2,1-*b*]pyrazole (II). However, as later pointed out, it is likely that steric hindrance (between the atoms distinguished by asterisks) influences the course of the reaction.



The title compound (I) crystallizes with two independent molecules in the unit cell. These two molecules are very similar except for the tilts of the external phenyl groups. Bond distances and interbond angles for (I) are shown in Fig. 1. The bond lengths indicate that resonance structures with a positive charge on N(3), with delocalization of the negative charge about the ring systems, may account for the observed molecular structure.

The two independent molecules exhibit conformational variability, probably as a result of finding different ways of relieving close contacts such as H(9)···H(13) and N(11)···C(21). A major difference lies in the orientation of the two phenyl groups relative

to the principal ring systems. As summarized in Fig. 2, in molecule *A* the external phenyl groups are approximately normal to the principal ring system while in molecule *B* they are tilted by approximately 20° from the normal. Relevant torsion angles are given in the caption to Fig. 2. It is not obvious that the variation in the tilts is caused by packing forces since there is ample room in the crystal for the accommodation of both orientations of the external phenyl groups. The difference in the bowing of the molecules is also striking:

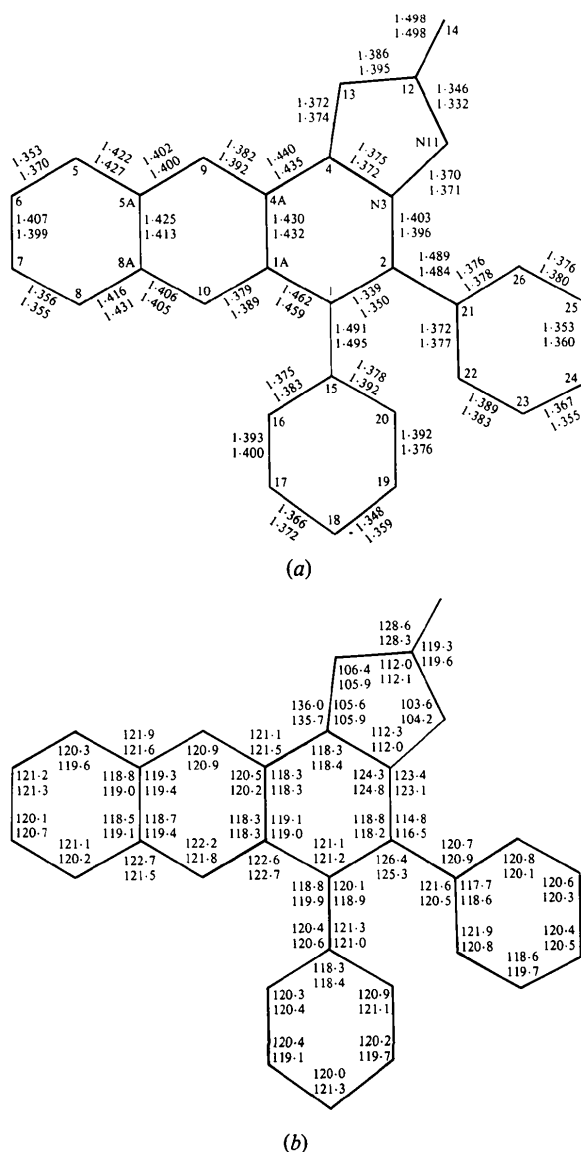


Fig. 1. (a) Labelling of the atoms and bond distances (Å). The average e.s.d. for a C-C or C-N bond length is 0.003 Å. Values for molecule *B* are below those for molecule *A*. The minimum and maximum C-H bond lengths are 0.87 Å for C(17)-H(C17) of molecule *A* and 1.07 Å for C(16)-H(C16) of molecule *B*. (b) Bond angles ($^\circ$). The average e.s.d. for an interbond angle involving C or N atoms is 0.2° . Values for molecule *B* are below those for molecule *A*.

the principal ring system of neither molecule is planar. The r.m.s. deviations of the atoms of the least-squares plane calculated using the coordinates of the C atoms of the naphthalene moiety in (I) [atoms C(5), C(6), C(7), C(8), C(9), C(10), C(14), C(4A), C(5A), C(8A)] are 0.02 and 0.03 Å for molecules *A* and *B*, respectively. However, molecule *A* is substantially more bowed than molecule *B* as evidenced, in part, by the deviations of atoms C(14) from these planes; these values are 0.63 Å for molecule *A* and 0.18 Å for molecule *B*.

The arrangement of symmetry-related molecules in the unit cell is dominated by a herring-bone pattern of the principal ring systems of the molecules. There is no overlapping of aromatic rings in planes 3.4 Å apart although the independent molecules pack with themselves in parallel planes across centers of symmetry in a remarkably similar manner. This is illustrated in Fig. 3. The separation between the planes is 3.16 Å for molecule *A* and 3.02 Å for molecule *B*. In this packing (Fig. 3), the closest approach is between symmetry-related atoms C(8); the C(8)⋯C(8) separation is

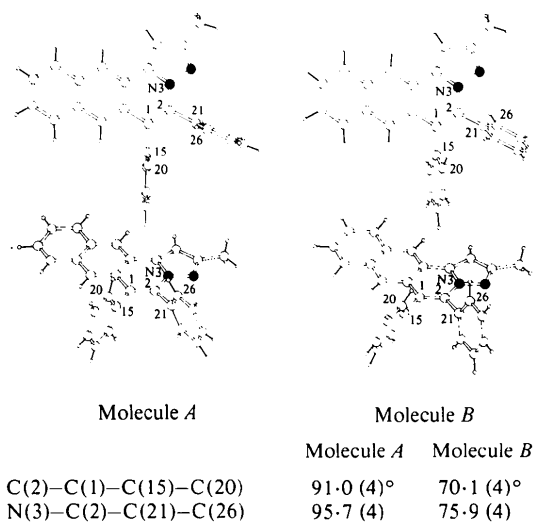


Fig. 2. Views of the conformations of the independent molecules. The conformations of the phenyl rings relative to the principal ring system are compared above.

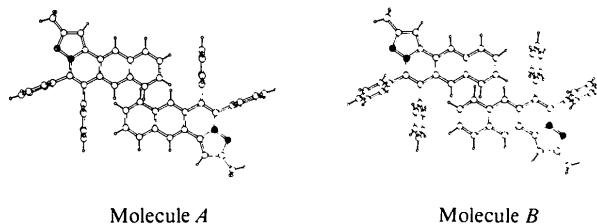


Fig. 3. Packing of the independent molecules with themselves across centers of symmetry. The principal ring systems of the molecules lie in parallel planes which are 3.16 and 3.02 Å apart for molecules *A* and *B* respectively.

3.456 (4) and 3.402 (4) Å for molecules *A* and *B* respectively.

A model of the desired reaction product, the diazasteroid (II), was generated by computer graphics (Badler *et al.*, 1979) using the coordinates for molecule *A* of the title compound as a starting point; the C(1)–C(1A) bonding constraint was removed and the C(1A)–C(4A)–C(4)–C(13) torsion angle was altered from approximately 0° in (I) to 180° in (II). Analysis of the geometry of this molecule (II) reveals steric interference between the indicated H atom and its neighboring phenyl group; in particular, the separation between the indicated H and phenyl C atoms [distinguished by asterisks in (II), the diazasteroid] is 1.8 Å while the sum of their van der Waals radii is 2.9 Å. This implies that severe buckling of the principal ring system would be required to relieve this close approach if the diazasteroid were formed. Thus the principal pathway of the reaction is determined by the lesser amount of strain or buckling in the observed major product. It is likely that the synthesis of the diazasteroid (II) is sterically inhibited for this reason.

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The Structure of 2,2-Dimethyl-3-ureido-6-phenoxyacetamidopenam*

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Abstract

C₁₆H₂₀N₄O₄S, *M_r* = 364.43, an active derivative, resistant to penicillinase, with a ureide moiety instead of a carboxy group, crystallizes in the orthorhombic space group *P*2₁2₁2₁ with *a* = 17.751 (6), *b* = 15.306 (4), *c* =

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6.493 (2) Å, *V* = 1764 Å³, *Z* = 4, *D_m* = 1.364, *D_c* = 1.371 Mg m^{−3}, *F*(000) = 768. *R* = 0.040 for 1704 observed independent reflections. The thiazolidine ring exhibits an envelope conformation with C(3) 0.52 Å out of the plane through the remaining four atoms. The β-lactam ring is folded 9° from planarity. Each molecule is hydrogen bonded to four neighbouring molecules. The resistance to β-lactamase is caused by the changed chemical properties of the compound rather than by shielding of the β-lactam.

* {3,3-Dimethyl-7-oxo-6-[(phenoxyacetyl)amino]-4-thia-1-azabicyclo[3.2.0]hept-2-yl}urea.