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MOLECULAR AND CRYSTAL STRUCTURE OF (1S,2R)-1-{2-[(1S)-1-(DIMETHYLAMINO)ETHYL]PHENYL} -1,2-DIPHENYLETHANE-1,2-DIOL

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The (R)-configuration of the carbinol center formed as a result of diastereospecific reduction of (2S)-2-{2-(1S)-1-(dimethylamino)ethyl]phenyl}-2-hydroxy-1,2-diphenylethanone is established by the XRD method. The analysis of shortened nonvalent intramolecular contacts testifies that the molecule is quite rigid, despite the presence of a large number of single valence bonds. Layered nature of molecular packaging is revealed.

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Keywords: aminoalcohols, aminoketoalcohols, reduction, stereoselectivity, configuration, atom-atom potentials, molecular agglomerates in crystals.

INTRODUCTION

The synthesis of chirally pure compounds is an urgent problem of modern organic chemistry. It is related to the production of catalysts for the asymmetric synthesis widely used nowadays to obtain chiral compounds and to design drugs whose pharmacological activity depends on their configuration.

The interest in the study of molecular agglomerates (finite or infinite ensembles of molecules which are most tightly bound in a crystal) is due to the fact that final agglomerates or fragments of molecular chains and layers are often maintained in the solutions or melts after the crystal is destroyed; also, they can pass from crystal to crystal during polymorphic phase transitions or in the course of solid-phase chemical reactions [1].

We earlier reported that N,N-dimethyl-1-phenylethanamine (**I**, readily available in both enantiomeric forms) can be used to obtain chirally pure aminoalcohols [2] which showed good asymmetrical activity in the reaction of enantioselective addition of diethylzinc to aromatic aldehydes [3]. An approach to estimate the stability of molecular agglomerates in a crystal was proposed in [4].

To continue these works, we studied the reduction of the previously obtained (2S)-2-{2-(1S)-1-(dimethylamino)ethyl]phenyl}-2-hydroxy-1,2-diphenylethanone (**II**) [5] by metal hydrides ($NaBH_4$, $LiAlH_4$, (*tert*-BuO)$_3$LiAlH) and showed that (1S,2R)-1-{2-[(1S)-1-(dimethylamino)ethyl]phenyl}-1,2-diphenylethane -1,2-diol (**III**) is formed with diastereomeric purities of 50%, 80%, and 100%, respectively.

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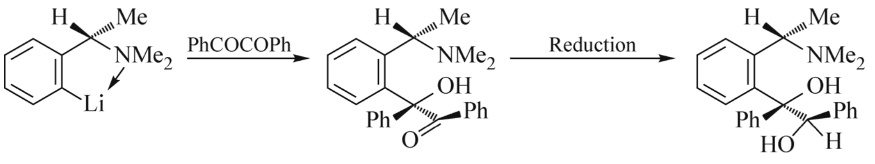

I **II** **III**

The effect of the chiral carbinol center (C-1, (S)-configuration) adjacent to the carbonyl group on the stereoselectivity of the reaction was estimated using the reduction of {2-(1S)-1-(dimethylamino)ethyl]phenyl}(phenyl)methanone by (*tert*-BuO)$_3$LiAlH which demonstrated low degree of stereoselectivity (below 50%).

To establish the configuration of the newly formed carbinol center in the obtained diastereomer **III,** the molecular structure of the latter was studied with the XRD method.

EXPERIMENTAL

The reduction of the aminoketoalcohols **II** was carried out in a water-alcohol environment (NaBH$_4$) or in the absolute ether (LiAlH$_4$, (*tert*-BuO)$_3$LiAlH).

23.23 mmol of absolute *tert*-butanol (distilled over P_2O_5 and double distilled over Na) was dropwise added to the stirred solution of 7.74 mmol of LiAlH$_4$ in 20 ml of absolute ether at 0 °C while stirred. The reaction mixture was kept for 30 min at 0 °C, then the solution of 1.94 mmol ketoamino alcohol **II** in 50 ml of absolute ether was added dropwise. The mixture was additionally kept for 30 min at 0 °C, 30 ml of water was decomposed at cooling, NaCl was added to saturation and extracted with ether (6×10 ml). After drying over MgSO$_4$, the ether was removed by distillation to obtain a crystalline substance, yield 85%, T_m 185° (from ethanol), $[\alpha]_D$ –118,4° (c 1, ethanol).

IR spectrum: ν_{OH} 3150-2400 cm^{-1} (OH group linked by the intramolecular hydrogen bond (BBC)), ν_{OH} 3610 cm^{-1} (free OH group), ν_{OH} 3530 cm^{-1} (dimeric OH group).

^{1}H NMR (400 MHz, CDCl$_3$, TMC) δ ppm: 0.98 d ($C\underline{H}_3$ CH, 3H, *J* 6.8), 1.98 s ($NC\underline{H}_3$ 6H), 2.44 s (benzyl $O\underline{H\ at\ C(2)}$, 1H) 3.54 q ($C\underline{H}$–CH$_3$, 1H, *J* 6.8), 5.51 s ($C\underline{H}$–OH, 1H), 6.9-8.15 m (arom. 14H); 10.0 s (benzhydryl $O\underline{H\ at\ C(1)}$, 1H). ^{13}C NMR spectrum (400 MHz, CDCl$_3$) δ ppm: 7.27 s. ($\underline{C}H_3$–CH), 38.34 wide s. (($\underline{C}H_3)_2N$), 57.02 ($\underline{C}H$–CH$_3$), 78.53 s. ($H\underline{C}OH$), 80.32 s. ($\underline{C}OH$), 127,4-146.0 (aromatic).

Found,%: C 80.07, H 7.65, N 3.67. $C_{24}H_{27}NO_2$. Calculated,%: C 79.75, H 7.53, N 3.87.

X-ray analysis of single crystals III. Rhombic crystals, $T = 293$ K: $a = 7.618(3)$ Å, $b = 9.461(5)$ Å, $c = 26.987(9)$ Å, $V = 1945(2)$ Å^3, space group $P2_12_12_1$, $Z = 4$, $d_{calc} = 1.234$ g/cm^3, $\mu = 0.078$ mm^{-1}. Unit cell parameters and the intensities of 1780 independent diffraction reflections were recorded on an automatic four-circle diffractometer Siemens P3/PC (λMoK_α, graphite monochromator, θ/2θ scanning, $\theta_{max} = 24°$). The absorption correction was ignored. The structure was solved by the direct method and refined by the least squares method with respect to F^2 in the anisotropic approximation for non-hydrogen atoms. Two hydrogen atoms of hydroxyl groups of the molecule **III** were localized using the difference electron density synthesis, their positions were refined in the isotropic approximation. The coordinates of the remaining H atoms were calculated geometrically and refined using a riding model. The final divergence factors were $R_1 = 0.0378$ and $wR_2 = 0.1051$ for 1686 diffraction reflections with $I > 2\sigma(I)$, $R_1 = 0.0412$, and $wR_2 = 0.1146$ for the whole array of independent diffraction reflections. All calculations were carried out using the SHELXTL software package [6].

CIF files containing complete data on structure **III** were deposited with the CCDC under the number 1588127 and can be freely obtained on request on the site ccdc.cam.ac.uk/data_request/cif.

RESULTS AND DISCUSSION

Aminodiol **III** was obtained as a result of the reduction of aminoketoalcohol **II** by the action of (*tert*-BuO)$_3$LiAlH; its structure was confirmed by IR and NMR spectroscopy data. It was shown that the reaction is diastereospecific, and the presence of the chiral (carbinol) center near the reduced carbonyl group significantly affects the stereoselectivity of the reaction which was estimated by ^{1}H NMR spectra. According to the XRD data, the formed chiral carbinol center in the obtained diastereomer **III** has a (R)-configuration.

Fig. 1 shows the perspective view of the molecule (according to the XRD data) with numbered non-hydrogen atoms. The intramolecular hydrogen bond O(1)–H(1)…N with geometric parameters O(1)–H(1) 0.97(4), H(1)…N 1.73(5), O(1)…N 2.679(3) Å, angle O(1)–H(1)…N 165(4)° is shown by a dashed line. This H-bond closes the 7-membered cycle C(1)–C(2)–C(3)–C(8)–N…H(1)–O(1) and therefore fixes the torsion angle O(1)–C(1)–C(2)–C(3). As a result, even small rotations of the aryl fragment of the C(2)…C(7) molecule around the C(1)–C(2) bond are substantially limited. Moreover, any rotations of the molecule fragments around single bonds C(1)–C(12), C(12)–C(13), and C(1)–C(19) are also limited by short non-valence contacts C…C, O…C, and C…H (Table 1) of the type 1…4, 1…5, and even 1…6. These contacts are shorter than the double geometric mean of the corresponding van der Waals radii [7].

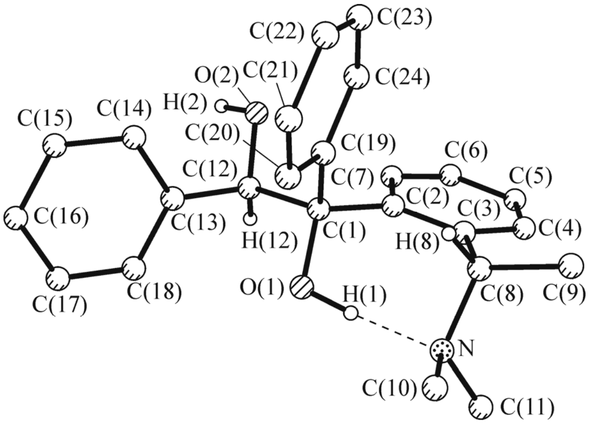

Fig. 1. Perspective view of molecule **III** with numbered atoms. Only hydrogen atoms of hydroxyl groups and chiral centers are shown.

TABLE 1. Some of the Shortened Intramolecular Nonvalent Contacts in the Molecule **III**

Contact	Type	Distance *d**, Å	Δ**, Å	Contact	Type	Distance *d*, Å	Δ, Å
O(1)…C(13)	1…4	2.77	0.20	O(2)…C(14)	1…4	2.80	0.17
O(1)…C(20)	1…4	2.80	0.17	O(2)…C(7)	1…5	2.87	0.10
C(7)…C(12)	1…4	2.90	0.52	C(2)…C(24)	1…4	2.97	0.45
C(13)…C(19)	1…4	3.05	0.37	C(3)…C(19)	1…4	3.18	0.24
C(8)…C(19)	1…5	3.22	0.20	C(12)…C(24)	1…4	3.29	0.13
C(14)…C(19)	1…5	3.29	0.13	C(13)…C(20)	1…4	3.32	0.10
C(14)…C(20)	1…6	3.32	0.10	C(19)…H(8)	1…4	2.48	0.34
C(9)…H(4)	1…5	2.49	0.33	C(12)…H(7)	1…5	2.49	0.33
C(9)…C(4)	1…4	2.88	0.54	–	–	–	–

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* Interatomic distance rounded to 0.01 Å.

** $\Delta = 2\sqrt{R_i \cdot R_j} - d$, where R_i and R_j are van der Waals radii of the atoms.

As a result, the relaxation of the molecule's steric strain caused by the repulsion of too closely spaced atoms of its fragments is due to the deformation of valence angles and valence bonds rather than the changes of the torsion angles. For example, tetrahedral valence angles C(2)–C(1)–C(12) and C(1)–C(12)–C(13) are increased to 113.2(2)° and 113.0(2)°, respectively, and the valence bond C(1)–C(12) is stretched to 1.570(4) Å. Note that the valence bond C(1)–C(12) is 0.014 Å longer than the average bond $(C^{\#})_3$–C–CH–$(C^{\#})_2$ [8].

According to the analysis of the Dirichlet packing polyhedron of molecule **III** performed by the procedure described in [9], the coordination number of the molecule in a crystal is 14. For each geometric molecular dimer (GMD) formed by the basic molecule with all the molecules of its first coordination environment, the energies of intermolecular interactions were calculated using the atom-atom potential model according to the formula $U_{\mathrm{M—M}} = \sum_{i,j} \varphi_{ij}$, where $\varphi_{ij} = -A_{ij} r_{ij}^{-6} + B_{ij} \exp(-C_{ij} r_{ij})$ are atom-atom potentials and A_{ij}, B_{ij}, C_{ij} are parameters of the interaction between the *i*th atom of the first molecule and the *j*th atom of the second molecule which are determined by the types of these atoms from the formulas $A_{ij} = \sqrt{A_{T_i} A_{T_j}}$, $B_{ij} = \sqrt{B_{T_i} B_{T_j}}$, and $C_{ij} = \sqrt{C_{T_i} C_{T_j}}$. All energy calculations were performed using the program [10], parameters A_T, B_T, and C_T for the atoms C, H, O, and N are cited from [11].

In [12], we suggested a new approach for the study and description of intermolecular interactions based on the analysis of the potentials of individual intermolecular atom-atom contacts. The contacts with the potential close to the minimum on the corresponding potential curve ($\varphi \le \varphi_{\mathrm{w}}$, where $\varphi_{\mathrm{w}} = \varphi(r_{\mathrm{w}})$ is the potential at the inflection point of the potential curve $\frac{\partial^2 \varphi(r_{\mathrm{w}})}{\partial r^2} = 0$) are referred to below as *potential well contacts* (PWCs). The left edge of the potential well is limited by the distance r_{l} such that $\varphi(r_{\mathrm{l}}) = \varphi_{\mathrm{w}}$. The contacts corresponding to the left side of the potential curve and having nonpositive atom-atom potentials are referred to as *left contacts* (LCs**),** and those with positive atom-atom potentials are referred to as *positive contacts* (PCs). Fig. 2 shows the potential curve with the indication of PWC, PC, and LC regions of atom-atom contacts C…C. Since atom-atom PWC contacts between the molecules are the strongest energy contacts, the number of PWCs between two adjacent molecules can be used to characterize the intensity and stability of intermolecular contacts. The presence of LCs and particularly PCs in intermolecular interactions may indicate the appearance of specific interactions (π-stacking, T-stacking, weak H-bonds) between the corresponding molecular fragments.

Let us consider GMDs, each consisting of the basic molecule and a molecule of its first coordination sphere. Obviously, the number of GMDs is equal to the coordination number (CN = 14). At the same time, there are only seven crystallographically independent GMDs within the first coordination sphere of the basic molecule.

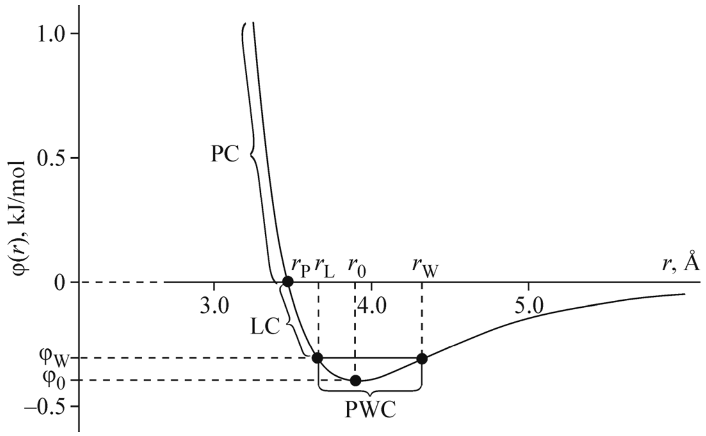

Fig. 2. The curve of the atom-atom potential interaction between two carbon atoms.

TABLE 2. Energy Characteristics of Pairwise Intermolecular Interactions Between Molecule **III** and the Molecules of its First Coordination Environment

№	Symmetry operation	GMD interaction energy, kJ/mol	Interaction energy of non-hydrogen atoms, kJ/mol	Number of PWCs of non-hydrogen atoms	Total energy of PWCs of non-hydrogen atoms, kJ/mol
1	$x+1, y, z$ $(x-1, y, z)$*	–29.5	–23.0	18	–6.5
2	$x, y+1, z$ $(x, y-1, z)$	–26.7	–20.6	17	–6.1
3	$x-1/2, -y-1/2, -z$ $(x+1/2, -y-1/2, -z)$	–23.5	–19.3	11	–4.2
4	$1-x, y+1/2, 1/2-z$ $(1-x, y-1/2, 1/2-z)$	–17.0	–15.9	3	–1.1
5	$-x, y+1/2, 1/2-z$ $(-x, y-1/2, 1/2-z)$	–13.8	–11.3	7	–2.5
6	$x+1/2, 1/2-y, -z$ $(x-1/2, 1/2-y, -z)$	–12.4	–11.0	4	–1.4
7	$x-1, y+1, z$ $(x+1, y-1, z)$	–9.7	–8.7	3	–1.0

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* The parentheses contain symmetry operations of symmetric analogs of original crystallographically independent GMDs.

Table 2 shows the following parameters for seven crystallographically independent GMDs: 1) symmetry operations that connect the basic molecule with the molecules from its first coordination sphere of this GMD and its symmetric analog; 2) intermolecular interaction energy in the GMD calculated by the method of atom-atom potentials ignoring the energy of electrostatic interaction; 3) part of this energy corresponding to the interaction of non-hydrogen atoms only; 4) number of PWCs between non-hydrogen atoms in the GMD, and 5) total energy of these PWCs.

The first GMD has 18 PWCs, which is only 2.5% of the total (729) contacts between non-hydrogen atoms. At the same time, the total energy of these 18 PWCs (–6.5 kJ/mol) is larger than 31% of the contact energy between non-hydrogen atoms. There is also another feature of intermolecular interaction in this dimer. Four atoms C(20), C(21), C(22), and C(23) of the phenyl ring of the basic molecule interact with eight atoms O(2A), C(12A), C(13A), C(14A), C(15A), C(16A), C(17A), and C(18A) of the flat fragment of the neighboring molecule (hereinafter, lettered numbering will be used for the atoms of the molecules from the first coordination sphere). The interaction of these two fragments of neighboring molecules involves 14 of 18 atom-atom PWCs. These contacts are shown by dashed lines in Fig. 3a. The total energy of intermolecular interactions of these 14 PWCs is –5.1 kJ/mol.

A special feature of intermolecular interactions in the first GMD is the presence of PCs of the C…H type with large positive potentials. For example, the contact between the C(22) atom of the basic molecule and the H(2A) atom of the hydroxyl group of the molecule of its first coordination sphere has the potential equal to +2.2 kJ/mol. As mentioned above, the presence of a PC (a contact with a positive energy of atom-atom interaction) indicates the possible presence of a specific interaction between these atoms. Geometric parameters of the C(22)…H(2A) contact are as follows: distance C(22)…O(2A)

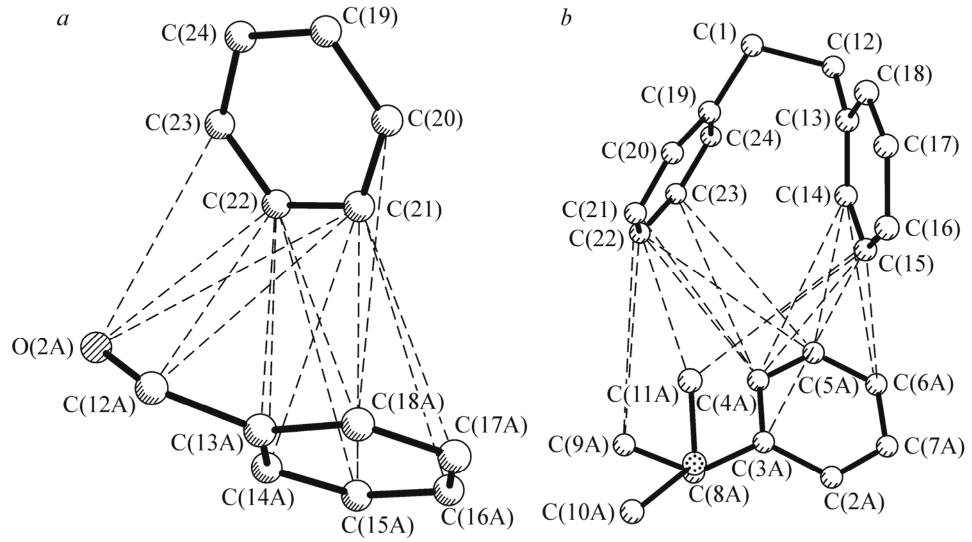

Fig. 3. Interaction of a fragment of the basic molecule with a fragment of the neighboring molecule in the first GMD (*a*), "chelate trap" in the second GMD (*b*).

is 3.47 Å, distance C(22)…H(2A) is 2.66 Å, and angle C(22)…H(2A)–O(2A) is 167°. According to the nomenclature proposed in [13], this contact is referred to as a H-bond of the O–H…π type localized on the C(22) atom of the basic molecule. Similarly, the hydrogen atom H(21A) of the phenyl of the molecule from the first coordination environment has four PCs with atoms C(13), C(16), C(17), C(18) of the phenyl of the basic molecules with a total energy of +0.73 kJ/mol. The energies of LCs between the H(21A) atom and the two remaining carbon atoms of this phenyl are close to zero to testify the possible presence of a weak delocalized hydrogen bond of the C_{ar}–H…π type with the following geometrical parameters: distance C(21A)…X is 3.46 Å, distance H(21A)…X is 2.79 Å, and angle C(21A)–H(21A)…X is 129°, where X is the centroid of the phenyl C(13)…C(18).

Intermolecular contacts of the first GMD and its symmetric analogue form a molecular chain of translationally identical molecules oriented along the crystallographic axis *a*. According to the nomenclature proposed in [1], this molecular chain is abbreviated as Bs(1) (beads) and is fully designated as $P_{c(X)}1$, $Z = 1$. It is stabilized by a large number of PWCs and H-bonds of O–H…π and C_{ar}–H…π types.

In the second crystallographically independent GMD, two phenyl fragments of the basic molecule actively interact with the neighboring aryl fragment. Six atoms of the basic molecule (C(14), C(15), C(16) on the one side and C(21), C(22), C(23) on the other side) hold in a chelate-like manner six atoms C(3A), C(4A), C(5A), C(6A), C(9A), C(11A) of the neighboring molecule (Fig. 3*b*) obtained by the basis translation along the crystallographic axis *b*. This "chelate trap" involves all 17 PWCs of the considered GMD with the total energy of intermolecular interaction equal to –6.1 kJ/mol. These 17 PWC are shown in Fig. 3*b* by dashed lines.

The second molecular dimer contains no PCs of the C…H and/or O…H type with a potential higher than +0.7 kJ/mol. Intermolecular contacts of the second GMD and its symmetric analog form a molecular chain of translationally identical molecules oriented along the crystallographic axis *b*. According to the nomenclature proposed in [1], this molecular chain is abbreviated as Bs(1) and is fully designated as $P_{c(Y)}1$, $Z = 1$. It is stabilized only by a large number of PWCs.

The third crystallographically independent GMD has 11 PWCs. The fragment of three non-hydrogen atoms C(5), C(6), and C(7) of the basic molecule is contained in the "chelate trap" formed by two fragments of the molecule of its first coordination sphere. The situation is almost the same as in the second GMD (Fig. 3*b*), but the "trap" is small in this case (containing only three non-hydrogen atoms). The third GMD has no PCs of the C…H and/or O…H type with a potential higher than +0.7 kJ/mol. The intermolecular contacts of the third GMD and its symmetric analog form a molecular chain

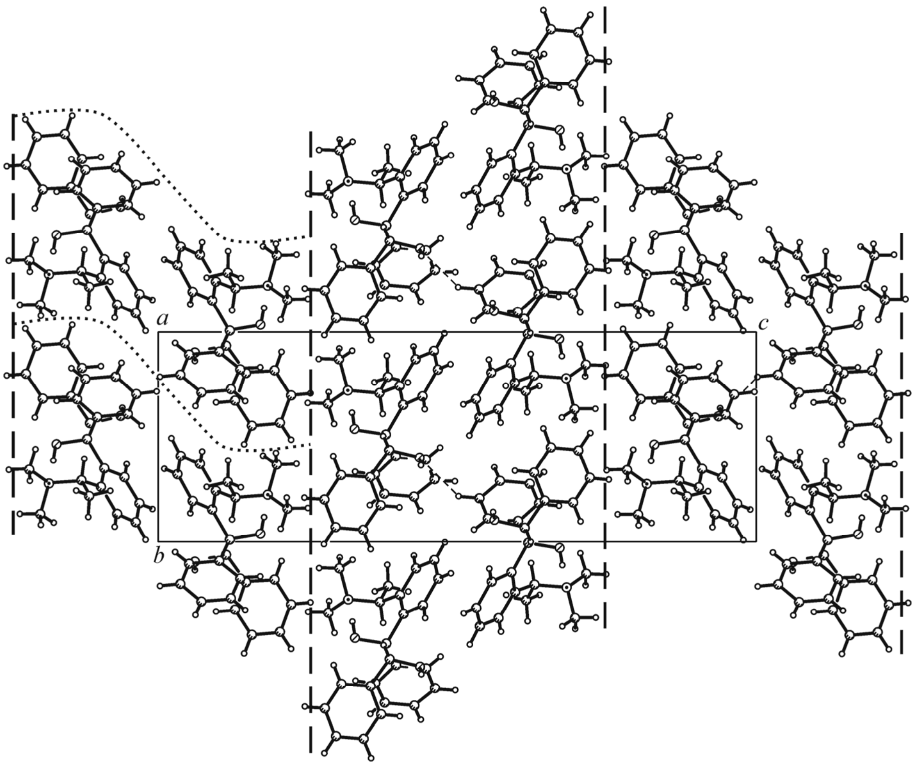

Fig. 4. Projection of the crystal structure **III** along the crystallographic *axis a.*

designated as SP(2_1) or simply SP (skating pace) according to the nomenclature proposed in [1]. Since this molecular chain is oriented along the crystallographic axis *a*, its full designation is $P_{c(X)}2_1$, $Z = 2(1)$.

Among the remaining four crystallographically independent GMDs of the basic molecule with the molecules of its first coordination sphere, the fifth and the sixth deserve special attention. In the fifth GMD, the fragment of three non-hydrogen atoms C(16), C(17), and C(18) of the basic molecule is in the "chelate trap" (7 PWC), and the sixth GMD has a PC with a positive potential of +1.6 kJ/mol between the H(23) atom of the basic molecule and the O(2A) atom. The geometrical parameters of this contact are as follows: distance C(23)…O(2A) is 3.26 Å, distance H(23)…O(2A) is 2.53 Å, angle C(23)–H(23)…O(2A) is 136°. According to the nomenclature proposed in [14], this contact is referred to as a weak H-bond of the C_{ar}–H…O type.

Note that the first three crystallographically independent GMDs are significantly different from the other four GMDs in terms of their integral energy characteristics (Table 2) (contact energy and interaction energy of non-hydrogen atoms) and differential energy characteristics (the number of PWCs of non-hydrogen atoms and the total energy of PWCs of non-hydrogen atoms). Consequently, these three GMDs, together with their symmetric analogs, can be considered as the main elements of the molecular agglomerate in the crystal structure **III**. Such an agglomerate is the molecular layer parallel to the crystallographic plane (0 0 1). The boundaries of these molecular layers are shown in Fig. 4 by dashed lines. Note that the energy of interaction between the molecules inside the layers significantly exceeds the energy of interaction between the molecules from adjacent layers. According to the nomenclature proposed in [1], the structural class of this molecular layer is referred to as $P_l2_{1(XY)}$, $Z = 2(1)$.

The most energy-intensive element of this molecular layer is the molecular chain oriented along the axis *a* (first and third GMDs with their symmetric analogs). The structural class of this molecular chain is $P_{c(X)}2_1$, $Z = 2(1)$, its boundaries are shown in Fig. 4 by dotted lines.

Thus, the crystal structure **III** refers to one of the two most common [1] subclasses of the structural class $P2_12_12_1$, $Z = 4(1)$ schematized as $1 - P_{c(X)}2_1, Z = 2(1)\uparrow\uparrow P_{l(XY)}\uparrow\downarrow P2_12_12_1, Z = 4(1)$.

CONCLUSIONS

It was shown that the reduction of aminoketoalcohol **II** by the action of (*tert*-BuO)$_3$LiAlH is diastereospecific, and the presence of the chiral (carbinol) center next to the reaction center significantly affects the stereoselectivity of the reduction. The XRD data testify that the newly formed chiral carbinol center in the diastereomer **III** has the (R)-configuration.

According to the analysis of intermolecular interaction energy and taking into account both integral (total intermolecular interaction energy in GMDs) and differential (PWC and PC) characteristics, the crystal structure **III** contains molecular agglomerates in the form of molecular chains $P_c2_{1(X)}$, $Z = 2(1)$ and molecular layers $P_l2_{1(XY)}$, $Z = 2(1)$.

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CONFLICT OF INTERESTS

The authors declare that they have no conflict of interests.

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