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Structure and Conformational Analysis of 5,5-Bis(bromomethyl)-2-[4-(dimethylamino)phenyl]-1,3-dioxane

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Abstract—The structure of 5,5-bis(bromomethyl)-2-[4-(dimethylamino)phenyl]-1,3-dioxane, a promising reagent for fine organic synthesis and a potential bactericidal compound, was investigated by ^{1}H and ^{13}C NMR spectroscopy and X-ray structural analysis. Both in the crystalline state and in solution, molecules of this compound have a *chair* conformation with an equatorial orientation of the aromatic substituent. Density functional theory calculations at the PBE/3ξ level of theory were used to determine the pathway of conformational transformations and the potential barriers for internal rotation of aromatic and $N(CH_3)_2$ groups both for the isolated molecule and for a chloroform solution. A conclusion was drawn that the nearest solvation shell of the studied 1,3-dioxane comprises a relatively small (up to four) number of solvent molecules.

Keywords: 1,3-dioxane, X-ray diffraction analysis, NMR, conformer, cluster model, computer simulation

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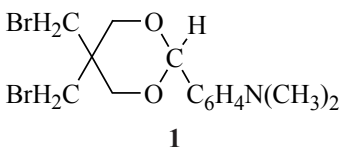
INTRODUCTION

Substituted 1,3-dioxanes belong to the classical models of conformational analysis [1, 2], and are used as reagents for fine organic synthesis [3–8], as well as for the design of new promising medicinal compounds, in particular, halogen- and nitrogen-containing analogs [9, 10]. Furthermore, 5,5-bis(halomethyl)-1,3-dioxanes contain 2 additional reaction centers: halogen atoms, which are capable of undergoing nucleophilic substitution reactions [11]. As shown in [12–14], 5,5-bis(halomethyl)-1,3-dioxanes characteristically undergo fast (on the NMR time scale) ring interconversions at room temperature. 2-Substituted analogs adopt a *chair* conformation with an equatorial substituent at the C^2 of the ring [15–17]. Due to the combination of the structural features, chemical properties, and composition (the presence of a halogen and a nitrogen atoms in the 1,3-dioxane molecule), such compounds can be considered as promising for solving the problems of conformational analysis and for the creation of objects with high biological activity. In this connection, the present is devoted to the study of structure and conformational transformations of a previously unknown 5,5-bis(bromomethyl)-2-[4-(dimethylamino)-phenyl]-1,3-dioxane (**1**) (Scheme 1) by means of ^{1}H and ^{13}C NMR spectroscopy, X-ray diffraction (XRD) analysis, and quantum-chemical calculations by the DFT PBE/3ζ method suitable for compounds of this

Scheme 1.



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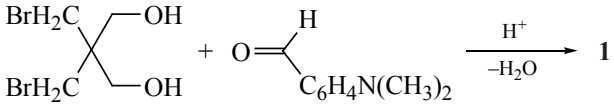
Scheme 2.



class [2] (PRIRODA software [18]), as well as to study the effect of the number of solvent molecules on the relative energies of minima and transition states on the potential energy surface (PES) of this compound (cluster model).

RESULTS AND DISCUSSION

Dioxane **1** was synthesized by the condensation of 2,2-bis(bromomethyl)propane-1,3-diol with *p*-(dimethylamino)benzaldehyde (Scheme 2).

Single-crystal XRD analysis of compound **1** was performed. The crystallographic data are presented in Experimental, and dioxane **1** was registered at the Cambridge Crystallographic Data Center (CCDC 2064773).

It was found that the molecule of acetal **1** adopts a *chair* conformation. Therewith, the molecules form orthorhombic crystals of the space group *Pbca* (Fig. 1). The heteroatomic part of the heteroring has expected C–O bond lengths (1.418–1.425 Å) and the bond angles close to 110°–112°. The torsion angles, too, has values characteristic of the *chair* conformation (Table 1) [2, 15–17]. Noteworthy is a characteristic *gauche* arrangement of the bromomethyl substituents, which has, to quantum-chemical calculations, the lowest energy compared to the alternative conformations of the C–Hal bonds in the substituents at the C^5 atom of the 1,3-dioxane ring [19]. Along with that, the aromatic substituent at the C^2 of the ring is almost coplanar to the heteroatomic plane of dioxane **1**, and the dihedral angle between the C^{11}–O^4–O^2–C^{15} fragment and the aromatic ring is 20.1(3)°. The $N(CH_3)_2$ substituent has a planar configuration of the nitrogen atom (the sum of the bond angles is 360°) and is expectedly coplanar to the aromatic ring; the C^{16}–N^3–C^6–C^9 torsion angle is 2.2(13)°.

The results of 1D and 2D ^{1}H and ^{13}C NMR spectroscopy in $CDCl_3$ solutions at room temperature (including NOESY, COSYHH, and HSQC techniques; Table 2) suggest that acetal **1** exists as a *chair* conformer. This is indicated by the diastereotopic character of the methylene protons at the magnetically equivalent C^4 and C^6 atoms in the heteroring (Δδ 0.4 ppm), which appear in the ^{1}H NMR spectrum as 2 doublets with ^2J –11.6 Hz. The methylene protons of the bromomethyl substituents at C^5 are magnetically nonequivalent (Δδ 0.7 ppm); the NOESY experiment showed that the axial CH_2Br protons give a signal in a weak field (Table 2). The most downfield heteroring carbon signal in the ^{13}C NMR spectrum belongs to C^2 (102.3 ppm); in the HSQC spectrum this signal correlates with the Ha signal at 5.4 ppm.

These results are confirmed by the conformational analysis of dioxane **1** in the PBE/3ζ approximation.

On the PES of this compound we localized minima corresponding the equatorial and axial *chair* (*Ce* and *Ca*) and 2,5-*twist* conformers (2,5-*T*), of which the first is the main minimum, as well as transition states TS-1 and TS-2, corresponding to half-*chair* conformations (Scheme 3). The calculated bond lengths and bond and torsion angles for conformer *Ce* are close to the respective values obtained by XRD analysis (Table 1).

Table 3 lists the relative energies of all forms corresponding to the stationary points on the PES of an isolated molecule of dioxane **1**, as well as for its solvent clusters.

The main difference between the theoretical data for the equatorial *chair* form of dioxane **1** and the results

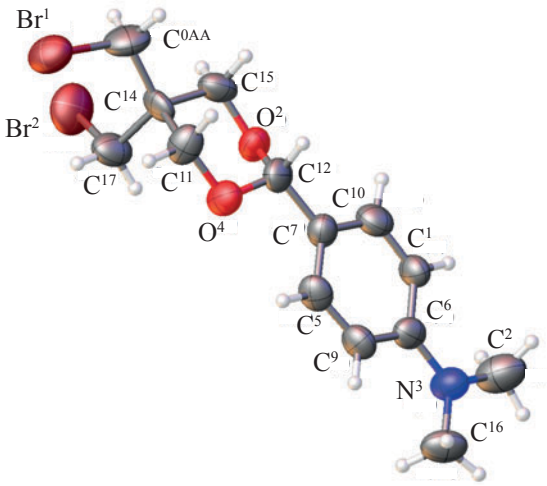


Fig. 1. Molecular structure of compounds **1**, with the atoms presented by thermal ellipsoids drawn at a 50% probability level.

Table 1. Selected bond lengths and bond and torsion angles in dioxane **1**[a]

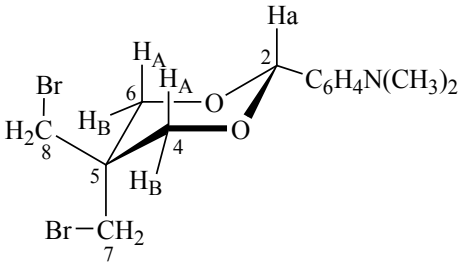
Bond	Bond length, Å		Bond angle	φ, deg		Torsion angle	τ, deg	
	calcd.	exptl.		calcd.	exptl.		calcd.	exptl.
Br_2–C_{17}	1.987	1.954(9)	O_2–C_{12}–O_4	110.3	110.0(7)	C_{12}–O_4–C_{11}–C_{14}	58.7	57.4(9)
O_2–C_{12}	1.428	1.418(9)	C_{12}–O_4–C_{11}	110.9	111.9(6)	C_{12}–O_2–C_{15}–C_{14}	–59.6	–58.8(9)
O_2–C_{15}	1.428	1.425(10)	C_{12}–O_2–C_{15}	110.9	110.2(6)	C_{11}–O_4–C_{12}–O_2	–62.0	–63.7(8)
O_4–C_{12}	1.433	1.418(9)	O_4–C_{11}–C_{14}	111.9	110.2(6)	C_{15}–O_2–C_{12}–O_4	62.5	62.9(8)
O_4–C_{11}	1.428	1.425(9)	O_2–C_{15}–C_{14}	111.6	112.5(7)	C_{11}–C_{14}–C_{15}–O_2	52.8	51.4(9)
C_7–C_{12}	1.500	1.497(11)	C_{11}–C_{14}–C_{15}	105.7	107.7(8)	C_{15}–C_{14}–C_{11}–O_4	–52.6	–49.9(8)
N_3–C_6	1.389	1.372(10)	Br_2–C_{17}–C_{14}	114.2	114.7(6)	C_{11}–C_{14}–C_{17}–Br_2	61.4	62.5(9)
N_3–C_2	1.456	1.438(10)	C_2–N_3–C_{16}	117.1	118.8(8)	C_{16}–N_3–C_6–C_9	13.1	2.2(13)

[a] Calculations were performed by the DFT PBE/3ζ method for an isolated molecule of the equatorial *chair* conformer.

of X-ray structural measurements is associated with the conformation of the aromatic substituent. In the crystal state, as noted above, this substituent is almost coplanar to the heteroatomic plane of the 1,3-dioxane ring; like what was observed in 2-phenyl- [16] and 2,2-diphenyl-1,3-dioxanes with a 5,5-dibromomethyl group [14] and unlike what was observed in 5,5-bis(bromomethyl)-2-(4-methoxyphenyl)-1,3-dioxane, where the aromatic group is oriented perpendicular to the corresponding heteroatomic plane [15]. However, the calculated data for both an isolated molecule of dioxane **1** and for its solvent clusters predict predominantly orthogonal orientation of the aromatic substituent and a low barrier to internal rotation (Table 3). The corresponding PES is similar to that described in detail [16] for the phenyl group, and the optimized **1**(*Ce*)@4 $CHCl_3$ system is shown in Fig. 2.

To obtain further evidence for the adequacy of the used calculation approximation, we examined the conformational characteristics of *N*,*N*-dimethylaniline as structural fragment of dioxane **1**. The calculated

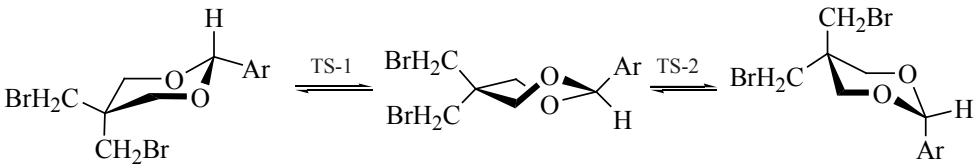
Table 2. ^1H and ^{13}C NMR data for dioxane **1** in $CDCl_3$



Proton	δ_C, ppm	C atom	δ_C, ppm
Ha	5.4	C^2	102.8
H_A	3.9–3.8 d (^2J 11.6 Hz)	C^4, C^6	71.9
H_B	4.3–4.2 d (^2J 11.6 Hz)	C^5	37.4
CH_2Br (*a*)	4.0 s	C^7	36.3
CH_2Br (*e*)	3.3 s	C^8	34.7
$(CH_3)_2N$	3.0	C_{arom}	113.2–151.3
C_6H_4	6.7 d; 7.4 d (^2J 8.7 Hz)	$(CH_3)_2N$	40.6

Scheme 3.

Minima



Transition states

Ar = C_6H_4*n*$N(CH_3)_2$.

barrier to rotation about the C–N bond (5.8 kcal/mol) is consistent with the experimental value established by ^{1}H NMR spectroscopy (5.1 ± 1.0 kcal/mol [20]); according to the gas electron diffraction data [1, 21], the energy minimum corresponds to a form with orthogonal orientation of the nitrogen LEP with respect to the benzene ring plane, and the transition state corresponds to a conformation with the LEP coplanar to the aromatic ring. The calculated lengths of the C_{arom}–N (1.393 Å) and N–CH_3 bonds (1.455 Å) are close to those obtained by gas electron diffraction: 1.396(14) and 1.460(12) Å [21]. It should also be noted the nitrogen atom has only weakly expressed pyramidal configuration: according to the calculation results, the sum of the corresponding bond angles is 354.5°, and the C_{arom}–C_{arom}–N–C torsion angle is 13.7°. In dioxane **1**, this substituent has analogous conformational characteristics (Table 3).

The closest minimum to the *Ce* form is conformer *Ca* for as isolated dioxane **1** molecule and and 2,5-*T* for its solvent clusters. In the latter case, the energy gap from the *Ce* form increases with increasing number of solvent molecules in the cluster; the main potential barrier to the conformational transformations of dioxane **1** (TS-2), as well as the barriers to internal rotation of the aromatic ring and the $N(CH_3)_2$ group also increase (Table 3). We have previously shown that the probably number of solvent molecules in a cluster with such saturated heterocycles as 1,3-dioxanes [14, 22], tetrahydro-1,3-oxazines [23], and 1,3,2-dioxaborinanes [24] should not be larger than 10 under normal conditions. In this case, comparison of the calculation results with the reported experimental barriers to interconvesion of substituted 1,3-dioxanes ($\Delta G^{\neq}_{298}$ 8–11 kcal/mol [1]) and to internal rotation of the $N(CH_3)_2$ group in the *N*,*N*-dimethylaniline fragment (5–6 kcal/mol [20]) gives us grounds to suggest that the number of chloroform molecules in the nearest solvation shell of dioxane **1** should not exceed 4.

It is also worth noting that the PES does not contain the intermediate minimum (1,4-*twist*) that is typical of the equilibrium of unsubstituted and 2-, 4-, 2,5- and 4,4-disubstituted 1,3-dioxanes [2].

EXPERIMENTAL

The NMR spectra were obtained on a Bruker Avance 400 spectrometer at 400.13 (^{1}H) and 100.62 (^{13}C) MHz, respectively, for $CDCl_3$ solutions; the chemical shifts

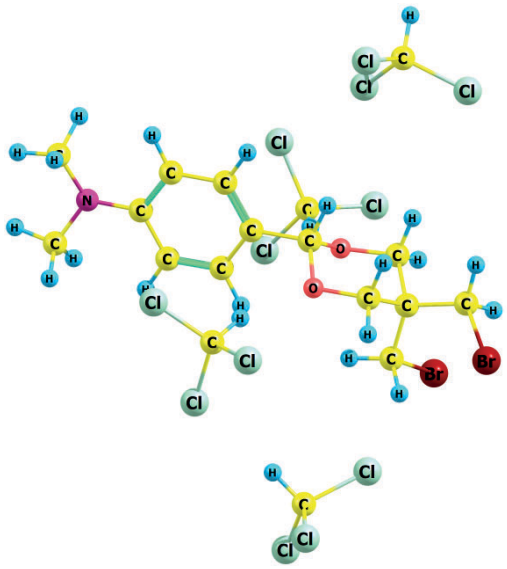


Fig. 2. Dioxane **1**(*Ce*)@4$CHCl_3$ cluster.

Table 3. Energy parameters of the conformational transformations of dioxane **1** and *N*,*N*-dimethylaniline by DFT PBE/3ζ calculations

Compound	ΔG^0_{298}, ($\Delta G^{\neq}_{298}$)[a], kcal/mol	ΔS^0_{298}, ($\Delta S^{\neq}_{298}$)[a], cal/mol·K
Isolated molecule 1:		
Ce (planar Ar)	0.65	–1.49
Ca	3.57	–3.57
2,5-*T*	4.09	0.46
TS-1	(9.77)	(–1.62)
TS-2	(11.10)	(–3.10)
Barrier to rotation about C–Ar (*Ce*)	(2.23)	(–8.42)
Barrier to rotation about C–Ar (*Ca*)	(6.00)	(–7.94)
Barrier to rotation about C–N(Me)$_2$ (*Ce*)	(6.60)	(–5.58)
1@4 $CHCl_3$:		
Ca	4.83	–2.77
2,5-*T*	4.26	3.58
TS-1	(9.12)	(1.35)
TS-2	(14.60)	(1.31)
Barrier to rotation about C–Ar (*Ce*)	(2.51)	(–2.68)
Barrier to rotation about C–N(Me)$_2$ (*Ce*)	(7.20)	(–5.56)
1@8 $CHCl_3$:		
Ca	5.87	–7.60
2,5-*T*	5.26	–4.35
TS-1	(10.81)	(–5.39)
TS-2	(14.64)	(–10.23)
Barrier to rotation about C–Ar (*Ce*)	(3.34)	(–5.68)
Barrier to rotation about C–N(Me)$_2$ (*Ce*)	(7.94)	(–5.87)
***N*,*N*-Dimethylaniline**	(5.81)	(–5.64)

[a] For dioxane **1**, relative to the *Ce* form.

were measured relative to residual proton and carbon signals of the solvent.

X-ray diffraction analysis was performed at 293(2) K on an XCalibur Eos automated four-circle diffractomere (graphite monochromator, MoK_α radiation, λ 0.71073 Å, ω-scanning, $2\theta_{max}$ 62°). Data acquisition and processing were performed using CrysAlis^{Pro} version 1.171.36.20 (an Oxford Diffraction). The structures were solved by the direct method and refined by full-matrix least squares with anisotropic displacement parameters for nonhydrogen atoms. Hydrogen atoms were located by difference Fourier synthesis and refined with isotropic displacement parameters. The calculations were performed using SHELX97 [25]. Orthorhombic crystal system; space group *Pbca*; unit cell parameters: *a* 12.941(2) Å, *b* 9.9881(17) Å, *c* 23.858(6) Å; β 90°, *V* 3083.7(10) Å^3, *Z* 8; ρ_{calc} 1.694 mg/mm^3, μ 5.255 mm^{-1}, *F*(000) 1568.0; scan range $4.644 < \theta < 58.694°$; $-16 \le h \le 17, -11 \le k \le 13, -12 \le l \le 29$; unique reflections 3601 (R_{int} 0.1255), *GOOF* 0.932; final divergence factors R_1 0.0272, wR_2 0.1451 [on reflections with $I_{hkl} > 2\sigma(I)$] and R_1 0.2321 and wR_2 0.2123 (on all reflections); $\Delta\rho_{min/max}$ 0.53/–0.64 eÅ^{-3}.

The geometry of the *chair* conformer of acetal **1** was optimized first by the AM1 method (HyperChem 8.0) [26] and then by the DFT PBE/3ζ method (PRIRODA [18]). The ring interconversion and the internal rotation of the aromatic and dimethylamino substituents were simulated by scanning the corresponding torsion angles. The potential barriers were determined by the transition state search algorithm implemented in PRIRODA. Stationary points on the PES were identified as transition states by the presence of one imaginary frequency in the corresponding Hessian matrix, and as minima, by the absence of imaginary frequencies in the latter. Model clusters were formed by successively adding

the molecule of solvent in the vicinity of 1,3-dioxane molecule **1** using HyperChem, and the resulting system was further optimized in the PBE/3ζ approximation.

5,5-Bis(bromomethyl)-2-[4-(dimethylamino)-phenyl]-1,3-dioxane (**1**). An equimolar mixture (0.02 mol, 5.24 g) of 2,2-bis(bromomethyl)propan-1,3-diol (Sigma–Aldrich) and 2.38 g of *p*-(dimethylamino)benzaldehyde in 50 mL of benzene in the presence of 0.1 g of *p*-toluenesulfonic acid was heated under reflux until water no longer collected in the Dean–Stark trap, washed in succession with 5% aqueous $NaHCO_3$ (10 mL) and water (2 × 10 mL), the solvent was distilled off, and the residue was twice recrystallized from 95% EtOH. Yield 4.88 g (62%), mp 145.5–146.5°C.

CONCLUSIONS

It was found by XRD analysis and NMR spectroscopy that 5,5-bis(bromomethyl)-2-(4-dimethylaminophenyl)-1,3-dioxane molecules adopt a *chair* conformation with an equatorial substituent at the ring C^2 atom. The pathway of conformational transformations in a chloroform solution, predicted by DFT PBE/3ξ calculations (cluster model), includes, along with the equatorial *chair* (the main minimum on the PES), local minima of the 2,5-*twist* and axial *chair* forms, as well as *half-chair* transition states. It was shown that the number of solvent molecules in the nearest solvation shell of the studied 1,3-dioxane is not larger than four.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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