

Comparison of Some Molecular Structures by Minimizing the Comparison Function

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Abstract: The geometric difference in the relative arrangement of atoms in molecules with the same chemical formula significantly affects the properties of the crystal. For quantitative comparison of the spatial geometric structure of two molecules, we used the method of optimal superposition of molecules through the minimization of a certain comparison function by rotating the molecules after superposing their centers of mass. The search for the minimum of the comparison function over Euler rotation angles is performed by the Rosenbrock method. The assumed criterion for comparing molecules allows us to quantify the proximity in the spatial structure of molecules. The implementation of the method is shown by comparing the structure of eight molecules in four crystalline substances.

Keywords: conformation, Euler angles, rotation matrix, optimization methods, Rosenbrock method

1. INTRODUCTION

The paper deals with the mathematical problem that arises in structural chemistry, namely: the numerical study of the spatial structure of molecules with the same chemical formula, which may differ in the geometry of the mutual arrangement of atoms. The study of specific crystals was carried out in the framework of a mathematical model for comparing two molecules, studied in [1, 2]. The specified model is reduced to a comparison of two objects consisting of N ordered points with rigid geometry that behave like rigid bodies in \mathbb{R}^3 . The comparison principle in this model is based on optimizing the alignment of these two objects by shifting and rotating. The optimal superposition of these objects involves the minimization over shifts and rotation angles of a certain comparison function of the geometry of the objects, which is the sum of the squares of the distances between the points of two objects with the same indices. It is proved that the minimum over shifts is achieved by superposing some characteristic points, conventionally called centers of mass of molecules. To minimize the [3–5] comparison function over rotation angles, the Rosenbrock zero-order method [6] is used. The results obtained are used to study the geometry of molecules in real crystal structures.

Four organic crystalline substances (I, II, III, IV) are investigated. Substances II-IV consist of molecules with the same chemical formula and bond structure (same graphs), substance I is only a part of this graph. In addition, substances II and III contain symmetrically independent molecules (IIa, IIb, IIc, IId, and IIIa, IIIb) that may have the same graph, but may differ in spatial structure, i.e., in the geometry of the arrangement of atoms. The problem arises of objectively comparing the geometry in the space of all these eight molecules and

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quantifying the differences that exist in them, since the standard characteristics – bond lengths (interatomic distances) and valence angles (angles between valence bonds) do not always show differences in the geometry of molecules. In addition, it may be necessary to compare fragments of different molecules. For this purpose, [1, 2] provides a method for pairwise quantitative comparison of the geometry of molecules based on minimizing the comparison function by shifting and rotating the molecules. Here is a brief description of the comparison method.

2. ASSUMED MATHEMATICAL MODEL

The study of molecules with the same chemical formula by comparing their geometries uses the concept of structure. Here is the definition of the structure adopted in [1, 2]

Definition 2.1:

A geometric structure, or in short – structure, will mean a rigid geometric construction of N ordered points in \mathbb{R}^3 with coordinates (x_i, y_i, z_i) , $i = 1, \dots, N$, whose movement in \mathbb{R}^3 is performed like the motion of a rigid body.

We assume that each i -th point of the structure has a weight coefficient $w_i \geq 0$, and $\sum_{i=1}^N w_i = W > 0$. Let $i_k, k = 1, \dots, K$ – all indices corresponding to non-zero weight coefficients w_i . Then

$$W = \sum_{i=1}^N w_i = \sum_{k=1}^K w_{i_k} > 0. \quad (2.1)$$

In accordance with [1, 2], we will associate the optimal criterion for superimposing two geometric structures with the minimum over shifts and rotation angles (Euler angles [7]) of the comparison function of the form

$$U(\mathbf{r}_{1,0}, \mathbf{r}_{2,0}, \varphi, \theta, \psi) = \sum_{i=1}^N w_i |\mathbf{r}_{1,i} - \mathbf{r}_{1,0} - Q(\mathbf{r}_{2,i} - \mathbf{r}_{2,0})|^2, \quad (2.2)$$

where the vectors $\mathbf{r}_{1,i}$ and $\mathbf{r}_{2,i}$ determine the position of points in the first and second structure, the vectors $\mathbf{r}_{1,0}$ and $\mathbf{r}_{2,0}$ determine the offsets of the corresponding points of the first and second structure from the coordinate center, $Q = Q(\varphi, \theta, \psi)$ — the rotation matrix for Euler angles (ψ — precession angle, θ — nutation angle, φ — self rotation angle):

$$Q = \begin{pmatrix} \cos \psi \cos \varphi - \sin \psi \sin \varphi \cos \theta & -\cos \psi \sin \varphi - \sin \psi \cos \varphi \cos \theta & \sin \psi \sin \theta \\ \sin \psi \cos \varphi + \cos \psi \sin \varphi \cos \theta & -\sin \psi \sin \varphi + \cos \psi \cos \varphi \cos \theta & -\cos \psi \sin \theta \\ \sin \varphi \sin \theta & \cos \varphi \sin \theta & \cos \theta \end{pmatrix} \quad (2.3)$$

Thus, the U function of the form (2.2) is the sum of the squares of the distances between “eponymous” points of two geometric structures with weights w_i after matching points defined by vectors $\mathbf{r}_{1,0}$ and $\mathbf{r}_{2,0}$, with the coordinate center and rotation of the second structure relative to the first.

By matching some characteristic points of two geometric structures, called “centers of mass” you can reduce the task of minimizing the comparison function over a full set of variables to finding the minimum of the U function over the rotation angles φ, θ, ψ .

The following theorem is proved in [1].

Theorem 2.1:

The minimum of the U function of the form (2.2) is achieved at the point corresponding to

“center of mass” of two geometric structures and is defined by vectors

$$\mathbf{r}_{j,0} = \frac{1}{W} \sum_{i=1}^N w_i \mathbf{r}_{j,i}, \quad j = 1, 2. \quad (2.4)$$

So, the minimum of the function (2.2) corresponds to the shift of “centers of mass” of geometric structures defined by the formula (2.4) to the origin. The function (2.2) can now be considered as a function of rotation angles

$$U(\varphi, \theta, \psi) = \sum_{i=1}^N w_i |\mathbf{r}_{1,i} - \mathbf{r}_{1,0} - Q(\varphi, \theta, \psi)(\mathbf{r}_{2,i} - \mathbf{r}_{2,0})|^2, \quad (2.5)$$

where $\mathbf{r}_{1,i}, \mathbf{r}_{2,i}$ – given coordinates of geometric structures, and “centers of mass” $\mathbf{r}_{1,0}$ and $\mathbf{r}_{2,0}$ are calculated using the formula (2.4). The minimum of the function (2.5) is determined by the rotation angles φ, θ, ψ .

Let the minimum of the function $U = U(\varphi, \theta, \psi)$ of the form (2.5) be reached at the point $(\varphi_0, \theta_0, \psi_0)$. In accordance with [1, 2], we will call the value

$$s = \left(\frac{U(\varphi_0, \theta_0, \psi_0)}{W} \right)^{1/2}. \quad (2.6)$$

the measure of proximity of two geometric structures. This value can be considered as a quantitative characteristic of the proximity of geometric structures, since it represents the average distance between points with the same indices in two structures after “superposing”.

We will call two geometric structures equal if they can be superposed by points with the same indices by various displacements of these structures as solids. As shown in [1], this superposition is achieved by minimizing the comparison function (2.5) and corresponds to $s = 0$.

We will call two structures approximately equal if

$$s = \left(\frac{1}{W} \min_{\varphi, \theta, \psi} U(\varphi, \theta, \psi) \right)^{1/2} = \left(\frac{U(\varphi_0, \theta_0, \psi_0)}{W} \right)^{1/2} \leq s_0, \quad (2.7)$$

where s_0 is the specified value (in applications, it is determined by the specific practical situation). The inequality $s \leq s_0$ will be called the criterion of proximity of structures.

Practical experience in studying the conformation of molecules, based on the results of comparing a significant number of structures [8, 9], resulted in the following conditional classification: $s \leq s_0 = 0, 1 \text{ \AA}$ – molecules are practically equal, $0, 1 \text{ \AA} < s \leq 0, 2 \text{ \AA}$ – molecules are close, $s > 0, 2 \text{ \AA}$ – molecules are different.

Note that if the minimum point is not unique and there is a point $(\varphi_1, \theta_1, \psi_1)$ such that $U(\varphi_1, \theta_1, \psi_1) = U(\varphi_0, \theta_0, \psi_0)$, then the value of s does not change and the non-uniqueness of the minimum point does not affect the proximity criterion of structures.

The test for comparing the geometry of two geometric structures consists of three stages: 1) shifting the center of mass of each geometric structure to the coordinate center; 2) minimizing the function (2.5) over angles; 3) calculating the value of s using the formula (2.7) and inferring the proximity of the structures. Additional information is provided by residual values $\Delta r_i = |\mathbf{r}_{1,i} - \mathbf{r}_{2,i}|$.

When comparing two structures in accordance with the algorithm 1)-3), determination of the minimum of the comparison function $U(\varphi, \theta, \psi)$ over rotation angles after superposing the centers of mass of structures is performed numerically.

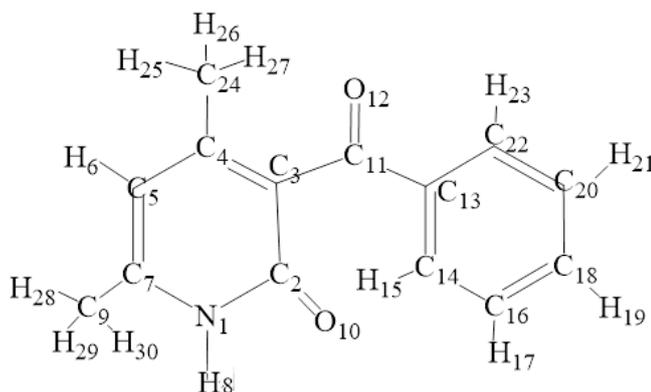


Fig. 3.1. Molecule $C_{14}H_{13}NO_2$ 4,6-dimethyl-3-(phenylcarbonyl) pyridin-2 (1H) -one (I).

3. NUMERICAL STUDY OF CRYSTAL STRUCTURES

This section presents the results of the numerical study comparing chemically identical molecules in a crystal by minimizing the comparison function (2.5). In this case, we will consider molecules with an ordered structure of N points-atoms as a geometric structure. The coordinates of the molecules in the crystal are obtained from X-ray analysis. In this study, the combined atoms in the molecules are assigned a weight of $w_i = 1$. The remaining atoms are assigned a weight of $w_i = 0$. The coordinates of the hydrogen atoms were not included in the calculations, since the accuracy of their determination is lower than that of other atoms and their presence is insignificant in the present task of superposing molecules, so they are assigned a weight of $w_i = 0$.

When comparing molecules, we will be interested in differences in the spatial structure of molecules with a single structural formula (graph). Since the comparison function (2.5) is not convex, the Rosenbrock zero-order method [6] is used to numerically minimize it. The program that implements the comparison algorithm 1)-3) uses the optimization library module [10] to minimize the comparison function (2.5) using the Rosenbrock method.

In this paper, we set the task of comparing the spatial structure of 4,6-dimethyl-3-(phenylcarbonyl) pyridin-2 (1H) -one (I) molecules with the chemical formula $C_{14}H_{13}NO_2$ where $N = 30$ and in 3-benzoyl-4,6-crystals-dimethyl-1-[2-(4-methylphenyl)-2-oxoethyl] pyridin-2 (1H)-one (II, III, IV) with the chemical formula $C_{23}H_{21}NO_3$, where $N = 48$. The composition, bonds and geometry of these molecules are schematically depicted in Fig. 3.1 and Fig. 3.2.

The atomic coordinates were obtained by the method of X-ray analysis [11]. The characteristics of these substances in crystallography are described as follows:

I $C_{14}H_{13}NO_2$ space group $P2_1/c$, $Z = 4$ (molecule occupies 1 position);

II $C_{23}H_{21}NO_3$ space group $P\bar{1}$, $Z = 8$ (four independent molecules a, b, c, d);

III $C_{23}H_{21}NO_3 \cdot \frac{1}{2}H_2O$ (two independent molecules a, b);

IV $C_{23}H_{21}NO_3 \cdot \frac{1}{2}H_2O$ space group $C2/c$, $Z = 8$ (molecule occupies one position).

Space group [12] describes all possible symmetries of an infinite number of periodically located points in three-dimensional space. The number Z shows the number of molecules in the unit cell. In crystals I and IV, the molecules occupy one system of positions, that is, they are transformed into each other using symmetry operations of the space group. In crystals II and III, the molecules occupy independent positions, respectively, four (IIa, IIb, IIc, IId) and two (IIIa, IIIb), that is, the molecules are not transformed into each other by symmetry operations of the space group of the crystal and therefore can be different in structure.

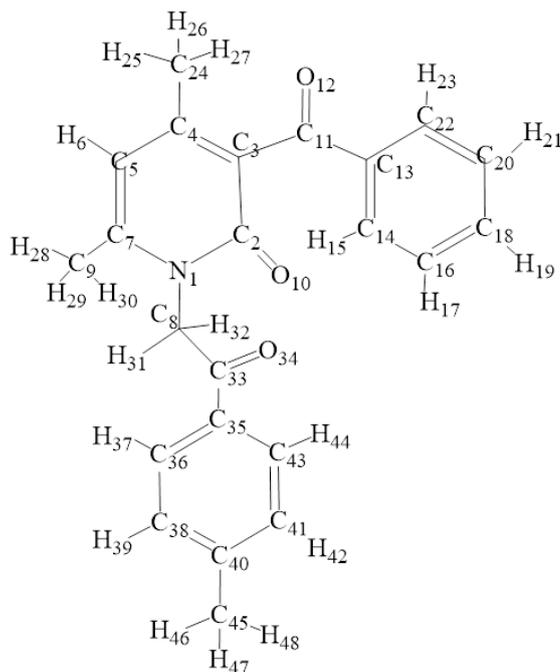


Fig. 3.2. Molecule $C_{23}H_{21}NO_3$, 3-benzoyl-4,6-crystals-dimethyl-1-[2-(4-methylphenyl)-2-oxoethyl] pyridin-2 (1H)-one (II, III, IV)

Table 3.1. Comparison of four independent molecules a, b, c, d in crystals II

Atom	The value of "residuals" Δr_i , characteristic s in crystals II						
	$a - b$	$a - c$	$a - d$	$b - c$	$b - c$	$b - d$	$c - d$
N 1	0.20	0.06	0.03	0.23	0.05	0.18	0.08
C 2	0.19	0.16	0.04	0.34	0.08	0.15	0.20
C 3	0.06	0.15	0.05	0.20	0.02	0.03	0.19
C 4	0.05	0.10	0.06	0.09	0.03	0.10	0.16
C 5	0.02	0.08	0.05	0.08	0.08	0.07	0.11
C 7	0.05	0.06	0.01	0.04	0.04	0.04	0.04
C 8	0.19	0.03	0.03	0.17	0.13	0.16	0.02
C 9	0.03	0.10	0.03	0.08	0.06	0.08	0.08
O 10	0.27	0.22	0.04	0.47	0.07	0.29	0.23
C 11	0.07	0.24	0.04	0.30	0.14	0.04	0.26
O 12	0.22	0.35	0.08	0.56	0.30*	0.14	0.42
C 13	0.09	0.15	0.06	0.24	0.44*	0.13	0.12
C 14	0.30	0.35	0.06	0.65	0.69*	0.24	0.41
C 16	0.42	0.46	0.16	0.88	0.92*	0.26	0.63
C 18	0.37	0.41	0.15	0.78	0.96*	0.22	0.56
C 20	0.23	0.24	0.06	0.45	0.77*	0.18	0.30
C 22	0.12	0.09	0.07	0.19	0.53*	0.09	0.10
C 24	0.18	0.15	0.11	0.20	0.03	0.24	0.26
C 33	0.16	0.12	0.08	0.20	0.34*	0.15	0.12
O 34	0.31	0.28	0.15	0.39	0.56*	0.22	0.21
C 35	0.10	0.10	0.06	0.18	0.50*	0.14	0.14
C 36	0.04	0.29	0.04	0.27	0.40*	0.06	0.32
C 38	0.13	0.33	0.04	0.38	0.65*	0.12	0.30
C 40	0.24	0.14	0.06	0.37	0.91*	0.21	0.17
C 41	0.28	0.25	0.06	0.43	1.06*	0.24	0.26
C 43	0.19	0.24	0.08	0.35	0.88*	0.18	0.21
C 45	0.32	0.27	0.11	0.57	1.06*	0.35	0.22
s	0.21	0.23	0.08	0.40	0.08	0.18	0.27

Note that a comparison of bond lengths and bond angles does not reveal differences in the spatial structure of molecules. In eponymic bonds, the differences in length are no more than $0,02\text{\AA}$, and in bond angles no more than 5° . Some differences are observed in individual torsion angles - up to 19° ; however, how substantially this affects the general geometry of the molecules is not always clear. Thus, it is not known in advance whether these molecules are similar in structure or whether their differences are significant. In this situation, there is a need for an objective, quantitative, comparison of the structure of molecules.

For this purpose, the technique described in the previous section was applied to the study of these molecules. Comparison of molecules was carried out by minimizing the comparison function (2.5). As already mentioned, the coordinates $\mathbf{r}_{1,i}, \mathbf{r}_{2,i}, i = 1, \dots, 48$ (for substances II - IV), $i = 1, \dots, 30$ (for substance I) for each pair of compared molecules were obtained on based on x-ray analysis data. All crystals (I - IV) are centrosymmetric (both left and right molecules are present), therefore, to compare some pairs, one of the molecules was taken with inversion. The centers of mass were determined by the formula (2.4). The comparison function (2.5) was minimized numerically using the Rosenbrock method over three Euler angles after superposing the centers of mass of the two molecules being compared.

The essential thing in our method of quantitative comparison of the spatial structure of molecules is the variation in the values of the weight factors w_i . The ability to superpose molecules with separate fragments is achieved by setting the values of $w_i = 1$ for compatible atoms and $w_i = 0$ for other atoms. This allows you to change the center of gravity of the molecules, combine the molecules along the closest or most significant parts and thereby more clearly visualise certain differences in the structure of the molecules and their parts. As already mentioned, in our calculations we set the values $w_i = 0$ for hydrogen atoms H .

In table 3.1 we present the results of applying the comparison algorithm 1) - 3) for matching 4 symmetrically independent molecules (a, b, c, d) that coexist in one crystalline substance II. Here, the residuals $\Delta r_i = |\mathbf{r}_{1,i} - \mathbf{r}_{2,i}|, i = 1, \dots, 48$, i.e., the distances between the eponymic atoms in the two molecules under comparison are calculated after matching (at the point of minimum of the comparison function U), as well as magnitude s - magnitude measure of proximity. Results are shown for non-hydrogen atoms. The (*) indicates atoms for which $w_i = 0$ was taken in this calculation.

Let us analyze the data obtained. In practice, only the pair of a-d molecules ($s = 0,08\text{\AA}$) are practically equal in their spatial structure; another pair of $b - d$ molecules ($s = 0,18\text{\AA}$) are close. Other pairs of molecules have greater or lesser differences. The largest difference in the structure of molecules, is in the $b - c$ pair ($s = 0,40\text{\AA}$). For this pair, another calculation was performed in which only for atoms of the central pyridine ring and atoms directly connected with it with indices $i = 1, \dots, 11, 24$ and weight $w_i = 1$. In this comparison, $s = 0,08\text{\AA}$, which means the equality of these fragments and, in addition, this comparison highlighted the differences in the rotation of the phenyl rings. The result of this comparison is presented in Fig. 3.3.

As the calculations showed, two symmetrically independent molecules a and b in crystal III ($s = 0,04\text{\AA}$), as well as pairs of molecules IV and IIIa ($s = 0,03\text{\AA}$), IV and IIIb ($s = 0,04\text{\AA}$) are almost identical. Calculations comparing molecules from IV with four independent molecules from crystal II indicated their significant differences in geometry. To identify differences for the same pairs of molecules, additional calculations were performed with varying weight factors. The Δr_i values for atoms with $w_i = 0$ are also marked with (*). The calculation results are given in Table 3.2.

The results of the comparison point to parts of the molecules where there are differences and make us look for geometric characteristics to visually describe these differences. These characteristics were found as the differences in the angles between the planes (. 3.3) - plane 1: through the atoms $NC_2C_3C_4C_5C_6$, plane 2: through the atoms $C_{13}C_{14}C_{16}C_{18}C_{20}C_{22}$, plane 3: through the atoms ($C_{35}C_{36}C_{38}C_{40}C_{41}C_{43}$).

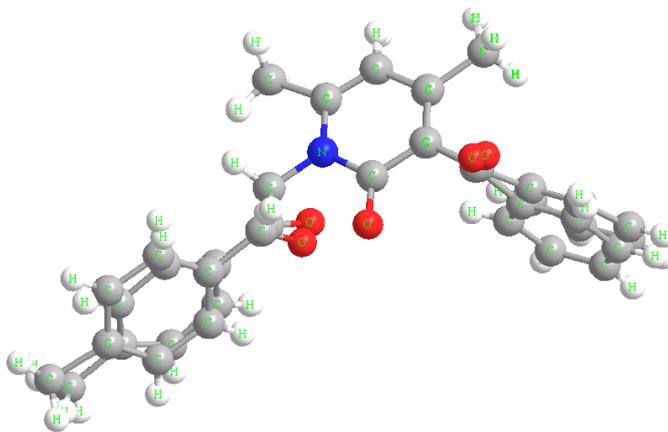


Fig. 3.3. The best combination of molecules IIb and IIc with $w_i = 1$ for $i = 1, \dots, 11, 24$.

Table 3.2. Comparison of a molecule from crystal IV with a, b, c, d molecules in crystal II.

Atom	The value of "residuals" Δr_i , characteristic s							
	IV&IIa	IV&IIa	IV&IIb	IV&IIb	IV&IIc	IV&IIc	IV&II d	IV&II d
N 1	0.43	0.04	0.38	0.03	0.41	0.02	0.41	0.02
C 2	0.31	0.01	0.31	0.03	0.38	0.05	0.29	0.04
C 3	0.22	0.02	0.16	0.04	0.33	0.02	0.17	0.05
C 4	0.35	0.06	0.40	0.04	0.43	0.04	0.29	0.02
C 5	0.44	0.06	0.47	0.06	0.47	0.08	0.40	0.05
C 7	0.45	0.01	0.41	0.04	0.40	0.06	0.44	0.04
C 8	0.49	0.06	0.46	0.13	0.50	0.03	0.51	0.06
C 9	0.57	0.10	0.57	0.09	0.55	0.13	0.58	0.07
O 10	0.43	0.04	0.50	0.03	0.40	0.06	0.44	0.05
C 11	0.13	0.08	0.17	0.06	0.22	0.17	0.13	0.13
O 12	0.08	0.29*	0.21	0.21*	0.36	0.50*	0.08	0.29*
C 13	0.43	0.34*	0.34	0.29*	0.56	0.72*	0.45	0.34*
C 14	0.27	0.17*	0.40	0.10*	0.48	0.69*	0.27	0.20*
C 16	0.42	0.40*	0.27	0.27*	0.84	1.14*	0.32	0.26*
C 18	0.99	0.92*	0.62	0.85*	1.40	1.66*	0.84	0.72*
C 20	1.36	1.15*	1.22	1.21*	1.60	1.73*	1.32	1.04*
C 22	1.06	0.85*	1.05	0.90*	1.15	1.25*	1.11	0.84*
C 24	0.42	0.07	0.61	0.07	0.51	0.05	0.38	0.04
C 33	0.30	0.45*	0.31	0.54*	0.39	0.29*	0.36	0.37*
O 34	0.35	0.46*	0.35	0.54*	0.60	0.09*	0.40	0.30*
C 35	0.26	0.84*	0.20	1.05*	0.36	0.68*	0.27	0.80*
C 36	0.18	0.83*	0.20	2.38*	0.35	0.93*	0.16	0.84*
C 38	0.39	1.28*	0.35	2.54*	0.69	1.37*	0.41	1.37*
C 40	0.78	1.80*	0.64	2.07*	0.88	1.53*	0.79	1.87*
C 41	0.87	1.82*	0.67	3.37*	0.81	1.30*	0.83	1.81*
C 43	0.58	1.36*	0.44	3.02*	0.55	0.88*	0.51	1.29*
C 45	1.14	2.34*	0.96	2.65*	1.38	2.18*	1.22	2.50*
s	0,60	0,05	0,54	0,06	0,72	0,08	0,59	0,05

Table 3.3. Angles (in degrees) between planes in molecules IIa, IIb, IIc, II d and molecule in crystal IV

Planes	IIa	IIb	IIc	II d	IV
Planes 1 2	84.4	85.9	78.2	89.4	86.7
Planes 1 3	86.5	87.8	71.7	85.7	71.2
Planes 2 3	55.4	51.8	61.8	52.5	84.1

In addition, we present in table 3.4 the distances between the far points of the C_{18} and C_{45} molecules.

The maximum distance is observed in molecules IIc and II d, the minimum - in IV. This illustrates the largest difference $s = 0,72\text{\AA}$ for the IIc - IV pair. Fig. 3.4 shows the

Table 3.4. Distances (in angstroms) between the “far points” C_{18} and C_{45} of the *IIa*, *IIb*, *IIc*, *II d* molecules in crystals II and in the crystal IV molecule.

	<i>IIa</i>	<i>IIb</i>	<i>IIc</i>	<i>II d</i>	IV
Distance $C_{18}C_{45}$	12.8	12.3	13.4	12.8	11.3

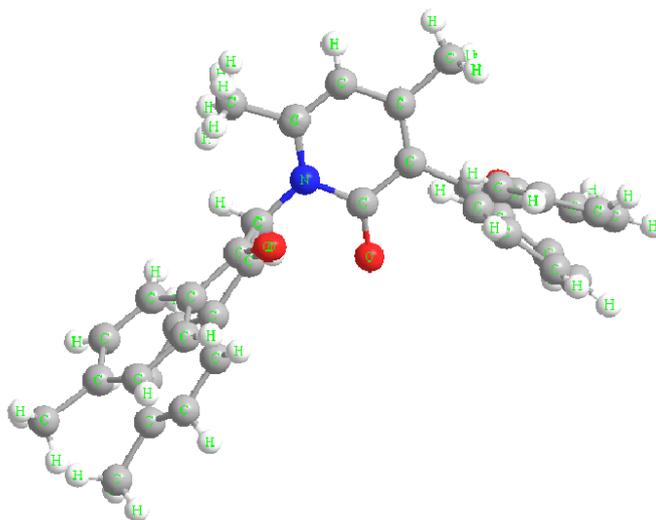


Fig. 3.4. The best combination of molecules *IIb* and IV with $w_i = 1$ for $i = 1, \dots, 11, 24$.

result of combining *IIc* - IV with $w_i = 1$ for the pyridine nucleus and the nearest atoms ($NC_2C_3C_4C_5C_7C_9C_{11}C_{24}O_2O_{10}$).

The application of the comparison algorithm 1) - 3) also works well for comparing molecules from I with the corresponding fragments of molecules *IIa*, *IIb*, *IIc*, *II d*, *IIIa*, *IIIb*, IV. The results are presented in Table 3.5. The table contains the calculated residuals $\Delta r_i = |\mathbf{r}_{1,i} - \mathbf{r}_{2,i}|$, $i = 1, \dots, 30$. The results are shown for non-hydrogen atoms (except for H_8 from crystal I).

Comparison of molecule I with fragments of molecules - IV, *IIIa*, *IIIb* gave the same results, $s = 0, 27\text{\AA}$ (there are some differences), which is explainable, since molecules IV, *IIIa*, *IIIb* are practically identical to each other in their geometry.

The molecule in crystal I has the biggest differences with molecule *IIc*, $s = 0, 54\text{\AA}$. To identify these differences, we use the same technique - variation of weighting factors. The calculation by combining the planes of the pyridine rings and the directly bonded C and O atoms gave $s = 0, 17\text{\AA}$ (parts of the fragments are close). This result indicates differences in the relative positions of the pyridine and phenyl rings. In this regard, the angles between plane 1 $s = 0, 17\text{\AA}$ and plane 2 ($C_{13}C_{14}C_{16}C_{18}C_{20}C_{22}$) are calculated. For the molecule of their crystal I, the angle is $81, 1^\circ$; the angle in *IIc* is the most different from it, which is $78, 2^\circ$. In addition, differences in the orientation of C = O bonds were found: differences in the torsion angles of $C_4C_3C_{11}O_{12}$, $O_{12}C_{11}C_{13}C_{22}$ and $C_3C_{11}C_{13}C_{22}$ are $19, 7^\circ$, $19, 9^\circ$ and $12, 5^\circ$, respectively.

4. CONCLUSION

The calculations presented here show the effectiveness of the technique used to study the geometry of molecules in crystals using the comparison function. Interesting facts were

Table 3.5. Comparison of molecule I with corresponding fragments of molecules IIa, IIb, IIc, IId, IIIa, IIIb, IV ((*) marked atoms for which $w_i = 0$ is calculated)

Atom	The value of "residuals" Δr_i , characteristic s							
	I&IIa	I&IIb	I&IIc	I&IId	I&IIIc	I&IIIb	I&IV	
N 1	0.28	0.27	0.46	0.05	0.24	0.19	0.20	0.20
C 2	0.37	0.39	0.45	0.07	0.36	0.30	0.31	0.31
C 3	0.20	0.23	0.26	0.04	0.19	0.15	0.13	0.13
C 4	0.33	0.33	0.45	0.04	0.29	0.15	0.14	0.15
C 5	0.37	0.37	0.45	0.08	0.34	0.24	0.24	0.24
C 7	0.17	0.24	0.21	0.10	0.18	0.13	0.15	0.14
O 8*	0.78*	0.68*	1.03*	0.52*	0.77*	0.77*	0.83*	0.69*
C 9	0.45	0.53	0.44	0.10	0.44	0.44	0.44	0.45
O 10	0.70	0.71	0.83	0.10	0.61	0.56	0.56	0.57
C 11	0.38	0.37	0.55	0.06	0.37	0.17	0.18	0.19
O 12	0.78	0.75	0.96	0.73*	0.75	0.37	0.37	0.36
C 13	0.10	0.13	0.03	0.97*	0.05	0.05	0.05	0.04
C 14	0.31	0.41	0.15	1.19*	0.33	0.14	0.13	0.12
C 16	0.16	0.23	0.17	1.96*	0.19	0.23	0.23	0.23
C 18	0.55	0.55	0.63	2.57*	0.46	0.31	0.31	0.31
C 20	0.73	0.83	0.78	2.39*	0.73	0.25	0.26	0.25
C 22	0.40	0.47	0.41	1.55*	0.45	0.08	0.09	0.09
C 24	0.62	0.56	0.88	0.08*	0.49	0.28	0.27	0.27
s	0.45	0.47	0.54	0.17	0.42	0.27	0.27	0.27

obtained - 3-benzoyl-4,6-dimethyl-1- [2- (4-methylphenyl) -2-oxoethyl] pyridin-2 (1H) - one molecules have the same conformation in different crystals of III and IV, and different conformation - in one crystal II.

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