Preferred Orientation of Crystallites in Tablets. IV.[1] Features of the Preferred Orientation Plane[2]

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Features of the preferred orientation plane of some organic crystals were studied from a quantum chemical point of view. The interaction energies in those crystal planes in which cleavage is possible were calculated by using the interaction energies between two molecules. The intermolecular interaction energies were calculated by the CNDO/2 (complete neglect of differential overlap) method. The preferred orientation planes, which have a tendency to orient themselves parallel to the upper surface of a tablet during compression, showed only small interaction energy. Thus, the preferred orientation of crystallites in a tablet was considered to occur by cleavage along that crystal plane which had small interaction energy during compression.

Keywords preferred orientation; compression; molecular orbital calculation; cleavage; intermolecular interaction energy; tablet

In previous papers,[1a,b] X-ray powder diffraction methods were presented to evaluate the preferred orientation of crystallites in tablets. We showed that particular planes, such as 100 in aspirin, 110 or 210 in salicylic acid, 002 in benzoic acid and 002 in nicotinic acid, had a tendency to orient parallel to the upper surface of a tablet during compression, so these planes were called the preferred orientation planes. It is well known that the (100) plane of an aspirin crystal is a cleavage plane.[3] Umeyama *et al.*[4] and Kim *et al.*[5] studied the (100) plane of aspirin crystal, which was determined to have the smallest interaction energy and the smallest specific surface energy by means of molecular orbital calculations (CNDO/2 method[6]) and the atom–atom potential method, respectively.

In the present study, in order to clarify the feature of the preferred orientation planes of salicylic acid, benzoic acid and nicotinic acid, the interaction energies in those crystal planes in which cleavage is possible were calculated by the CNDO/2 method (complete neglect of differential overlap method).

Methods

Crystallographic data (lattice constants, space group and the positional parameters of atoms) of salicylic acid,[7] benzoic acid,[8] and nicotinic acid[9] were used in the literature. CNDO/2 molecular orbital calculations were carried out using a Hewlett–Packard HP9816S model 216 computer using the BASIC program.[10] The Cartesian coordinates of atoms of molecules were generated from lattice constants, positional coordinates and appropriate symmetry operations. The thermal motion of atoms was neglected and optimization of geometry was not performed in the calculation.

Intermolecular interaction energy between molecules A and B (ΔE_{AB}) was calculated as follows:

$$\Delta E_{AB} = E_{AB} - (E_A + E_B) \quad (1)$$

where E_{AB} is the total energy of the complex of molecules A and B, and E_A and E_B are total energies of the isolated molecules. The intermolecular interaction energies were calculated for all of the pairs of the central molecule and its surrounding molecules positioned within 7 Å in the nearest atom–atom distance. The intermolecular interaction energy was considered to be zero between molecules more than 7 Å distant from each other. The interaction energies in the planes possible for cleavage was calculated approximately from the interaction energies between two molecules, as reported by Umeyama *et al.*[4] The interaction energy across the plane (p) of the crystal was calculated from Eq. 2,

$$\Delta E_p = \frac{100}{Cf} \sum_i \Delta E_{1i} \quad (2)$$

where ΔE_{1i} is the interaction energy between the 1st molecule on one side of the plane and the i-th molecule on the other side of the plane. The numbers of i for the calculation of ΔE_p are listed in Tables II, V and VIII. Cf is a cross section of the plane (p) parallel to (hk1) plane in a unit cell (Tables III, VI and IX), and $100/Cf$ is a correction factor for the calculation of the energy in the definite area (kcal/(mol·100 Å^2)). A structure with a pattern in which one molecule on one side of the plane interacts with many molecules on the other side of the plane is called "an interaction type".[4] Since the number of interaction types in the plane (p) is one or more, the interaction energy in the cleavage plane was calculated as the mean value of ΔE_p for the individual interaction type.

Results and Discussion

Salicylic Acid Crystals of salicylic acid are monoclinic with $a = 11.52$ Å, $b = 11.21$ Å, $c = 4.92$ Å and $\beta = 90.83°$, and with space group $P2_1/a$.[7] Four molecules are contained in a unit cell. Table I shows the fractional coordinates of 38 salicylic acid molecules and the interaction energies (kcal/mol) between the 1st molecule, which was positioned in the center, and each of the other molecules by the CNDO/2 method. Since molecule 1 forms two hydrogen bonds with molecule 8, the interaction energy between them is −21.13 kcal/mol (most stabilizing). Figures 1 and 2 show the crystal structure of salicylic acid projected on (001) and (010) planes, respectively. There are five planes (planes I—V) on which cleavage is possible in the crystal lattice. No planes offering the possibility of cleavage parallel to the a axis existed.

The number of "interaction types" in planes I and III is four, and in the planes II, IV and V, two. The interaction energies in planes I—V were evaluated as the mean value of the interaction energies in (I-1, I-2, I-3 and I-4), (II-1 and II-2), (III-1, III-2, III-3 and III-4), (IV-1 and IV-2) and (V-1 and V-2), respectively. Table II shows the molecular numbers used to calculate the interaction energies in plane I-1 to V-2. Table III shows the indices of crystal planes corresponding to planes I—V, as well as correction factors and the interaction energies in the definite area (kcal/(mol·100 Å^2)) in planes I—V, respectively.

Since the interaction energy of a hydrogen bond is larger than that of van der Waals bonding, the interaction

TABLE I. Fractional Coordinates of the 38 Salicylic Acid Molecules and Interaction Energies (kcal/mol) between the 1st Molecule and Each of the Remaining 37 Molecules Calculated by Using the CNDO/2 Method

Molecule no.	Fractional coordinates			ΔE	Molecule no.	Fractional coordinates			ΔE
1	$x+0.5$	$0.5-y$	z		20	$-x$	$-y$	$\bar{z}$	+0.04
2	$0.5-x$	$y-0.5$	$-1-z$	+0.02	21	$-x$	$\bar{y}$	$\bar{z}$	+0.04
3	$0.5-x$	$y-0.5$	$-z$	−0.08	22	$-x$	$-y$	$2-z$	+0.03
4	$0.5-x$	$y-0.5$	$\bar{z}$	−0.13	23	$-x$	$\bar{y}$	$2-z$	+0.03
5	$0.5-x$	$y-0.5$	$2-z$	+0.04	24	$\bar{x}$	$-y$	$-1-z$	−0.01
6	$0.5-x$	$y+0.5$	$-z$	−0.28	25	$\bar{x}$	$\bar{y}$	$-1-z$	−0.01
7	$0.5-x$	$y+0.5$	$\bar{z}$	−1.89	26	$\bar{x}$	$-y$	$-z$	−0.27
8	$0.5-x$	$y+0.5$	$2-z$	−21.13	27	$\bar{x}$	$\bar{y}$	$-z$	−0.27
9	$1.5-x$	$y-0.5$	$-z$	−0.02	28	$\bar{x}$	$-y$	$\bar{z}$	−0.81
10	$1.5-x$	$y+0.5$	$-z$	−0.01	29	$\bar{x}$	$\bar{y}$	$\bar{z}$	−0.81
11	$1.5-x$	$y+0.5$	$\bar{z}$	+0.05	30	$\bar{x}$	$-y$	$2-z$	−0.19
12	x	y	$z-1$	−0.06	31	$\bar{x}$	$\bar{y}$	$2-z$	−0.19
13	$x+1$	y	$z+1$	−0.06	32	$x+0.5$	$-0.5-y$	$z-1$	−0.04
14	x	y	z	−0.31	33	$x+0.5$	$1.5-y$	$z+1$	−0.04
15	$x+1$	y	z	−0.31	34	$x+0.5$	$0.5-y$	$z-1$	−0.34
16	x	y	$z+1$	−0.37	35	$x+0.5$	$0.5-y$	$z+1$	−0.34
17	$x+1$	y	$z-1$	−0.37	36	$x+0.5$	$0.5-y$	$z+2$	+0.05
18	x	y	$z+2$	0.00	37	$x+0.5$	$0.5-y$	$z-2$	+0.05
19	$x+1$	y	$z-2$	0.00	38	$0.5-x$	$y+0.5$	$3-z$	−0.07

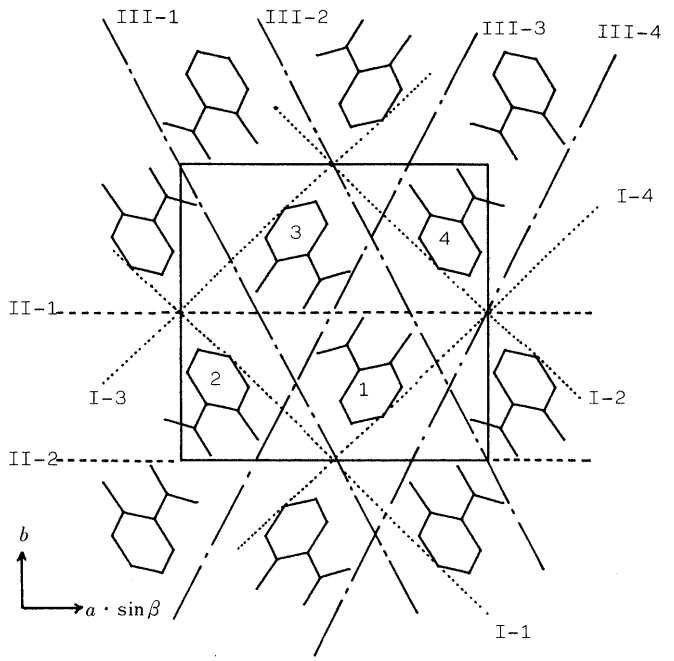

Fig. 1. Crystal Structure of Salicyclic Acid Projected along [001] and Three Planes (I—III) Offering the Possibility of Cleavage of Salicyclic Acid

Fractional coordinate: (1) $x+0.5$, $0.5-y$, z; (2) x, y, z; (3) $0.5-x$, $y+0.5$, $\bar{z}$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

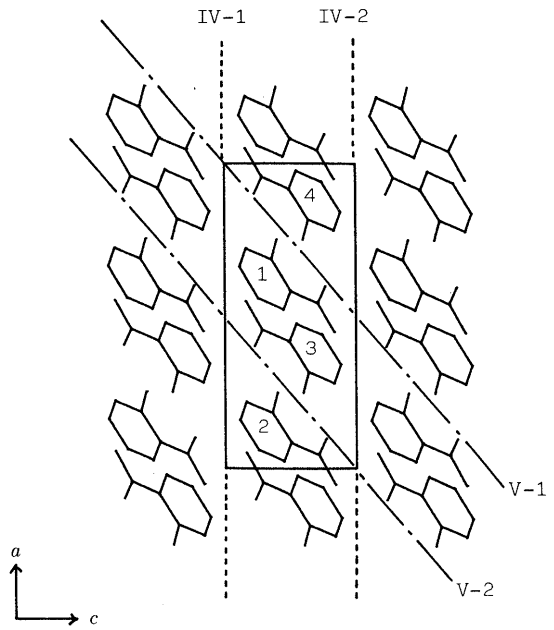

Fig. 2. Crystal Structure of Salicyclic Acid Projected along [010] and Two Planes (IV, V) Offering the Possibility of Cleavage of Salicyclic Acid

Fractional coordinates: (1) $x+0.5$, $0.5-y$, z; (2) x, y, z; (3) $0.5-x$, $y+0.5$, $\bar{z}$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

energies in planes II—V was larger than that in plane I. Thus, the interaction energy in plane I was less stable than in any of the other planes. This result indicates that plane I may have a marked tendency to cleave in salicylic acid crystals.

Considering the result that the preferred orientation plane in aspirin coincided with the cleavage plane, plane I might be the preferred orientation plane in salicylic acid crystals. It was found that either the 110 or 210 plane of salicylic acid was the preferred orientation plane.[1b] These results suggest that the preferred orientation of salicylic acid crystallites occurred by cleavage along the {110} planes during compression.

Benzoic Acid Crystals of benzoic acid are monoclinic with $a=5.510$ Å, $b=5.157$ Å, $c=21.973$ Å and $\beta=97.41°$, and with space group $P2_1/c$.[8] Four molecules are contained in a unit cell. Table IV shows the fractional coordinates of 37 benzoic acid molecules and the interaction energies (kcal/mol) between the 1st molecule and each of the other molecules. The 1st molecule forms two hydrogen bonds with the 33rd molecule, and the intermolecular interaction energy between them was −18.64 kcal/mol. Figure 3 shows the crystal structure of benzoic acid projected on (010). There are five planes (planes I—V) on which cleavage is possible in the crystal. No planes offering

the possibility of cleavage parallel to both the *a* and *c* axes existed.

The number of "interaction types" in planes I and II is one, and in planes III, VI and V, two. The interaction energies in planes III, IV and V were evaluated as the mean value of the interaction energies of (III-1 and III-2), (IV-1 and IV-2) and (V-1 and V-2), respectively. Table V shows the molecular numbers used to calculate the

Table II. Salicylic Acid Numbers Used to Calculate the Interaction Energy in Planes I-1 to V-2

Plane	Salicylic acid number
I-1	2, 3, 4, 5, 12, 14, 16, 18, 20, 22, 32
I-2	10, 11, 25, 27, 29, 31, 33
I-3	21, 23, 33
I-4	2, 3, 4, 5, 9, 10, 11, 13, 15, 17, 19, 24, 26, 28, 30, 32
II-1	6, 7, 8, 10, 11, 21, 23, 25, 27, 29, 31, 33, 38
II-2	2, 3, 4, 5, 9, 20, 22, 24, 26, 28, 30, 32
III-1	2, 3, 4, 5, 12, 14, 16, 18, 20, 21, 22, 23, 32
III-2	9, 10, 11, 13, 15, 17, 19, 25, 27, 29, 31, 33
III-3	6, 7, 8, 12, 14, 16, 18, 20, 21, 22, 23, 33, 38
III-4	9, 10, 11, 13, 15, 17, 19, 24, 26, 28, 30, 33
IV-1	3, 6, 9, 10, 12, 17, 26, 27, 32, 34
IV-2	5, 8, 13, 16, 22, 23, 30, 31, 33, 35
V-1	5, 8, 11, 13, 15, 28, 29, 30, 31, 33, 35
V-2	3, 6, 12, 14, 20, 21, 32, 34

Table III. Indices of Crystal Plane,[a] Correction Factor (*Cf*) and Interaction Energies (kcal/(mol·100 Å^2)) in the Five Planes Offering the Possibility of Cleavage of Salicylic Acid Crystals

Plane	Indices of crystal plane	Correction factor (*Cf*)	Interaction energy
I	(110)	*cd*	−1.34
II	(020)	*ac*	−22.94
III	(210)	*ec*	−11.64
IV	(001)	*ab*	−9.28
V	(201)	*bf*	−14.53

a) One of the indices of the crystal plane corresponding to planes I—V in a set of symmetrically equivalent crystal planes. *a*, *b* and *c* represent the lattice constants of salicylic acid crystal. *d*, *e* and *f* are the longer diagonal lines of the parallelogram constructed by (*a* and *b*), (*a*/2 and *b*) and (*a*/2 and *c*), respectively.

Table IV. Fractional Coordinates of the 37 Benzoic Acid Molecules and Interaction Energies (kcal/mol) between the 1st Molecule and Each of the Remaining 36 Molecules Calculated by Using the CNDO/2 Method

Molecule no.	Fractional coordinates			ΔE	Molecule no.	Fractional coordinates			ΔE
1	$\bar{x}$	$y+0.5$	$0.5-z$		20	$-x$	$y+0.5$	$0.5-z$	−0.25
2	$x-1$	y	z	+0.04	21	$2-x$	$y+0.5$	$0.5-z$	−0.25
3	$x-1$	$y+1$	z	+0.04	22	$-x$	$y+1.5$	$0.5-z$	−0.47
4	x	$y-1$	z	−0.02	23	$2-x$	$y-0.5$	$0.5-z$	−0.47
5	x	$y+2$	z	−0.02	24	$-x$	$y+2.5$	$0.5-z$	−0.05
6	x	y	z	−0.13	25	$2-x$	$y-1.5$	$0.5-z$	−0.05
7	x	$y+1$	z	−0.13	26	$\bar{x}$	$y-0.5$	$0.5-z$	−0.60
8	$x+1$	$y+2$	z	−0.06	27	$\bar{x}$	$y+1.5$	$0.5-z$	−0.60
9	$x+1$	$y-1$	z	−0.06	28	$x-1$	$1.5-y$	$z+0.5$	−0.10
10	$x+1$	y	z	−0.19	29	x	$0.5-y$	$z+0.5$	−0.15
11	$x+1$	$y+1$	z	−0.19	30	x	$1.5-y$	$z+0.5$	−0.37
12	$x+2$	y	z	+0.01	31	x	$2.5-y$	$z+0.5$	−0.09
13	$x+2$	$y+1$	z	+0.01	32	$x+1$	$-0.5-y$	$z+0.5$	−0.10
14	$\bar{x}$	$\bar{y}$	$-z$	+0.03	33	$x+1$	$0.5-y$	$z+0.5$	−18.64
15	$\bar{x}$	$\bar{y}$	$\bar{z}$	+0.03	34	$x+1$	$1.5-y$	$x+0.5$	−0.86
16	$\bar{x}$	$2-y$	$-z$	+0.03	35	$x+1$	$2.5-y$	$z+0.5$	−0.02
17	$\bar{x}$	$2-y$	$\bar{z}$	+0.03	36	$x+2$	$0.5-y$	$z+0.5$	+0.32
18	$-x$	$y-0.5$	$0.5-z$	+0.11	37	$x+2$	$1.5-y$	$z+0.5$	−0.17
19	$2-x$	$y+1.5$	$0.5-z$	+0.11					

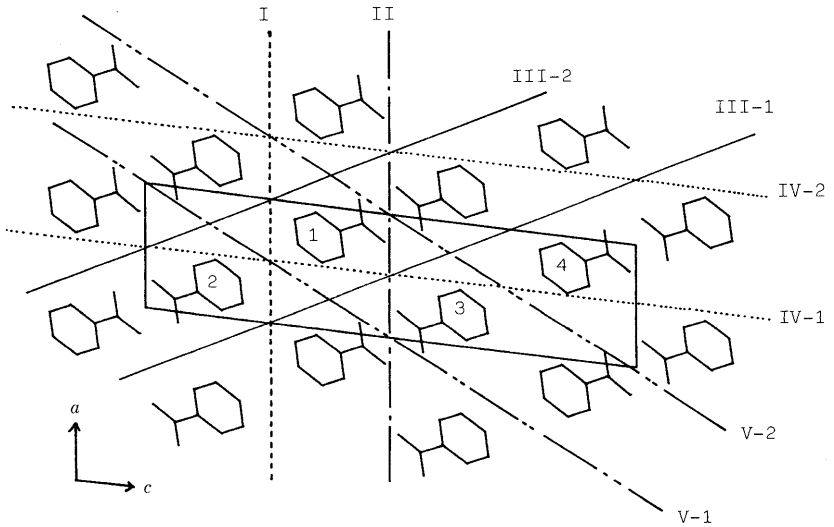

Fig. 3. Crystal Structure of Benzoic Acid Projected along [010] and Five Planes (I—V) Offering the Possibility of Cleavage of Benzoic Acid
Fractional coordinates: (1) $\bar{x}$, $y+0.5$, $0.5-z$; (2) x, y, z; (3) x, $0.5-y$, $0.5+z$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

interaction energies in planes I to V-2. Table VI shows the indices of crystal planes corresponding to the planes I—V, as well as the correction factors and the interaction energies in the definite area (kcal/(mol·100 Å^2)) in planes I—V, respectively. Because the interaction energies in planes I, III and IV were smaller than those in planes II and V, planes I, III and IV were considered to be cleave easily. All intermolecular interaction energies across plane I were less than −0.19 kcal/mol, while the largest intermolecular interaction energies, across plane III and across plane IV, were −0.47 kcal/mol, (molecules 1 and 22) and (molecules 1 and 23), respectively. These results may indicate that although the interaction energies in the definite area in planes III and IV were relatively small, cleavage was not easy along these planes. Furthermore, since the molecular density on the plane IV is low (Fig. 3), the stability of the plane IV is considered to be poor. Thus, cleavage along plane IV would not occur. For plane III, it might be necessary to take into account the contribution of electrostatic, exchange repulsion, charge transfer interaction energies and so on, to the total intermolecular interaction energy.

Table V. Benzoic Acid Numbers Used to Calculate the Interaction Energy in Planes I to V-2

Plane	Benzoic acid number
I	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16
II	15, 17, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37
III-1	2, 3, 15, 17, 18, 20, 22, 24, 28, 29, 30, 31
III-2	8, 9, 10, 11, 12, 13, 14, 16, 19, 21, 23, 25, 36, 37
IV-1	2, 3, 4, 5, 6, 7, 18, 20, 22, 24, 28, 29, 30, 31
IV-2	12, 13, 19, 21, 23, 25, 36, 37
V-1	2, 3, 4, 5, 6, 7, 14, 16, 18, 20, 22, 24, 28
V-2	12, 13, 15, 17, 19, 21, 23, 25, 32, 33, 34, 35, 36, 37

Table VI. Indices of Crystal Plane,[a] Correction Factor (*Cf*) and Interaction Energies (kcal/(mol·100 Å^2)) in the Five Planes Offering the Possibility of Cleavage of Benzoic Acid Crystals

Plane	Indices of crystal plane	Correction factor (*Cf*)	Interaction energy
I	(002)	*ab*	−2.25
II	(002)	*ab*	−70.80
III	(10$\bar{2}$)	*bd*	−1.04
IV	(100)	*bc*	−0.92
V	(102)	*be*	−17.08

a) One of the indices of the crystal plane corresponding to planes I—V in a set of symmetrically equivalent crystal planes. *a*, *b* and *c* represent the lattice constants of benzoic acid crystal. *d* and *e* are the longer diagonal line of the parallelogram constructed by (*a* and $-c/2$) and (*a* and $c/2$), respectively.

Table VII. Fractional Coordinates of the 34 Nicotinic Acid Molecules and Interaction Energies (kcal/mol) between the 1st Molecule and Each of the Remaining 33 Molecules Calculated by Using the CNDO/2 Method

Molecule no.	Fractional coordinates			*ΔE*	Molecule no.	Fractional coordinates			*ΔE*
1	x	$0.5-y$	$z+0.5$		18	$-1-x$	$y-0.5$	$0.5-z$	−0.05
2	x	y	z	−0.41	19	$-1-x$	$y+0.5$	$0.5-z$	+0.02
3	$x-1$	y	$z+1$	−0.41	20	$-x$	$y-0.5$	$0.5-z$	−0.85
4	$x+1$	y	$z+1$	−0.11	21	$-x$	$y-0.5$	$1.5-z$	−0.11
5	$x-1$	y	z	−0.11	22	$-x$	$y+0.5$	$0.5-z$	−0.19
6	$x+1$	y	z	+0.01	23	$-x$	$y+0.5$	$1.5-z$	+0.02
7	$x-1$	y	$z+1$	+0.01	24	$\bar{x}$	$y-0.5$	$0.5-z$	−0.18
8	x	$y-1$	z	+0.11	25	$\bar{x}$	$y-0.5$	$1.5-z$	−0.13
9	x	$y-1$	$z+1$	+0.11	26	$\bar{x}$	$y+0.5$	$0.5-z$	0.00
10	$-x$	$-y$	$-z$	−0.03	27	$\bar{x}$	$y+0.5$	$1.5-z$	+0.02
11	$-x$	$\bar{y}$	$-z$	−0.03	28	$2-x$	$y-0.5$	$1.5-z$	0.00
12	$-x$	$-y$	$\bar{z}$	−0.45	29	x	$1.5-y$	$z+0.5$	−0.01
13	$-x$	$\bar{y}$	$\bar{z}$	−0.45	30	x	$-0.5-y$	$z+0.5$	−0.01
14	$\bar{x}$	$-y$	$\bar{z}$	−9.07	31	$x+1$	$0.5-y$	$z+0.5$	−0.13
15	$\bar{x}$	$\bar{y}$	$\bar{z}$	−9.07	32	$x-1$	$0.5-y$	$z+0.5$	−0.13
16	$2-x$	$-y$	$\bar{z}$	−0.01	33	$x+1$	$0.5-y$	$z+1.5$	+0.02
17	$2-x$	$\bar{y}$	$\bar{z}$	−0.01	34	$x-1$	$0.5-y$	$z-0.5$	+0.02

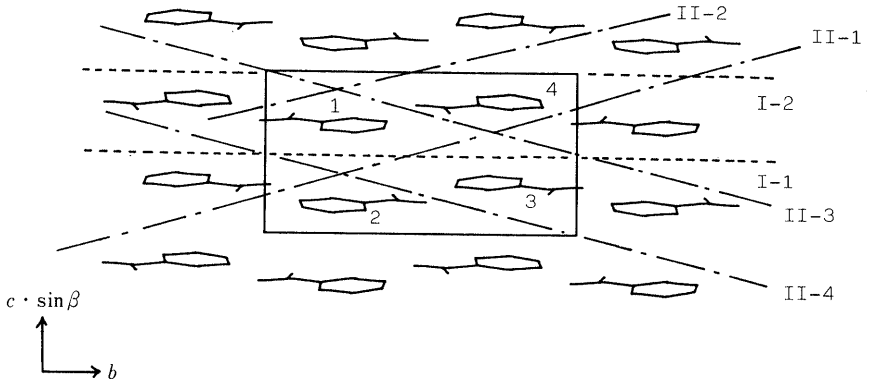

Fig. 4. Crystal Structure of Nicotinic Acid Projected along [100] and Two Planes (I, II) Offering the Possibility of Cleavage of Nicotinic Acid

Fractional coordinates: (1) x, $0.5-y$, $0.5+z$; (2) x, y, z; (3) $\bar{x}$, $y+0.5$, $0.5-z$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

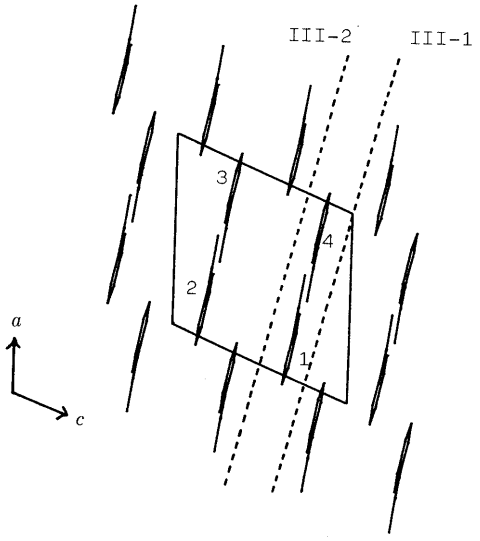

Fig. 5. Crystal Structure of Nicotinic Acid Projected along [010] and One Plane (III) Offering the Possibility of Cleavage of Nicotinic Acid

Fractional coordinates: (1) x, $0.5-y$, $0.5+z$; (2) x, y, z; (3) $\bar{x}$, $y+0.5$, $0.5-z$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

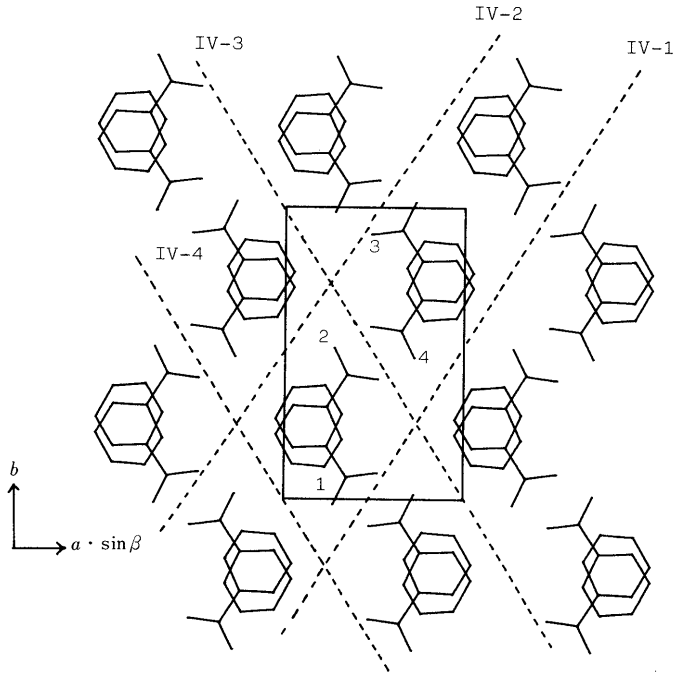

Fig. 6. Crystal Structure of Nicotinic Acid Projected along [001] and One Plane (IV) Offering the Possibility of Cleavage of Nicotinic Acid

Fractional coordinates: (1) x, $0.5-y$, $0.5+z$; (2) x, y, z; (3) $\bar{x}$, $y+0.5$, $0.5-z$; (4) $\bar{x}$, $\bar{y}$, $\bar{z}$.

It was found that the 002 plane of benzoic acid was the preferred orientation plane.[1b] The preferred orientation of benzoic acid crystallites was considered to occur primarily by cleavage along the (002) planes (plane I) during compression.

Nicotinic Acid Crystals of nicotinic acid are monoclinic with $a=7.16$ Å, $b=11.70$ Å, $c=7.24$ Å and $\beta=104.2°$, and with space group $P2_1/c$.[9] Four molecules are contained in a unit cell. Table VII shows the fractional coordinates of 34 nicotinic acid molecules, and the interaction energies (kcal/mol) between the 1st molecule and each of the other molecules. The 1st molecule forms an O–H···N hydrogen bond with the 14th and 15th molecules, and the intermolecular interaction energy between hydrogen bonded molecules was -9.07 kcal/mol. Figures 4—6 show the crystal structure of nicotinic acid projected on planes (100), (010) and (001), respectively. There are four planes (planes I—IV) on which cleavage is possible in the crystal.

Since the numbers of "interaction types" in planes I—IV are two, four, two and four, respectively, the interaction energies in the these planes were evaluated as the mean value of the interaction energies of (I-1 and I-2), (II-1, II-2, II-3 and II-4), (III-1 and III-2), (IV-1, IV-2, IV-3 and IV-4), respectively. Table VIII shows the molecular numbers used to calculate the interaction energies in planes I-1 to IV-4. Table IX shows the indices of the crystal plane corresponding to planes I—IV, as well as the correction factor and the interaction energies in the definite area (kcal/(mol·100 Å^2)) in planes I—IV, respectively. The interaction energy in plane I, corresponding to the (002) plane, was the smallest in planes I—IV.

It was found that the (002) plane of nicotinic acid was the preferred orientation plane.[1b] The preferred orientation of nicotinic acid crystallites was considered to occur by cleavage along the (002) planes (plane I) during compression.

In conclusion, the preferred orientation planes of some organic crystals were found to agree with the plane having only small interaction energy in the crystal lattice as determined by quantum chemical calculations. The preferred orientation during compression was considered to occur by the cleavage of crystals along those planes with small interaction energy.

TABLE VIII. Nicotinic Acid Numbers Used to Calculate the Interaction Energy in Planes I-1 to IV-4

Plane	Nicotinic acid number
I-1	2, 5, 6, 8, 10, 11, 18, 19, 20,22, 24, 26, 34
I-2	3, 4, 7, 9, 21, 23, 25, 26, 28, 33
II-1	2, 5, 6, 10, 11, 19, 23, 26, 29, 34
II-2	3, 4, 7, 9, 12, 14, 16, 21, 23, 25, 27, 28, 30, 33
II-3	3, 4, 7, 13, 15, 17, 21, 23, 25, 27, 28, 29, 33
II-4	2, 5, 6, 8, 10, 11, 18, 20, 24, 30, 34
III-1	3, 4, 7, 9, 12, 13, 21, 23, 25, 27, 28, 32, 33
III-2	2, 5, 6, 8, 10, 11, 16, 17, 18, 19, 20, 22, 24, 26, 31, 34
IV-1	4, 6, 8, 9, 14, 16, 17, 24, 25, 28, 31, 33
IV-2	5, 7, 11, 13, 19, 22, 23, 29, 30
IV-3	4, 6, 15, 26, 27, 28, 29, 31, 33
IV-4	3, 5, 7, 8, 9, 10, 12, 18, 19, 20, 21, 30, 32, 34

TABLE IX. Indices of Crystal Plane,[a] Correction Factor (Cf) and Interaction Energies (kcal/(mol·100 Å^2)) in the Four Planes Offering the Possibility of Cleavage of Nicotinic Acid Crystals

Plane	Indices of crystal plane	Correction factor (Cf)	Interaction energy
I	(002)	ab	−1.37
II	(012)	ad	−5.74
III	(10$\bar{4}$)	ce	−2.43
IV	(110)	cf	−5.36

a) One of the indices of the crystal plane corresponding to planes I—IV in a set of symmetrically equivalent crystal planes. a, b and c represent the lattice constants of nicotinic acid crystal. d, e and f are the longer diagonal line of the parallelogram constructed by (b and $c/2$), (a and $-c/4$) and (a and b), respectively.

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