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OD CHARACTER AND POLYTYPIC FEATURES OF THE STRUCTURE OF THE MOLECULAR CRYSTAL (1R,3S)-DIMETHYL 2-OXOCYCLOHEXANE-1,3-DICARBOXYLATE

Abstract - *OD* character and polytypic features of the structure of the molecular crystal (1R,3S)-dimethyl 2-oxocyclohexane-1,3-dicarboxylate. The crystals of the molecular structure of (1R,3S)-dimethyl 2-oxocyclohexane-1,3-dicarboxylate (*meso*-dicarboxylate) display OD character. They are built up by sequences of equivalent layers, which may follow each other in two different ways, pairs of adjacent layers being geometrically equivalent. Disordered or ordered (polytypes) sequences result. Through the application of the OD procedures the common symmetry properties of the various sequences (OD groupoid family) are found. Moreover the symmetry and metrics of the two main polytypes (MDO structures) and the peculiar features of the complex diffraction pattern are derived.

Key words - *meso*-dicarboxylate, OD structures, polytypism, MDO structures, family structure, diffraction pattern

Riassunto - *Carattere OD e aspetti politipici della struttura del cristallo molecolare (1R,3S)-dimetil 2-oxocicloesano-1,3-dicarbossilato.* I cristalli del composto molecolare (1R,3S)-dimethyl 2-oxocyclohexane-1,3-dicarboxylate (*meso*-dicarboxylate) dispiegano carattere OD. Infatti essi sono costituiti da sequenze di strati equivalenti, che possono susseguirsi l'un l'altro secondo due distinte modalità, coppie di strati adiacenti risultando, comunque, sempre geometricamente equivalenti. Attraverso l'applicazione delle procedure OD, si ricavano le proprietà di simmetria comuni alle diverse sequenze (OD groupoid family). Inoltre si ottengono simmetria e metrica dei due politipi principali (strutture MDO) e si calcolano gli aspetti peculiari del complesso diffrattogramma.

Parole chiave - *meso*-dicarboxylate, strutture OD, politipismo, strutture MDO, struttura di famiglia, diffrattogramma complesso

OD CHARACTER OF THE CRYSTALS OF *MESO*-DICARBOXYLATE

The paper on 'Allotwinning in a molecular crystal: (1R,3S)-dimethyl 2-oxocyclohexane-1,3-dicarboxylate' by Jahangiri *et al.* (2013) presents a lot of evidences that point to the OD character of the studied compound (*meso*-dicarboxylate): presence of rows of diffuse spots (Fig. 3 in the paper), non-space-group absences, presence of two polytypes, twinning.

In fact the two structures described in the paper by Jahangiri *et al.* (2013) are members of an OD family

built up by equivalent layers, more precisely they are the two MDO (Maximum Degree of Order) structures in that family.

The single layer is characterized by layer group symmetry $P m c 2_1$, with translation vectors **b**, **c**, third basic vector (not a translation vector) \mathbf{a}_0 (b = 4.7233, c = 11.6835, $a_0 = 9.4721$ Å).

Layers with symmetry $P(m)c2_1$ (the parenthesis denotes the direction of missing periodicity) follow each other (Fig. 1) related by the set of σ -operations (σ -operations are those relating adjacent layers; λ -operations are the symmetry operations of the single layer) listed in the second row of the symbol (OD groupoid family symbol):

$$\begin{array}{cccc}
P & (m) & c & 2_1 \\
\{ (n_{1,-1/2}) & n_{1/2,2} & 2_{1/2} \} \\
\end{array} \tag{1}$$

It may be useful to recall that the symbols of the partial operations (POs) are in keeping with the symbols used for normal space group operations. Therefore $2_{1/2}$ in the third position in (1) is the symbol for a twofold rotation with translational component c/4. As regards the glides, the most general glide operation is denoted $n_{r,s}$; the order of the indices is chosen so that the directions to which *n* and the two indices refer follow in a cyclic way; the indices are only of interest *modulo* 2; thus an index *r* may be replaced by r + 2 or r - 2 and the same occurs for *s*. Consequently $n_{1/2,2}$ in the second position is the symbol for a glide normal to **b**, with translational component $c/4+a_0$ and $n_{1,1/2}$ in the first position is the symbol for a glide normal to a_0 , with translational component **b**/2 - **c**/4.

Subsequent layers along the direction normal to the **b**,**c** layer follow each other related by the glide normal to \mathbf{a}_0 with translational component either $\mathbf{b}/2 - \mathbf{c}/4$, or $\mathbf{b}/2 + \mathbf{c}/4$. Pairs of glides obtained in both ways are geometrically (and therefore energetically) equivalent (*principle of OD structures*). The ordered or disordered succession of the two operations give rise to infinite polytypes (ordered sequences) or disordered arrangements, respectively.

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Fig. 1 - Two adjacent layers in the OD family of *meso*-dicarboxylate (carbon atoms in blue, oxygen atoms in red; hydrogen atoms are not indicated). The λ operations are drawn with black colour, whereas the σ operations are drawn with red colour. The pair of layers, related by the glide operation $n_{1,-1/2}$ normal to \mathbf{a}_0 , is represented down **b**, with **c** vertical.

Particularly interesting (and stable) are those structures in which not only pairs of layers, wherever taken, are geometrically equivalent (*principle of OD structures*), but also triples of layers are geometrically equivalent (*principle of MDO structures*) (Dornberger-Schiff, 1964). Those structures correspond to regular sequences of operations.

Two such structures may be formed in the present family:

MDO1, characterized by the sequence of glides normal to a_0 : $/n_{1,-1/2}/n_{1,-1/2}/n_{1,-1/2}/\dots$ [the sequence $n_{1,1/2}/n_{1,1/2}/n_{1,1/2}/n_{1,1/2}/\dots$ gives rise to the same structure (MDO1), twin related with MDO1, twin plane (100)].

MDO2, characterized by the sequence of glides normal to a_0 : $/n_{1,-1/2}/n_{1,-1/2}/n_{1,-1/2}/n_{1,-1/2}/\dots$

Symmetry and metrics of the two MDO structures

MDO1. The application of two successive operations $n_{1,-1/2}$ gives rise to a *C* centred unit cell, with translation $\mathbf{a} = 2\mathbf{a_0} - \mathbf{c}/2$ (a = 19.82 Å; $\beta = 107.1^\circ$). All the layers present a *c* glide, which is a total operation of the

whole structure, which thus presents *C*1*c*1 symmetry. The other operators (*m* normal to \mathbf{a}_0 and $\mathbf{2}_1$ parallel to **c**) are lost.

MDO2. The alternate application of $n_{1,1/2}$ and $n_{1,1/2}$ gives rise to a primitive unit cell with $\mathbf{a} = 2\mathbf{a}_0$. In this structure not only the *c* glide, but also *m* normal to \mathbf{a}_0 and 2_1 parallel to **c** are valid for the whole structure, which thus has space group symmetry $Pmc2_1$.

The relation between the two MDO structures, and more generally among the various possible polytypes in the family, may be easily appreciated by observing that layers related by the operators $n_{1,1/2}$ and $n_{1,1/2}$ are translationally equivalent and related by stacking vectors $\mathbf{t_1} = \mathbf{a_0} + \mathbf{b}/2 - \mathbf{c}/4$ and $\mathbf{t_2} = \mathbf{a_0} + \mathbf{b}/2 + \mathbf{c}/4$, respectively. In the orthorhombic polytype the two stacking vectors regularly alternate, whereas in the monoclinic polytype the $\mathbf{t_1}$ vector is constantly applied (the constant application of the vector $\mathbf{t_2}$ gives rise to the twin structure), The discussion of the diffraction effects in the whole family (Appendix) is made easier by the translational equivalence of the layers.

Symmetry and metrics of the family structure

All the disordered or ordered structures in a family display diffraction patterns with common reflections, which present the same positions and intensities in all the structures of the family and are always sharp; they are denoted as *family reflections* and define the *family structure*.

In the present case the family reflections correspond to those indicated by the authors as 'the most prominent reflections... indexed by an orthorhombic cell *Imm2*, a = 18.9441, b = 4.7233, c = 5.8418 Å'.

As a matter of fact, the symmetry of the family structure may be derived from the symmetry operations (λ and σ) of the OD family, taking into account the metrical relationships between corresponding vectors in the family structure and in the single layer. These relationships are here indicated, if **A**, **B**, **C** are the vectors of the family structure:

$$\mathbf{A} = 2\mathbf{a}_0$$
$$\mathbf{B} = \mathbf{b}$$
$$\mathbf{C} = \mathbf{c}/2$$

Consequently the symmetry operations of the family structure may be derived from the λ and σ operations of the layer, multiplying by 2 the indices that in (1) refer to the direction **c** and dividing by 2 those referring to the direction **a**:

$$\begin{array}{cccc} (m) & n_{1,0} & 2_1 \\ (n_{1,-1/2}) & n_{1/2,2} & 2_{1/2} \end{array}$$
(2a)

By applying the indicated changes, we obtain

which may be definitely written as:

 $\begin{array}{cccc} m & m & 2 \\ n & n & 2_1 \end{array} (2c)$

These are the operations of the space group *Imm*2, confirming the findings of Jahangiri *et al.* (2013).

DIRECT DERIVATION OF THE OD GROUPOID FAMILY

The careful study carried on by Jahangiri *et al.* (2013) presents all the necessary elements for an *a-priori* derivation of the OD groupoid family of the studied crystal, and subsequently to obtain metrics and symmetry of the MDO structures which are simultaneously present in it.

The direction of missing periodicity is clearly indicated, on the basis of an examination of Fig. 3 in the paper by Jahangiri *et al.* (2013), as \mathbf{a}^* , in the orientation assumed by the authors.

Moreover the authors have found the orthorhombic cell defined by the 'most prominent reflections', corresponding to those with l = 2n, reflections which are always sharp, at difference from those corresponding to values of l = 2n+1. The first ones define the cell of the 'family structure', using the OD terminology, with space group symmetry *Imm2*, with A = 18.9441, B = 4.7233, C = 5.8418 Å.

The single structural layer displays translation vectors $\mathbf{b} = \mathbf{B}$, $\mathbf{c} = 2\mathbf{C}$ (based on the preceding considerations, which indicated that the 'family structure' corresponds to the reflections with l = 2n), and $\mathbf{a}_0 = \mathbf{A}/2$ as third basis vector (not a translation vector). The OD theory consents to derive the number p of layers per basic translation of the family structure in the direction corresponding to the missing periodicity (translation \mathbf{A} in the present case); details are given in Dornberger-Schiff and Fichtner 1972) and in Ferraris *et al.* (2008).

A careful examination of the whole diffraction pattern, including both the sharp 'family reflections' and the diffuse 'superstructure' reflections, reveals that reflections h0l are present only for even l values. This rule, valid for the general reflections and not limited to the family reflections, can only be due to symmetry elements of the single layer (λ -operations). It is the only registered absence (apart, obviously, from that registered for the 00l reflections which are present only for l = 2n) and points to a symmetry of the single layer of the type:

 $P - c 2_1$

Looking at the symmetry operations of the family structure (2c) we may conclude that the layer group symmetry of the single layer is:

 $P(m) c 2_1$

It seems now proper to recall that one of the most important results of the OD theory was the systematic derivation of the sets of σ -operations compatible with the symmetry of each layer group (group of λ -operations). The λ -POs and the corresponding σ -POs build up the OD groupoid family of the OD compound under study.

The availability of a complete Table of those families, which includes 400 hundred members, is extremely useful in describing and discussing OD structures, to derive the MDO structures, to sketch the corresponding diffraction patterns and to decipher the generally complex patterns of OD crystals. Moreover they sometimes provide – when supported by proper crystal chemical reasoning – a formidable help in guessing reliable structural arrangements.

A first derivation of OD-groupoid families has been carried on by Dornberger-Schiff (1964). Subsequently a new procedure for listing all the OD-groupoid families has been presented (Dornberger-Schiff and Fichtner, 1972; Fichtner, 1977). A list of the monoclinic and orthorhombic OD families is presented also in the book by Ferraris *et al.* (2004). As in the quoted papers the direction of missing periodicity is assumed as the **c** direction, it is necessary – in the present case – to exchange the **a** and **c** directions, passing from the layer group $P(m)c2_1$ to the layer symmetry $P2_1a(m)$, for which the following OD groupoid symbols are given (Dornberger-Schiff and Fichtner, 1972):

$$P 2_{1} a (m) P 2_{1} a (m) \{2_{r,1} n_{2,r-1} (n_{r,s})\} \{n_{s,2} 2_{s} (2_{2})\}$$
(3)

The choice is easy: in fact the symmetry operations of the family structure point to the presence of twofold axes 2 and 2_1 in the **c** direction, which becomes **a** direction in the new orientation, thus immediately excluding the second OD groupoid family in (3).

It is now possible to derive also the values of the parameters r and s. To this aim both the λ and σ operators in the first symbol in (3) are considered and the translational component of any glide and screw are modified in agreement with the passing from the dimensions of the single layer to those of the 'family structure'. Thus we have to double the translational components which refer to the **a** axis and divide by 2

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those referring to the axis **c**. Then assuming $r = \frac{1}{2}$, s = 1, the operators reproduce those found in the 'family structure':

$$2_2 n_{0,2} m$$
 $2 m m$ $2 m m$

$$2_{2r} n_{1,2r} n_{2r,s} \qquad 2_1 n_{1,1} n_{1,1} \qquad 2_1 n n$$

By substituting the obtained values of r and s in the first symbol of (3) we definitely obtain the correct OD groupoid family symbol:

$$\begin{array}{cccc} P & 2_1 & a & (m) \\ \{2_{-1/2} & n_{2,-1/2} & (n_{1/2,1})\} \end{array}$$

The symbol, after transformation by exchange of **a** and **c**, becomes:

$$\begin{array}{ccc} P & (m) & c & 2_1 \\ & & \{(n_{1,1/2}) & n_{-1/2,2} & 2_{-1/2}\} \end{array}$$

and, by inverting the **c** direction, we obtain the symbol: P(m) = c - 2

$$\begin{array}{ccc} (m) & c & 2_1 \\ \\ \{(n_{1,-1/2}) & n_{1/2,2} & 2_{1/2}\} \end{array}$$

which is just the symbol (1) we have derived by looking at the crystal structure of the compound. Once the OD groupoid family has been obtained we may discuss the order-disorder character of the family, derive the MDO structures, namely those characterized by regular sequences of operations, obtaining their metrics and symmetries.

CONCLUSIONS

In the first part of this paper we have shown how the OD approach consents a clear presentation of the structural features of the studied compound, and a deep understanding of the relationships between the two main polytypes, as well as of the complex diffraction pattern. We have indicated the common symmetry properties of the disordered and ordered sequences (polytypes) of the building layer, properties summarized in the OD groupoid family symbol.

Moreover, in the final part we have shown how the OD groupoid family could be derived without knowledge of the crystal structure, but just through a careful observation of the diffraction features of the crystal and taking advantage of the tools and procedures which OD theory has developed.

Once more, this example shows how the theory favours a deep insight into the various related phenomena of one dimensional disorder, twinning, allotwinning, polytypism, and how it presents a comprehensive interpretation of the diverse anomalous features frequently displayed by the diffraction patterns of OD crystals.

Appendix. Diffraction effects in the crystals of meso-dicarboxylate

The Fourier transform of the whole structure may be derived summing up the contributions of the single layers

$$\mathbf{F}(\mathbf{r}^*) = \boldsymbol{\Sigma}_{\mathbf{p}} \, \mathbf{F}_{\mathbf{p}}(\mathbf{r}^*)$$

The Fourier transform can be different from zero only in points ηkl (indices referred to the orthorhombic cell with $\mathbf{a}_{ort} = 2\mathbf{a}_0$, $\mathbf{b}_{ort} = \mathbf{b}$, $\mathbf{c}_{ort} = \mathbf{c}$, where \mathbf{a}_0 , \mathbf{b} , \mathbf{c} are the basis vectors of the single layer) of the reciprocal lattice. The sequence of layers may be periodic or aperiodic; consequently the Fourier transform may be different from zero for discrete values of η or for any value η , respectively, and we shall observe either diffraction patterns with only sharp spots, or diffraction patterns with diffuse streaks; moreover, as a disordered structure may contain ordered domains, we may also observe sharp maxima placed on diffuse streaks. For a correct interpretation of the diffraction patterns of an OD structure a fundamental role is played by those reflections which are independent from the kind of sequence and are indicated as 'family reflections'. In the studied compound all the layers are translationally equivalent; the translation which connects adjacent layer is

$$\mathbf{t}_{q} = \mathbf{a}/2 + \mathbf{b}/2 + (\beta_{q}/4)\mathbf{c}$$
 with $\beta_{q} = \pm 1$

The position of the layer $\rm L_p$ relative to $\rm L_0$ may be calculated as it follows

$$L_p = L_{p-1} + [1/2, 1/2, \beta_q/4] = L_0 + [p/2, p/2, (\Sigma_q \beta_q)/4]$$

The sum $\Sigma_q \beta_q$ is even or odd according to whether *p* is even or odd; therefore it may be substituted with

$$\Sigma_{\rm q} \beta_{\rm q} = 2m_{\rm p} + p \qquad (A.1)$$

with $m_{\rm p}$ integers depending on the the kind of succession.

$$L_p = L_0 + [p/2, p/2, m_p/2 + p/4]$$

Therefore the Fourier transform of the layer L_p is related to that of L_0 by the relation

$$F_{p}(\eta kl) = F_{0}(\eta kl) \exp \left\{2\pi i [\eta p/2 + kp/2 + lm_{p}/2 + lp/4]\right\}$$

and the Fourier transform of the structure is

$$F(\eta kl) = \sum_{p} F_{p}(\eta kl) = S(\eta kl) F_{0}(\eta kl) \quad (A.2)$$

with

$$S(\eta kl) = \sum_{p} \exp \{2\pi i [\eta/2 + k/2 + l/4]p + lm_p/2\} (A.3)$$

For l = 2L the expression $S(\eta kl)$ simply becomes

$$S(\eta kl) = \sum_{n} \exp \left\{ 2\pi i \left[(\eta + k + L)/2 \right] p \right\}$$

With a large number of layers this expression vanishes except for integral values b of η for which

$$b + k + \mathbf{L} = 2n \qquad (A.4)$$

Therefore any polytype or disordered sequence of the family under study will present, as a common feature, sharp reflections for even l values and those reflections will fulfil rule (A.4), outlining the cell of the family structure, with parameters a = 18.9441, b = 4.7233, c = 5.8418 Å and I centring.

The diffraction patterns of the various polytypes (patterns which differ only in the reflections with l = 2n + 1) will be obtained from the expression (A.2) and (A.3), on the basis of the actual sequence of layers.

For the polytype MDO2 the layers follow each other with alternation of $\beta_q = +1$ and $\beta_q = -1$. Therefore, after a sequence of an even number of layers, $\Sigma_q \beta_q = 0$, which requires $2m_p = -p$ in (A.1). Substituting $m_p = -p/2$ in (A.3) we obtain:

$$S(\eta kl) = \sum_{n} \exp \{2\pi i [\eta/2 + k/2] p\}$$

With a large number p (= 2n) of layers this expression vanishes except for integral values h of η .

For the polytype MDO1 the layers regularly follow each other with $\beta_q = -1$. With a sequence of *p* layers $\Sigma_q \beta_q = -p$, which requires $m_p = -p$ in (A.1). The expression (A.3) is now:

$$S(\eta kl) = \sum_{n} \exp \{2\pi i [\eta/2 + k/2 - l/4]p\}$$

With a large number p of layers it vanishes except for half integer values b' of η , for which

$$2b' + 2k - l = 4n$$

Therefore for l = 4n + 1, we shall have reflections at half integer values b' of η subject to the condition: 2b'+2k = 4m + 1; for l = 4n + 3 we shall have reflections at half integer values b' of η subject to the condition: 2b'+ 2k = 4m - 1.

Half integer values of h occur because the reference cell is the orthorhombic one. Actually the distribution

of reflections just indicated outlines a monoclinic cell with $\mathbf{a}_{mon} = \mathbf{a}_{ort} - \mathbf{c}_{ort}/2$, $\mathbf{b}_{mon} = \mathbf{b}_{ort}$, $\mathbf{c}_{mon} = \mathbf{c}_{ort}$ and *C* centring.

It is easy to show that when the layers follow each other with $\beta_q = +1$ the distribution of reflections correspond to the twin structure, polytype MDO1'.

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