(c) La première couche glisse de $+\frac{1}{4}a$, la deuxième reste immobile, la troisième glisse de $+\frac{1}{4}a$, la quatrième couche reste immobile, etc. (Fig. 12c).

Il y a rupture d'un des sommets d'octaèdre toutes les deux couches. Celle solution demande les plus petits glissements, au maximum $\frac{1}{4}$ de a. La morphologie reste monoclinique, avec perturbation de la surface de (100).

(2) *Glissement de $\frac{1}{4}a$ dans le sens négatif de l'axe* [100]

Il y a dans ce cas, rupture d'un sommet pour tous les octaèdres. Il nous paraît peu vraisemblable. Il y a, comme précédemment deux possibilités:

(a) La cinquième couche garde sa position initiale, le maximum de déplacement étant de $\frac{3}{4}a$, avec conservation de la morphologie monoclinique, et perturbation à la surface de (100) (Fig. 13a).

(b) La cinquième couche se déplace de a, les mouvements atomiques deviennent de plus en plus grands, la morphologie devient cubique la face (100) devient une face (1$\bar{1}$0) cubique avec une perturbation à la surface (Fig. 13b).

Ce qui nous permettrait de déterminer le mode de glissement, parmi les différentes possibilités, serait l'étude de la morphologie et des perturbations de la surface. Cela n'est malheureusement pas possible, vu le mode d'obtention de ces cristaux.

Conclusion

La propriété remarquable de cette transition est de se faire sans destruction de la structure. Les ions Na^+ et ClO_3^- gardent leur même environnement octaédrique, avec le même mode d'empilement, bien qu'au niveau des atomes Na et O, il y ait un changement de coordinence. Le mouvement de glissement par couche, rappelant celui des transitions martensitiques, peut être envisagé de différentes façons. Bien que nous n'ayons aucun critère expérimental permettant le choix entre les différents processus décrits, le mode 1(b) nous paraît le plus vraissemblable. Dans ce cas, les atomes conservent leur environnement, mais les déplacements deviennent de plus en plus grands au fur et à mesure que la transition se propage dans le cristal. Il ne paraît pas impossible que le processus puisse différer d'un échantillon à l'autre, de nombreux facteurs pouvant intervenir, tels que la taille de l'échantillon, les contraintes, l'adhérence à une surface.

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Analysis of Orientationally Disordered Structures.
III. Positive Definiteness of Orientational Distribution Functions

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Abstract

In previous publications [Press & Hüller (1973). Acta Cryst. A29, 252–256; Press (1973). Acta Cryst. A29, 257–263], the analysis of molecular crystalline structures by symmetry-adapted surface harmonics has been discussed. Implications of both molecular and site symmetry have been emphasized. Here the question is raised whether the magnitude of symmetry-allowed expansion coefficients is subject to constraints or not. Obvious restrictions result from the requirement that the density distribution at a molecular site has to be positive definite. Even stronger conditions are imposed by the requirement that the orientational distribution function $g(\tau)$ has to be positive definite, too. The area in parameter space for parameter values which are in agreement with the strong conditions is shown. Physically meaningful expansion coefficients are guaranteed by starting from a symmetry-allowed rotational potential $V(\tau)$.

I. Orientational probability distribution

The structure analysis of crystals containing small rigid molecules or polyatomic ions is simplified considerably by the use of symmetry-adapted surface harmonics (Lage & Bethe, 1947). The probability density function of finding the scattering centres (electrons in the case of X-rays, or nuclei in the case of neutrons) on concentric

spheres around the molecular centre is expanded into a series of symmetry-adapted surface harmonics (Kurki-Suonio, 1967; Seymour & Pryor, 1973; Press & Hüller, 1973). The rotational structure factor $F_{rot}(Q)$ of a molecule then is obtained in terms of the same set of harmonics, with the polar angles θ_Q and φ_Q of the momentum transfer Q as arguments. The method has recently been applied to NH_3 molecules (Eckert & Press, 1979) rotating with one orientational degree of freedom around the axis of their dipole moment, to the linear molecules H_2 (Press, 1973), N_2 (Press & Hüller, 1978), OH^- (Bleif, 1978; Bleif & Dachs, 1979) and to the tetrahedral molecules CD_4, NH_4^+ (Press, 1973), CBr_4 (More, Lefèbvre & Fouret, 1977; Dolling, Powell & Sears, 1979), and $C_{10}H_{16}$ (adamantane) (Amoureux & Bée, 1979), and to the octahedral molecules MoF_6 (Levy, Sanger, Taylor & Wilson, 1974) and SF_6 (Dolling, Powell & Sears, 1979).

Both the site symmetry and the molecular symmetry impose conditions on the expansion coefficients of the probability density. To exhibit these conditions the probability density has been expanded in two coordinate systems (Press & Hüller, 1973). The first one is fixed in the molecule – it rotates with the molecule, the second one is fixed in the crystal. The transformation properties of the symmetry-adapted surface harmonics from one coordinate system to the other determine which expansion coefficients vanish. A very detailed analysis of the rôle of symmetry in a surface harmonics expansion is found in the paper by Yvinec & Pick (1979). These authors also consider improper rotations which had not been taken into account previously. In the context of orientational structures improper rotations do not lead to new evidence, however.

In the following we will discuss the restrictions which are imposed on the expansion coefficients by the condition that a physically acceptable probability density must be positive everywhere. The investigation will go beyond the usual postulate of a positive-definite distribution (More, Lefèbvre & Fouret, 1977; Dolling, Powell & Sears, 1979) of scattering centres by demanding a positive-definite distribution function for the molecular orientations. This is a very general condition which has to be fulfilled for neutron and X-ray scattering, for any shape of molecule, and for any site symmetry. For clarity, the discussion will, however, be restricted to: (i) the case of neutron scattering where the scattering centres may be represented by δ functions at the positions of the scattering nuclei; (ii) a single shell of nuclei with radius ρ (= distance of the atoms from the centre of mass of the molecule) and (iii) tetrahedral or octahedral molecules at a lattice site with cubic symmetry.

The probability density $a(r)$ of scattering centres weighted with the scattering length (the scattering-length density) then can be separated as follows:

$$a(r) = a(\theta,\varphi)\delta(r - \rho)/r^2. \tag{1.1}$$

The appropriate set of surface harmonics for expanding the angular part of the probability density are the cubic harmonics (Lage & Bethe, 1947) $K_{lm}(\theta,\varphi)$. The expansion reads

$$a(\theta,\varphi) = \sum_{lm} c_{lm} K_{lm}(\theta,\varphi). \tag{1.2}$$

The coefficients c_{lm} are directly obtained from a diffraction experiment. It has been pointed out in § III of Press & Hüller (1973) that $a(\theta,\varphi)$ may be derived from the probability density $f(\omega)$. $f(\omega)$ denotes the probability density of finding a molecule in an orientation defined by the Euler angles $\omega = \xi, \eta, \zeta$. Instead of Euler angles in this paper the less customary but more convenient quaternions (Klein & Sommerfeld, 1897; Hund, 1928; Hüller & Kane, 1974), $\tau = (\tau_1, \tau_2, \tau_3, \tau_4)$, will be used to describe the orientation of a molecule. The quaternions are restricted to the surface of the four-dimensional unit sphere and therefore $\sum_{i=1}^{4} \tau_i^2 = 1$. If expressed in terms of quaternions, the orientational density distribution $f(\omega)$ will be called $g(\tau)$. The scattering-length density $a(\theta,\varphi)$ is derived from $g(\tau)$ by means of an integration $\oint d\tau$ on the surface of the four-dimensional unit sphere:

$$a(\theta,\varphi) = \oint d\tau\, g(\tau)\, b(\theta,\varphi;\tau). \tag{1.3}$$

Here $b(\theta,\varphi;\tau)$ is the scattering-length density for the orientation of the molecule which is specified by the quaternion τ. $b(\theta,\varphi;\tau)$ is a sum of δ functions at the positions (θ,φ) which are occupied by nuclei for the special orientation of the molecule.

If $g(\tau)$ is positive definite, the same holds for $a(\theta,\varphi)$. The reverse, however, is not always true. Therefore the requirement that $a(\theta,\varphi)$ must be positive definite is only a necessary, but not a sufficient condition. We must impose the further condition that $g(\tau)$ is positive definite.

$g(\tau)$ is expanded in terms of the symmetry-adapted cubic rotator functions (Hüller & Kane, 1974; James & Keenan, 1959), $H_{mm'}^l(\tau)$:

$$g(\tau) = \frac{1}{2\pi^2} \sum_{lmm'} (2l + 1) A_{mm'}^{(l)} H_{mm'}^{(l)}(\tau). \tag{1.4}$$

If Euler angles are used (Press & Hüller, 1973, 1974), the normalization factor is $(2l + 1)/8\pi^2$. [It has been omitted in equation (3.6) of Press & Hüller, 1973.]

In the special case of tetrahedral or octahedral molecules at a cubic crystal site, only a few of the coefficients $A_{mm'}^{(l)}$ are non-zero:

$$g(\tau) = \frac{1}{2\pi^2} [1 + 9A_{11}^{(4)} H_{11}^{(4)}(\tau) + 13A_{11}^{(6)} H_{11}^{(6)}(\tau)$$

$$+ 17A_{11}^{(8)} H_{11}^{(8)}(\tau) \ldots]. \tag{1.4a}$$

The right hand side of (1.4a) must be positive for all values of τ. If we suppose, for the moment, that all the terms of order $l \geq 10$ are negligible, then the right-hand

side of (1.4a) can be evaluated for a certain value $\tilde{\tau}$ of τ. Then $g(\tilde{\tau}) \geq 0$ leads to an inequality for the coefficients $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$. To calculate $H_{11}^{(4)}(\tau)$ and $H_{11}^{(6)}(\tau)$ we use the analytical forms of Hüller & Kane (1974); an expression for $H_{11}^{(8)}(\tau)$ is given in the Appendix. The latter function has also been obtained in terms of Euler angles (Amoureux, 1978). Table 1 gives the values of $H_{11}^{(4)}(\tau)$, $H_{11}^{(6)}(\tau)$, and $H_{11}^{(8)}(\tau)$ for four different values of $\tilde{\tau}$. For the first one, namely $\tilde{\tau} = (0,0,0,1)$, the three functions $H_{11}^{(4)}(\tau)$, $H_{11}^{(6)}(\tau)$ and $H_{11}^{(8)}(\tau)$ assume their maximum value $+1$. Thus the condition $g(\tilde{\tau}) \geq 0$ excludes the possibility that $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ simultaneously adopt large negative values. To obtain bounds for positive values of the coefficients, the next three values of $\tilde{\tau}$ have been chosen such that $H_{11}^{(4)}(\tau)$, $H_{11}^{(6)}(\tau)$ and $H_{11}^{(8)}(\tau)$, respectively, acquire their minimal values. From Table 1, four inequalities are obtained which may be represented by four planes in the $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ space. Each plane divides the space into an allowed and a forbidden region. The region of space which is allowed by all four conditions has the shape of the distorted tetrahedron shown in Fig. 1. Of course, it includes the origin which represents a uniform distribution over all orientations of the molecule. The requirement that the triplet $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ has to fall

Table 1. *Values of the cubic rotator functions* $H_{11}^{(l)}(\tau)$ *for different orientations*

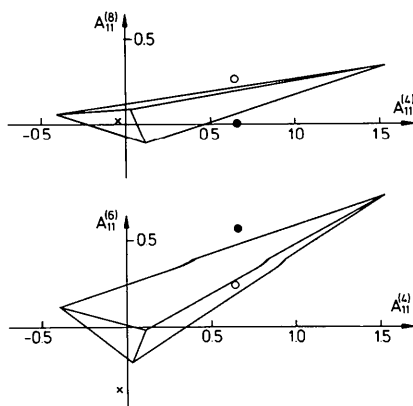| $\tilde{\tau}$	$H_{11}^{(4)}(\tau)$	$H_{11}^{(6)}(\tau)$	$H_{11}^{(8)}(\tau)$
$(0, 0, 0, 1)$	$+1$	$+1$	$+1$
$(x, x, x, 0), x = 1\sqrt{3}$	$-13/27$	$+103/243$	$+169/729$
$\{[(1 - x)/2]^{1/2}, 0, 0,$ $[(1 + x)/2]^{1/2}\}, x = 1/\sqrt{2}$	$+1/6$	$-3/4$	$+17/24$
$[x, x, x, (1 - 3x^2)^{1/2}],$ $x = 0.1651$	$+0.134$	$+0.048$	-0.558

Fig. 1. The distorted tetrahedron in $A_{11}^{(4)}$, $A_{11}^{(6)}$, and $A_{11}^{(8)}$ space, into which experimentally determined points must fall if the terms beyond $l = 8$ in (1.4a) are negligible. Crosses denote CBr_4 (More, Lefèbvre & Fouret, 1977), open circles denote SF_6 (Dolling, Powell & Sears, 1979) and full circles denote adamantane (Amoureux & Bée, 1979).

into the distorted tetrahedron of Fig. 1 was derived under the assumption that $A_{11}^{(10)}$, $A_{mm'}^{(12)}$, ... are all zero.

If a set of experimentally determined values of $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ falls outside the allowed region, three conclusions are possible:

(I) The translational and rotational motions of the molecules are strongly coupled. To arrive at (1.2), the assumption was made that the probability density of finding a scattering centre at the position $\mathbf{r}$ can be expressed as a product of a translational part and a rotational part $a(\theta,\varphi)$. If such a separation is not possible, (1.2) becomes more involved. It might be replaced by a double series for the angular and translational degrees of freedom of the molecule. Problems of this kind have been encountered in the study of the rotational motion of the NO_3 group in KNO_3 (Lefèbvre, 1978) and may be important in the study of KCN where the importance of rotation–translation coupling has been demonstrated recently (Michel & Naudts, 1977; Fontaine, Pick & Yvinec, 1977).

(II) A second possible conclusion would be that the higher-order terms in (1.4) may not be neglected. Their importance can then be estimated from the distance of the point from the allowed region.

(III) The experimentally determined parameters c_{lm} (which determine $A_{mm'}^{(l)}$) may be wrong. One should also investigate if a variation of the experimentally determined parameters within the error bars allows the construction of a positive-definite $g(\tau)$.

For an explicit discussion of experimental results, one needs a relation between the coefficients c_{lm} of (1.2) which are determined in a diffraction experiment and the coefficients $A_{mm'}^{(l)}$ of (1.4). If $b(\mathbf{r}')$ represents the scattering-length density of the shell of atoms in a (primed) coordinate system rotating with the molecule (Press & Hüller, 1973), its expansion in terms of cubic harmonics reads

$$b(\mathbf{r}') = \sum_{lm'} b_{lm'}^{S} K_{lm'}(\theta', \varphi')\, \delta(r' - \rho)/r'^2. \quad (1.5)$$

S represents the symmetry of the molecule. We have restricted the discussion to either tetrahedral, $S = T$, or octahedral, $S = O$, molecules. The coefficients $b_{lm'}^{S}$ are well known (Press, 1973):

$$b_{41}^{T} = -\sqrt{7/3},\ b_{61}^{T} = +4\sqrt{26/9},\ b_{81}^{T} = +\sqrt{561/27},$$

$$b_{41}^{O} = +\sqrt{21/2},\ b_{61}^{O} = +\sqrt{26/4},\ b_{81}^{O} = +\sqrt{561/8}.$$

The coefficients c_{lm} and $b_{lm'}^{S}$ are related to each other by the equation

$$c_{lm} = \sum_{m'} A_{mm'}^{(l)}\, b_{lm'}^{S}. \quad (1.6)$$

As has been mentioned before, there is only a single $A_{mm'}^{(l)}$ of order $l = 4$, 6 and 8 for cubic site symmetry ($m3m$). Equation (1.6) can be used for determining $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ from published values of c_{41}, c_{61}, and c_{81}.

These values of $A_{11}^{(4)}$, $A_{11}^{(6)}$ and $A_{11}^{(8)}$ are shown in Fig. 1 for CBr_4 (More, Lefèbvre & Fouret, 1977), SF_6 (Dolling, Powell & Sears, 1979) and $C_{10}H_{16}$ (Amoureux & Bée, 1979). It is seen that in all three cases terms of order $l \geq 10$ are needed to obtain an angular probability distribution $g(\gamma)$ which is positive everywhere. In CBr_4 the scattering-length density $a(\mathbf{r})$ becomes slightly negative in (1,1,1) directions if one uses only the three measured coefficients c_{41}, c_{61}, and c_{81}: it decreases to -0.8 times its average value of $1/4\pi$. We now look into the angular probability distribution $g(\tau)$ which is the basic distribution in problems of rotational motion of molecules. From Fig. 1 we see that the set of three parameters $A_{11}^{(4)}$, $A_{11}^{(6)}$, and $A_{11}^{(8)}$ are rather far from the allowed region. The following inequality is most seriously violated:

$$g[\tau = (0,0,0,1)] = \frac{1}{2\pi^2} (1 + 9A_{11}^{(4)} + 13A_{11}^{(6)} + 17A_{11}^{(8)})$$

$$\geq 0. \qquad (1.7)$$

It is connected with the first line in Table 1. From the values $A_{11}^{(4)} = -0.05$, $A_{11}^{(6)} = -0.373$ and $A_{11}^{(8)} = +0.021$, we obtain $g[\tau = (0,0,0,1)] = (-1/2\pi^2) \times 4.9$; i.e. at $\tau = (0,0,0,1)$, the probability function $g(\tau)$ is minus five times its average value of $1/2\pi^2$. This suggests that higher-order terms should be important. In order to compensate for the negative value of $g(\tau)$ at $(0,0,0,1)$, one needs: $21A_{11}^{(10)} + 25 \sum_{mm'} A_{mm'}^{(12)} \ldots \geq 4.9$.

II. Rotational potential

In the following, a method will be outlined which guarantees from the start that the angular distribution function $g(\tau)$ is positive definite. We start from the angular potential $V(\tau)$ which is also expanded into cubic rotator functions:

$$V(\tau) = C_{11}^{(4)} H_{11}^{(4)}(\tau) + C_{11}^{(6)} H_{11}^{(6)}(\tau). \qquad (2.1)$$

To avoid long expressions the notation $h_4(\tau) = H_{11}^{(4)}(\tau)$, $h_6(\tau) = H_{11}^{(6)}(\tau)$ etc. will be used in the following. Only terms up to order $l = 6$ are considered, but an extension to higher-order terms is straightforward. For high temperatures ($k_B T \gg \hbar\omega_{lib}$, ω_{lib} = librational frequency), the molecules behave like classical rotors. The orientational distribution function then can be written (Filter & Biem, 1975)

$$g(\tau) = w(\tau)/\oint w(\tau) \, d\tau, \qquad (2.2)$$

where the unnormalized distribution $w(\tau)$ is given by a Boltzmann factor

$$w(\tau) = \exp[-\beta V(\tau)], \text{ where } \beta = 1/k_B T; \qquad (2.3)$$

$g(\tau)$ cannot become negative. The problem is to determine the coefficients $A_{11}^{(4)}$, $A_{11}^{(6)}$, $A_{11}^{(8)} \ldots$ of the probability distribution $g(\tau)$ (see 1.4) from the coefficients $C_{11}^{(4)}$ and $C_{11}^{(6)}$ of the potential. To this end we abbreviate $\beta C_{11}^{(4)} = B_4$ and $\beta C_{11}^{(6)} = B_6$ and expand the exponential in (2.3):

$$w(\tau) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sum_{m=0}^{n} \binom{n}{m} B_4^m B_6^{n-m}$$

$$\times [h_4(\tau)]^m [h_6(\tau)]^{n-m}, \qquad (2.4)$$

each term in (2.4) is expanded into a series of cubic rotator functions using

$$[h_4(\tau)]^m [h_6(\tau)]^{m'} = a_0^{mm'} + a_4^{mm'} h_4(\tau)$$

$$+ a_6^{mm'} h_6(\tau) + \ldots, \qquad (2.5)$$

where

$$a_0^{mm'} = (m, m'), \quad a_4^{mm'} = 9(m + 1, m'),$$

and

$$a_6^{mm'} = 13(m, m' + 1),$$

with

$$(m, m') = \frac{1}{2\pi^2} \oint d\tau [h_4(\tau)]^m [h_6(\tau)]^{m'}. \qquad (2.6)$$

$w(\tau)$ thus becomes

$$w(\tau) = w_0 + w_4 h_4(\tau) + w_6 h_6(\tau) + \ldots. \qquad (2.7)$$

The coefficients w_i for $i = 0, 4, 6, \ldots$ are defined by

$$w_i = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sum_{m=0}^{n} \binom{n}{m} b_i^{mn} B_4^m B_6^{n-m}, \qquad (2.8)$$

with $b_0^{mn} = (m, n - m)$, $b_4^{mn} = (m + 1, n - m)$ and $b_6^{mn} = (m, n - m + 1)$. The denominator $\oint w(\tau) \, d\tau = w_0/2\pi^2$ in (2.2) is found from $\oint d\tau h_4(\tau) = \oint d\tau h_6(\tau) = 0$. Comparing (1.4a) and (2.2) with the use of (2.7), we therefore find

$$A_{11}^{(4)} = w_4/w \text{ and } A_{11}^{(6)} = w_6/w_0, \qquad (2.9)$$

which is the desired expression of $A_{11}^{(4)}$ and $A_{11}^{(6)}$ in terms of powers of $B_4 = \beta C_{11}^{(4)}$ and $B_6 = \beta C_{11}^{(6)}$. To evaluate (2.8) the integrals (m, m') have to be known. We have found exact values for (m, m') up to order $m + m' = 5$ by direct integration of (2.6) and approximate values for $m, m' \leq 10$ by a Monte Carlo method.* Should it be necessary to calculate (m, m') for even higher values of m and m', one can use the asymptotic formula $(m, m') \simeq 24 \, N^{-3/2} \pi^{-1/2}$ with $N = 40m/3 + 28m'$ to obtain approximate values for the integrals.

In a typical refinement calculation, $C_{11}^{(4)}$ and $C_{11}^{(6)}$ would be the adjustable parameters which by (2.9) determine the expansion coefficients $A_{11}^{(4)}$, $A_{11}^{(6)}$, ... and thus the intensity of Bragg reflections. The advantage of this method, which starts from a rotational potential is threefold: (i) the expansion coefficients $A_{11}^{(4)}$, $A_{11}^{(6)}$, ... represent the first new terms in an expansion of $g(\tau)$ which automatically is positive definite; (ii) the coefficients $C_{11}^{(4)}$ and $C_{11}^{(6)}$ define the orientational potential, a quantity with immediate physical significance; (iii) the analysis of diffraction experiments at different temperatures can be used to check the consistency of the orientational potential.

APPENDIX

The cubic rotator function $H_{11}^{(8)}(\tau)$ in terms of quaternions

Functions of order $l = 3$, 4, and 6 are found in Hüller & Kane (1974).

$$
\begin{aligned}
H_{11}^{(8)} = {} & A_1(\tau_1^{16} + \tau_2^{16} + \tau_3^{16} + \tau_4^{16}) \\
& + A_2(\tau_1^{10}\,\tau_2^2\,\tau_3^2\,\tau_4^2 + \tau_2^{10}\,\tau_3^2\,\tau_4^2\,\tau_1^2 \\
& \quad + \tau_3^{10}\,\tau_4^2\,\tau_1^2\,\tau_2^2 + \tau_4^{10}\,\tau_1^2\,\tau_2^2\,\tau_3^2) \\
& + A_3(\tau_1^8\,\tau_2^8 + \tau_1^8\,\tau_3^8 + \tau_1^8\,\tau_4^8 + \tau_2^8\,\tau_3^8 + \tau_2^8\,\tau_4^8 \\
& \quad + \tau_3^8\,\tau_4^8) \\
& + A_4(\tau_1^6\,\tau_2^6\,\tau_3^2\,\tau_4^2 + \tau_1^6\,\tau_3^6\,\tau_2^2\,\tau_4^2 + \tau_1^6\,\tau_4^6\,\tau_2^2\,\tau_3^2 \\
& \quad + \tau_2^6\,\tau_3^6\,\tau_1^2\,\tau_4^2 \\
& \quad + \tau_2^6\,\tau_4^6\,\tau_1^2\,\tau_3^2 + \tau_3^6\,\tau_4^6\,\tau_1^2\,\tau_2^2) \\
& + A_5\,\tau_1^4\,\tau_2^4\,\tau_3^4\,\tau_4^4 \\
& + A_6(\tau_1^{14} + \tau_2^{14} + \tau_3^{14} + \tau_4^{14}) \\
& + A_7(\tau_1^{12} + \tau_2^{12} + \tau_3^{12} + \tau_4^{12}) \\
& + A_8(\tau_1^{10} + \tau_2^{10} + \tau_3^{10} + \tau_4^{10}) \\
& + A_9(\tau_1^8 + \tau_2^8 + \tau_3^8 + \tau_4^8) \\
& + A_{10}(\tau_1^6 + \tau_2^6 + \tau_3^6 + \tau_4^6) \\
& + A_{11}(\tau_1^4 + \tau_2^4 + \tau_3^4 + \tau_4^4) \\
& + A_{12} \\
& + A_{13}(\tau_1^6\,\tau_2^6 + \tau_1^6\,\tau_3^6 + \tau_1^6\,\tau_4^6 + \tau_2^6\,\tau_3^6 + \tau_2^6\,\tau_4^6 + \tau_3^6\,\tau_4^6) \\
& + A_{14}\,\tau_1^2\,\tau_2^2\,\tau_3^2\,\tau_4^2.
\end{aligned} \tag{A.1}
$$

The coefficients A_ν are:

$A_1 = +8320/3$

$A_2 = +29120$

$A_3 = +16640/3$

$A_4 = +757120/3$

$A_5 = +1164800$

$A_6 = -33280/3$

$A_7 = +163072/9$

$A_8 = -46592/3$

$A_9 = +22960/3$

$A_{10} = -22400/9$

$A_{11} = +1960/3$

$A_{12} = -767/9$

$A_{13} = -23296/9$

$A_{14} = -8960.$

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