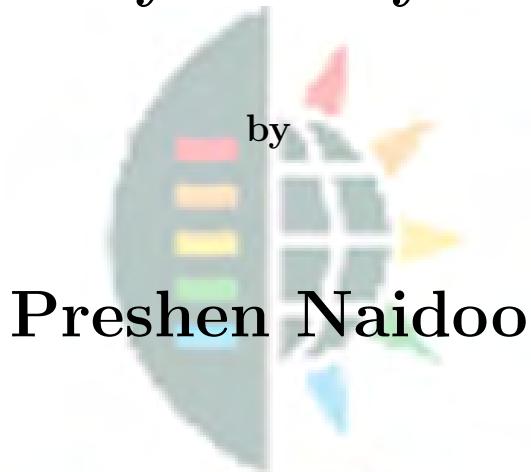


# **Second Kerr–effect virial coefficients of non-dipolar molecules with axial and lower symmetry**



*Dissertation submitted in partial fulfillment of the  
academic requirements for the degree of  
Master of Science in Physics in the  
School of Chemistry and Physics,  
University of kwaZulu-Natal.*

Supervisor: Dr. V. W. Couling



# **Declaration**

This dissertation describes the work undertaken at the School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg Campus under the supervision of Dr V W Couling between January 2015 and December 2016.

I, Preshen Naidoo, declare that the work reported in this dissertation is my own research, unless specifically indicated to the contrary in the text. This dissertation has not been submitted in any form, for any degree or examination to any other university.

Signed .....

I hereby certify that this statement is correct

Signed .....

Dr V W Couling

Supervisor

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# Abstract

The molecular theory of the second Kerr-effect virial coefficient  $B_K$  describing the effects of interacting pairs of molecules on the molecular Kerr constant for molecules with non-linear symmetry is reviewed, and then extended to include higher-order contributions arising from field gradient effects and molecular electric quadrupole moment contributions in the molecular interactions.

This investigation has been limited to non-dipolar species, where the permanent electric quadrupole moment is the leading multipole moment, making these molecules a useful test of the quadrupole-induced-dipole contributions. (In dipolar species, the quadrupole contributions will likely be masked by the generally much-larger contributions arising from the permanent electric dipole moment.) The resulting expressions for contributions to  $B_K$  are evaluated numerically (using Gaussian quadrature) for the non-dipolar molecules C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> and CO<sub>2</sub>.

C<sub>2</sub>H<sub>6</sub> and CO<sub>2</sub> are axially-symmetric molecules, while C<sub>2</sub>H<sub>4</sub> is of lower ( $D_{2h}$ ) symmetry. Attempts to approximate C<sub>2</sub>H<sub>4</sub> to axial symmetry in calculations of  $B_K$  have yielded values which significantly underestimate the measured data. Inclusion of the full molecular symmetry in the molecular-tensor theory yields a substantial improvement in agreement with experimental results. For CO<sub>2</sub> and C<sub>2</sub>H<sub>4</sub>, both of which have relatively large quadrupole moments and polarizability anisotropies, the series of quadrupole-induced-dipole interaction terms are found to contribute significantly to  $B_K$ , often in excess of 50%, while for C<sub>2</sub>H<sub>6</sub>, which has a relatively tiny quadrupole moment and polarizability anisotropy, the dipole-induced-dipole terms dominate, contributing in excess of 99% to  $B_K$ .

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# Chapter 1

## Review and Introduction

### 1.1 Review: Birefringence in the Kerr Effect

#### 1.1.1 The Kerr Effect

When a substance, which is optically isotropic, is placed in a region with a strong uniform electric field, the substance becomes birefringent. This effect was discovered by the Reverend John Kerr in 1875 when he observed the birefringence induced in glass when placed in a strong electric field [1]. Only gaseous media will be considered in this work, where the field-induced birefringence arises through both the partial alignment of the permanent molecular multipole moments as well as the distortion of the electronic structure of the molecules in the presence of the external static electric field. The Kerr constant  $K$  of a homogeneous substance is defined by the relation

$$n_{\parallel} - n_{\perp} = \lambda K E^2, \quad (1.1)$$

which illustrates that the magnitude of the effect is found to be proportional to the square of the electric field strength  $E$ .  $n_{\parallel}$  is the refractive index for light when the polarization vector is parallel to the direction of the applied electric field, while  $n_{\perp}$  is the refractive index for light with the polarization vector perpendicular to the applied field. If linearly-polarized light enters this now-anisotropic medium

propagating at right angles to the direction of  $E$ , the induced birefringence will cause it to emerge from the medium elliptically polarized. The relative phase retardation, in radians, between the parallel and perpendicular components of the light-wave electric vector is

$$\phi = \frac{2\pi l}{\lambda} (n_{\parallel} - n_{\perp}), \quad (1.2)$$

where  $l$  is the distance which the light traverses in the birefringent medium and  $\lambda$  is the wavelength of the light.

### 1.1.2 Interaction Properties, Effects of the Density

The effect of two-body or higher-order interactions on optical properties is often expressed by a virial expansion. The dependence of a measurable molecular-optic property  $Q$  of a real gas on the molar volume  $V_m$  is written as [2]

$$Q = A_Q + \frac{B_Q}{V_m} + \frac{C_Q}{V_m^2} + \dots, \quad (1.3)$$

where  $A_Q$ ,  $B_Q$  and  $C_Q$  are the first, second and third virial coefficients, respectively, which are independent of  $V_m$ , but are functions of frequency and temperature. The first virial coefficient  $A_Q$  describes the isolated molecule contribution to  $Q$ . The second virial coefficient  $B_Q$  describes the excess contribution to  $Q$  due to the interactions of molecular pairs, while the third virial coefficient  $C_Q$  describes contributions from the interaction of molecular triplets.

## 1.2 Introduction and the aims of this work

One of the principal goals in molecular optics is the experimental and theoretical determination of the electromagnetic properties of individual molecules. This

is often achieved via experimental investigation of the interaction between light and macroscopic samples of matter, and then coupling such measurements with suitable molecular-tensor theories to relate the macroscopic observables to the molecular property tensors of the molecules in the sample [3–8].

The measurement of the electro-optical Kerr effect of gases is an important tool used to determine electric properties such as the polarizability and hyperpolarizability tensors. These electric properties provide an insight into the structure and charge distribution of molecules [3, 9, 10]. Careful consideration must be taken of the fact that in a typical gas sample the molecules cannot be treated as though they are independent systems, since the presence of molecular interactions can affect the bulk properties of the sample, sometimes substantially modifying them from those of an ideal gas. Pressure dependence studies can yield useful insights into intermolecular interaction properties, allowing for testing of the long-range model of intermolecular forces, thus making the Kerr electro-optic effect a very useful technique. The Kerr effect in gases is, in general, very small in comparison to that in liquids and solids. Thus making density-dependent contributions to the effect are extremely difficult to measure with high accuracy and precision. This explains the relative scarcity in experimental data in the case of gases.

This work reviews the molecular-tensor theory of the Kerr effect developed by Couling and Graham [11, 12]. Subsequent work by Graham and Hohls [13] attempted to extend this theory to include quadrupole-induced-dipole contributions to  $B_K$ , though this work was never published, and has been found to contain catastrophic errors, some of the contributing terms not having been accounted for. The present investigation extends the molecular-tensor theory of the Kerr-effect of Couling and Graham to include higher-order contributions arising from field gradient effects and electric quadrupole moment contributions in the molecular interactions. This theory is developed in Chapter 2, and in Chapter 3 is applied to three non-dipolar species for which experimental  $B_K$  data are available, namely  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$  and  $\text{CO}_2$ . For  $\text{C}_2\text{H}_4$  and  $\text{CO}_2$ , which both have a

relatively large permanent quadrupole moment and polarizability anisotropy, the new higher-order contributions are found to often be quite substantial, sometimes contributing more than 50% to  $B_K$ . The calculated  $B_K$  values are compared with the available measured data, and are found to be in reasonable agreement after inclusion of the new contributions.

While experimental investigations of the Kerr effect exist for other molecules such as  $\text{CS}_2$ ,  $\text{C}_6\text{H}_6$ ,  $\text{C}_6\text{H}_3\text{F}_3$  and  $\text{C}_6\text{F}_6$  [14, 15], the observations have been made at relatively low pressures, so that second Kerr-effect virial coefficients were not detectable. With the new theory, it will be possible to predict the  $B_K$  data for a range of non-dipolar species which might be profitable for future measurement.

# Chapter 2

## Theory of the Kerr Effect

### 2.1 Introduction

In 1875, Kerr observed that when an isotropic medium is placed in a strong uniform electric field, it will generally become birefringent [1]. In this particular review the investigation shall be limited to gaseous media, where the application of a strong, uniform applied field gives rise to anisotropy in the molecular distribution either resulting from intrinsic anisotropy in the individual molecules, or because anisotropy is induced in the molecules due to the applied field itself. The main focus of the Kerr-effect measurements in gases is to be able to determine molecular polarizabilities and hyperpolarizabilities, as well the determination of the Kerr-effect virial coefficients. In order for these properties to be determined, mathematical relationships between the macroscopic experimental observables and molecular-property tensors are required. Such relationships allow for the molecular-property tensors to be extracted from the measured data. In 1955, Buckingham and Pople [9] were able to develop such a theory for gases comprised of axially-symmetric molecules at low pressure. Buckingham extended this theory to dense gases of axially-symmetric molecules [10]. In 1995, Buckingham's theory was extended by Couling and Graham to include gases comprised of molecules with symmetry lower than axial, and also including higher-order molecular-interaction terms to ensure convergence to a meaningful result [11, 12]. This theory will be reviewed as part of this MSc project, in preparation for

the inclusion of the new quadrupole-induced-dipole (QID) molecular-interaction terms. This thesis is primarily concerned with inclusion of these higher-order QID molecular-interaction terms and investigation of their relative contribution to the second Kerr-effect virial coefficient  $B_K$  of non-dipolar molecules.

When an isotropic gas sample is placed in the presence of a strong uniform electric field the gas becomes birefringent. This phenomenon is known as the quadratic electro-optic (or Kerr) effect, and the molar Kerr constant  $_mK$  of a gas is defined as [9]

$$_mK = \frac{6n(n_{\parallel} - n_{\perp})V_m}{(n^2 + 2)^2(\varepsilon_r + 2)^2 E^2}, \quad (2.1)$$

where  $V_m$  is the molar volume of the gas sample,  $n$  is the isotropic refractive index,  $(n_{\parallel} - n_{\perp})$  is the difference in refractive indices for light polarized parallel and perpendicular to the applied electric field, and  $\varepsilon_r$  is the dielectric constant of the gas. The virial expansion of the molar Kerr constant is [10]

$$_mK = A_K + \frac{B_K}{V_m} + \frac{C_K}{V_m^2} + \dots, \quad (2.2)$$

where  $A_K$ ,  $B_K$  and  $C_K$  refer to the first, second and third Kerr-effect virial coefficients respectively. These coefficients are functions of temperature and the frequency of the probing electromagnetic radiation.

## 2.2 Non-interacting molecules

Consider an isotropic fluid contained inside a Kerr cell to which a static electric field is applied. In order for the forces acting on the permanent and induced multipoles of the molecules to be minimized they will tend to orient themselves to the applied electric field. The medium becomes birefringent due to the resulting anisotropy. If a linearly-polarized light beam were to pass through this medium,

the emergent light would be elliptically polarized. This is caused by the phase difference  $\phi$  induced between the coherent resolved components of the incident beam linearly-polarized perpendicular and parallel to the direction of the applied electric field [9]. When the azimuth of the linearly-polarized incident beam has an angle of  $\frac{\pi}{4}$  radians relative to the applied field the phase difference induced is at a maximum. A light beam with wavelength  $\lambda$  that propagates through a birefringent medium of path length  $l$  will experience an induced phase difference,  $\phi$ , of

$$\phi = \frac{2\pi l (n_{\parallel} - n_{\perp})}{\lambda}. \quad (2.3)$$

Suppose the light beam, which is now elliptically polarized, is passed through a quarter-wave plate which has its fast axis set at an azimuth of  $\frac{\pi}{4}$ . The emergent light beam shall then be linearly polarized with its plane of polarization offset from  $\frac{\pi}{4}$  by  $\frac{\phi}{2}$ . The relationship between the induced phase difference and the Kerr effect is given by

$$\phi = 2\pi K l E^2, \quad (2.4)$$

where the Kerr constant  $K$ , which can be negative or positive, depends on the specific sample that is being investigated, its temperature, and the wavelength of the light beam. The Kerr constant  $K$  is defined as

$$K = \frac{(n_{\parallel} - n_{\perp})}{\lambda E^2}. \quad (2.5)$$

A Cartesian laboratory frame  $O(x, y, z)$  is considered to be fixed in a Kerr cell such that  $x$  and  $y$  are set perpendicular and parallel to the direction of the applied field respectively, with  $z$  in the direction of the beam propagating through the cell. In the case of dilute fluids, where the molecular interactions are negligible, the induced oscillating dipole moment  $\mu_i^{(p)}$  of molecule  $p$  will result

only from the oscillating electric field  $\mathcal{E}_{0i}$  of the light beam. Now since the fluid experiences an application of a strong static electric field  $E_i$  the optical-frequency polarizability  $\alpha_{ij}$  is modified to a new effective polarization  $\pi_{ij}$  which can be written as

$$\pi_{ij} = \frac{\partial \mu_i}{\partial \mathcal{E}_{0i}} = \alpha_{ij} + \beta_{ijk} E_k + \frac{1}{2} \gamma_{ijkl} E_k E_l + \dots . \quad (2.6)$$

Here, all tensors refer to the molecule-fixed axes  $O(1, 2, 3)$  of molecule  $p$ . The subscripts  $i, j, \dots$  indicate tensor components. When a suffix appears twice in the same term, the Einstein summation convention is used, requiring a summation over Cartesian components with respect to that term. The applied field causes a distorting effect on the polarizability which can be described by the first and second hyperpolarizability tensors  $\beta_{ijk}$  and  $\gamma_{ijkl}$ . Frequency doubling and frequency tripling are caused by the first hyperpolarizability and second hyperpolarizability, respectively. These describe the dipole moments (induced by a light-wave field) that oscillate at twice and three times the incident frequency respectively. The increase in moment per unit increase in the field is measured by  $\pi_{ij}$ . This effective polarizability has components parallel and perpendicular to the direction of the biasing field with respect to the laboratory frame given by

$$\pi_{xx} = \pi_{ij} a_i^x a_j^x \quad (2.7)$$

and

$$\pi_{yy} = \pi_{ij} a_i^y a_j^y \quad (2.8)$$

, respectively. Here  $a_i^x$  refers to the direction cosine between the  $x$  space-fixed and the  $i$  molecule-fixed axes and  $a_i^y$  refers to the direction cosine between the  $y$  space-fixed and the  $i$  molecule-fixed axes. The differential polarizability in the presence of the biasing field for a molecule held in a fixed spatial configuration  $\tau$  is given by

$$\begin{aligned}\pi(\tau, E) &= \pi_{ij} (a_i^x a_j^x - a_i^y a_j^y) \\ &= \left( \alpha_{ij} + \beta_{ijk} E a_k^x + \frac{1}{2} \gamma_{ijkl} E a_k^x E a_l^x + \dots \right) (a_i^x a_j^x - a_i^y a_j^y),\end{aligned}\quad (2.9)$$

where  $E_i$  has been written as  $E a_i^x$ . Since the molecule is tumbling in space, this quantity needs to be averaged over all configurations in the presence of the biasing influence of  $E_i$ . The rotational motion of the molecules can be treated classically at typical experimental temperatures. A Boltzmann-type weighting factor can be employed to perform the average over molecular configuration, since the light wave's period of oscillation is much smaller than the time taken for the molecules to rotate. The Boltzmann-type weighting factor is given by

$$\bar{\pi} = \frac{\int \pi(\tau, E) e^{-U(\tau, E)/k_B T} d\tau}{\int e^{-U(\tau, E)/k_B T} d\tau}, \quad (2.10)$$

where  $U(\tau, E)$  refers to the potential energy of the molecule in a specific configuration  $\tau$  in the presence of the biasing field. In molecule-fixed axes this becomes

$$\begin{aligned}U(\tau, E) &= U^0 - \mu_i^{(0)} E_i - \frac{1}{2} a_{ij} E_i E_j - \frac{1}{6} b_{ijk} E_i E_j E_k + \dots \\ &= U^0 - \mu_i^{(0)} E a_i^x - \frac{1}{2} a_{ij} E^2 a_i^x a_j^x - \frac{1}{6} b_{ijk} E^3 a_i^x a_j^x a_k^x + \dots.\end{aligned}\quad (2.11)$$

Here the field-free molecular potential energy is denoted by  $U^0$ , while the permanent dipole of the molecule is denoted by  $\mu_i^{(0)}$ , and  $a_{ij}$  refers to the molecule's static polarizability, with  $b_{ijk}$  referring to the molecule's static first-order hyperpolarizability, etc. The difference between the refractive indices becomes

$$n_x - n_y = \frac{2\pi N_A}{4\pi\epsilon_0} \bar{\pi}, \quad (2.12)$$

where  $N_A$  is Avogadro's number. The relation between the induced birefringence and the biasing electric field requires the average differential polarizability to be

evaluated. In order for this to be achieved, the biased averages are converted into isotropic averages by Taylor expanding  $\bar{\pi}$  in powers of  $E$ :

$$\bar{\pi} = A + B E + C E^2 + \dots , \quad (2.13)$$

where

$$A = (\bar{\pi})_{E=0} ,$$

$$B = \left( \frac{\partial \bar{\pi}}{\partial E} \right)_{E=0}$$

and

$$C = \frac{1}{2} \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} .$$

The isotropic average  $\langle X \rangle$  of a quantity  $X(\tau, E)$  with  $E = 0$  is given by

$$\langle X \rangle = \frac{\int X(\tau, 0) e^{-U^0/k_B T} d\tau}{\int e^{-U^0/k_B T} d\tau} . \quad (2.14)$$

In order to obtain expressions for  $A$ ,  $B$  and  $C$ , determination of the isotropic averages of the direction cosines is required. These general results are provided by Buckingham and Pople [9] and by Barron [5] as follows:

$$\left\{ \begin{array}{l} \langle a_i^x \rangle = \langle a_i^y \rangle = \langle a_i^z \rangle = 0 \\ \langle a_i^x a_j^x \rangle = \langle a_i^y a_j^y \rangle = \langle a_i^z a_j^z \rangle = \frac{1}{3} \delta_{ij} \\ \langle a_i^x a_j^x a_k^x \rangle = \langle a_i^y a_j^y a_k^y \rangle = \langle a_i^z a_j^z a_k^z \rangle = \frac{1}{6} \varepsilon_{ijk} \end{array} \right\} \quad (2.15)$$

and

$$\left\{ \begin{array}{l} \langle a_i^x a_j^x a_k^x a_l^x \rangle = \frac{1}{15} (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ \langle a_i^y a_j^y a_k^x a_l^x \rangle = \frac{1}{30} (4\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \\ \langle a_i^z a_j^z a_k^x a_l^x \rangle = \frac{1}{30} (4\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \end{array} \right\}. \quad (2.16)$$

When  $E = 0$ ,  $A$  becomes zero since  $\langle \pi \rangle = 0$ , and therefore no birefringence is induced in the fluid. Differentiating equation (2.10) with respect to  $E$  and putting  $E = 0$  gives

$$B = \left( \frac{\partial \bar{\pi}}{\partial E} \right)_{E=0} = \left\langle \frac{\partial \pi}{\partial E} \right\rangle - \frac{1}{k_B T} \left\langle \pi \frac{\partial U}{\partial E} \right\rangle, \quad (2.17)$$

where

$$\left\{ \begin{array}{l} \left( \frac{\partial \pi}{\partial E} \right)_{E=0} = \beta_{ijk} a_k^x (a_i^x a_j^x - a_i^y a_j^y) \\ \left( \frac{\partial U}{\partial E} \right)_{E=0} = -\mu_i^{(0)} a_i^x \end{array} \right\}. \quad (2.18)$$

Both of the terms in equation (2.17) average to zero over all directions of  $a_i^x$ , so that the leading non-vanishing term for the differential polarizability is  $C$

$$C = \frac{1}{2} \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} = \frac{1}{2} \left\langle \frac{\partial^2 \pi}{\partial E^2} \right\rangle - \frac{1}{2k_B T} \left\langle 2 \frac{\partial \pi}{\partial E} \frac{\partial U}{\partial E} + \pi \frac{\partial^2 U}{\partial E^2} \right\rangle + \frac{1}{2(k_B T)^2} \left\langle \pi \left( \frac{\partial U}{\partial E} \right)^2 \right\rangle. \quad (2.19)$$

Differentiating equations (2.9) and (2.11) twice with respect to  $E$  and setting the field to zero gives

$$\left\{ \begin{array}{l} \left( \frac{\partial^2 \pi}{\partial E^2} \right)_{E=0} = \gamma_{ijkl} a_k^x a_l^x (a_i^x a_j^x - a_i^y a_j^y) \\ \left( \frac{\partial U^2}{\partial E^2} \right)_{E=0} = -\alpha_{ij} a_i^x a_j^x \end{array} \right\}. \quad (2.20)$$

Equation (2.16) gives

$$\langle a_i^x a_j^x a_k^x a_l^x - a_i^y a_j^y a_k^x a_l^x \rangle = \frac{1}{30} (-2\delta_{ij}\delta_{kl} + 3\delta_{ik}\delta_{jl} + 3\delta_{il}\delta_{jk}) \quad (2.21)$$

such that

$$\left\{ \begin{array}{l} \frac{1}{2} \left\langle \frac{\partial^2 \pi}{\partial E^2} \right\rangle = \frac{1}{2} \gamma_{ijkl} \langle a_i^x a_j^x a_k^x a_l^x - a_i^y a_j^y a_k^x a_l^x \rangle \\ = \frac{2}{30} \gamma_{iijj}, \end{array} \right\}, \quad (2.22)$$

$$\left\{ \begin{array}{l} -\frac{1}{2k_B T} \left\langle 2 \frac{\partial \pi}{\partial E} \frac{\partial U}{\partial E} + \pi \frac{\partial^2 U}{\partial E^2} \right\rangle = \frac{1}{k_B T} \beta_{ijk} \mu_l^{(0)} \langle a_i^x a_j^x a_k^x a_l^x - a_i^y a_j^y a_k^x a_l^x \rangle \\ + \frac{1}{2k_B T} \alpha_{ij} a_{kl} \langle a_i^x a_j^x a_k^x a_l^x - a_i^y a_j^y a_k^x a_l^x \rangle \\ = \frac{2}{15k_B T} \beta_{iij} \mu_j^{(0)} + \frac{1}{15k_B T} (\alpha_{ij} a_{ij} - 3\alpha a), \end{array} \right\}, \quad (2.23)$$

and

$$\left\{ \begin{array}{l} \frac{1}{2(k_B T)^2} \left\langle \pi \left( \frac{\partial U}{\partial E} \right)^2 \right\rangle = \frac{1}{2(k_B T)^2} \alpha_{ij} \mu_k^{(0)} \mu_l^{(0)} \langle a_i^x a_j^x a_k^x a_l^x - a_i^y a_j^y a_k^x a_l^x \rangle \\ = \frac{3}{15(k_B T)^2} (\alpha_{ij} \mu_i^{(0)} \mu_j^{(0)} - \alpha (\mu^{(0)})^2), \end{array} \right\}, \quad (2.24)$$

where  $\alpha = \alpha_{ii}$  and  $a = a_{ii}$ . Consequently,

$$\frac{1}{2} \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} = \frac{2}{30} \gamma_{iijj} + \frac{2}{15k_B T} \beta_{iij} \mu_j^{(0)} + \frac{1}{15k_B T} (\alpha_{ij} a_{ij} - 3\alpha a) + \frac{3}{15(k_B T)^2} (\alpha_{ij} \mu_i^{(0)} \mu_j^{(0)} - \alpha (\mu^{(0)})^2), \quad (2.25)$$

so that equation (2.13) becomes

$$\bar{\pi} = \left\{ \frac{2}{30} \gamma_{iijj} + \frac{2}{15k_B T} \beta_{iij} \mu_j^{(0)} + \frac{1}{15k_B T} (\alpha_{ij} a_{ij} - 3\alpha a) + \frac{3}{15(k_B T)^2} (\alpha_{ij} \mu_i^{(0)} \mu_j^{(0)} - \alpha (\mu^{(0)})^2) \right\} E^2 . \quad (2.26)$$

The mean dynamic and static polarizabilities are given by [5]

$$\begin{cases} \alpha = \frac{1}{3} (\alpha_{11} + \alpha_{22} + \alpha_{33}) \\ a = \frac{1}{3} (a_{11} + a_{22} + a_{33}) \end{cases} . \quad (2.27)$$

The definition of the Kerr constant proposed by Otterbein [16] in the limit of low density becomes

$$_m K = \lim_{V_m \rightarrow \infty} \left\{ \frac{2(n_x - n_y) V_m}{27(4\pi\varepsilon_0) E^2} \right\}_{E=0} = \frac{2\pi N_A}{27(4\pi\varepsilon_0)} \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} . \quad (2.28)$$

Invoking equations (2.12) and (2.25) gives

$$_m K = \frac{2\pi N_A}{405(4\pi\varepsilon_0)} \left\{ 2\gamma_{iijj} + \frac{1}{k_B T} \left[ 4\beta_{iij} \mu_j^{(0)} + 2(\alpha_{ij} a_{ij} - 3\alpha a) \right] + \frac{3}{(k_B T)^2} (\alpha_{ij} \mu_i^{(0)} \mu_j^{(0)} - \alpha (\mu^{(0)})^2) \right\} . \quad (2.29)$$

This equation is a generalized form of the Langevin-Born equation [9] which takes into account the effects that high field strengths have on the polarizability. For molecules that have a high symmetry this general equation becomes greatly simplified.

The temperature-independent contribution to the Kerr effect, proportional to the second hyperpolarizability, accounts for a measurable Kerr constant for atoms like helium as well as for isotropically polarizable molecules such as methane. Although the Langevin-Born theory predicts a zero effect for these systems, the molar Kerr constant is in fact non-zero, and is given by

$$_m K = \frac{4\pi N_A}{81(4\pi\varepsilon_0)} \gamma^K . \quad (2.30)$$

$\gamma^K$  refers to the second Kerr hyperpolarizability, defined by

$$\gamma^K = \frac{1}{10} (3\gamma_{ijij} - \gamma_{iiji}) . \quad (2.31)$$

## 2.3 Interacting molecules

The above Langevin-Born and Buckingham-Pople [9] theory of electro-optical birefringence bears reference specifically to assemblies of non-interacting molecules, and in order to take into account dense fluids where intermolecular interactions are present, it needs to be modified. The molecular Kerr constant is given as per equation (2.2),

$$_mK = A_K + \frac{B_K}{V_m} + \frac{C_K}{V_m^2} + \dots , \quad (2.32)$$

where the coefficients  $A_K$ ,  $B_K$  and  $C_K$  refer to the first, second and third Kerr-effect virial coefficients. These describe the contributions made to the molar Kerr constant by non-interacting molecules, interacting pairs of molecules and interacting triplets, respectively.

The low density molar Kerr constant  $A_K$  is given by

$$A_K = \lim_{V_m \rightarrow \infty} (_mK) ,$$

while  $B_K$  describes the contribution arising from interacting pairs of molecules to  $_mK$ :

$$B_K = \lim_{V_m \rightarrow \infty} (_mK - A_K) V_m . \quad (2.33)$$

In 1955, Buckingham presented a statistical-mechanical theory of  $B_K$  for molecules

with axial-symmetry [10]. Buckingham and Orr extended this theory, in 1969, to include additional effects of polarizability and angle-dependent repulsive forces to calculate values of  $B_K$  for  $\text{CH}_2\text{F}_2$ ,  $\text{CH}_3\text{F}$  and  $\text{CHF}_3$  [17]. Their experimental values obtained approximate agreement for  $\text{CH}_3\text{F}$ , while the calculated values for  $\text{CHF}_3$  were found to be far too small [17]. They attributed this to the effects of short-range interactions on the polarizability and potential energy, arguing that the measurements of  $B_K$  for polar gases probably would not yield any useful information about the nature of intermolecular forces. In 1983, Buckingham *et al.* resolved this conflict between experiment and theory for the fluromethanes [18]. The collision-induced polarizability was included into the theory and this in fact was found to be the dominant contributor to  $B_K$ . A reasonable fit to the measured data for the fluromethanes over a range of temperature was achieved by using a simple Stockmayer-type potential. The limiting factor of this theory was the large uncertainty of around 50% in the experimental values. Couling and Graham, in 1995, developed a complete molecular-tensor theory of  $B_K$  for interacting molecules with general symmetry [11, 12]. This theory will now be reviewed, and will simultaneously be extended to include the quadrupole-induced-dipole interaction terms, followed by their application to non-dipolar molecules of axial and lower symmetry.

For an ideal gas in the presence of a strong electric field  $E_x$ , the molecular theory of the Kerr effect gives the difference in refractive index as

$$n_x - n_y = \frac{2\pi N_A}{(4\pi\epsilon_0) V_m} \bar{\pi}, \quad (2.34)$$

where  $\bar{\pi}$  is the average over all configurations of  $\pi_{ij} (a_i^x a_j^x - a_i^y a_j^y)$  of a representative isolated molecule in the presence of the biasing influence of the field  $E_x$ . The contribution given by a representative molecule 1 to the difference in refractive index,  $(n_x - n_y)$ , is modified by the presence of a neighbouring molecule 2. For a pair of interacting molecules in a specific relative configuration  $\tau$ , the contribution of molecule 1 to the induced birefringence at a particular moment will be

half of the total contribution of the interacting pair:

$$\frac{1}{2} \left\{ \frac{2\pi N_A}{(4\pi\epsilon_0) V_m} \pi^{(12)}(\tau, E) \right\}. \quad (2.35)$$

Here,

$$\pi^{(12)}(\tau, E) = \pi_{ij}^{(12)} (a_i^x a_j^x - a_i^y a_j^y), \quad (2.36)$$

where  $\pi_{ij}^{(12)}$  is the differential polarizability (in molecule-fixed axes) of the interacting pair. Initially the two molecules are allowed to rotate as a rigid whole in the presence of the biasing electric field  $E_i$ , the interacting pair being treated as held in a fixed relative configuration  $\tau$ . This gives a biased orientational average  $\overline{\pi^{(12)}(\tau, E)}$  which, by Taylor expansion in powers of  $E$ , can subsequently be converted into isotropic averages. The leading surviving term, unsurprisingly, is in  $E^2$ ,

$$\overline{\pi^{(12)}(\tau, E)} = \frac{1}{2} \left( \frac{\partial^2 \overline{\pi^{(12)}(\tau, E)}}{\partial E^2} \right)_{E=0} E^2, \quad (2.37)$$

where

$$\begin{aligned} \frac{1}{2} \left( \frac{\partial^2 \overline{\pi^{(12)}(\tau, E)}}{\partial E^2} \right)_{E=0} &= \frac{1}{2} \left\langle \frac{\partial^2 \pi^{(12)}}{\partial E^2} \right\rangle - \frac{1}{2k_B T} \left\langle 2 \frac{\partial \pi^{(12)}}{\partial E} \frac{\partial U^{(12)}}{\partial E} + \pi^{(12)} \frac{\partial^2 U^{(12)}}{\partial E^2} \right\rangle \\ &\quad + \frac{1}{2(k_B T)^2} \left\langle \pi^{(12)} \left( \frac{\partial U^{(12)}}{\partial E} \right)^2 \right\rangle. \end{aligned} \quad (2.38)$$

Here,  $U^{(12)}(\tau, E)$  refers to the potential energy of the interacting pair of molecules in the presence of the applied field  $E_i$ . Extrapolating the ideal-gas definition of the molecular Kerr constant which was proposed by Otterbein [16], provided in equation (2.28), to higher densities, the molar Kerr constant becomes

$$_mK = A_K + \int_{\tau} \frac{2\pi N_A}{27(4\pi\varepsilon_0)} \left\{ \frac{1}{2} \left( \frac{\partial^2 \bar{\pi}^{(12)}(\tau, E)}{\partial E^2} \right)_{E=0} - \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} \right\} P(\tau) d\tau. \quad (2.39)$$

Here,  $P(\tau) d\tau$  refers to the probability of molecule 1 having a neighbour in the range  $(\tau, \tau + d\tau)$ . The intermolecular potential  $U^{(12)}(\tau)$  is related to this probability by

$$P(\tau) = \frac{N_A}{\Omega V_m} e^{-(U^{(12)}(\tau)/k_B T)}, \quad (2.40)$$

where  $\Omega = V_m^{-1} \int d\tau$  is the integral over the orientational coordinates of the neighbouring molecule 2. By comparing equations (2.32) and (2.39), the second Kerr-effect virial coefficient is found to be

$$B_K = \frac{2\pi N_A^2}{27\Omega(4\pi\varepsilon_0)} \int_{\tau} \left\{ \frac{1}{2} \left( \frac{\partial^2 \bar{\pi}^{(12)}(\tau, E)}{\partial E^2} \right)_{E=0} - \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} \right\} e^{-(U^{(12)}(\tau)/k_B T)} d\tau. \quad (2.41)$$

For the more general case of molecules with symmetry lower than axial, the Euler angles and the intermolecular displacement  $R$  (as detailed in Appendix A.1) are best used to express the interaction coordinates such that  $B_K$  can be written as [11, 12]

$$\begin{aligned} B_K = & \frac{N_A^2}{216\pi^2(4\pi\varepsilon_0)} \int_{R=0}^{\infty} \int_{\alpha_1=0}^{2\pi} \int_{\beta_1=0}^{\pi} \int_{\gamma_1=0}^{2\pi} \int_{\alpha_2=0}^{2\pi} \int_{\beta_2=0}^{\pi} \int_{\gamma_2=0}^{2\pi} \\ & \times \left\{ \frac{1}{2} \left( \frac{\partial^2 \bar{\pi}^{(12)}(\tau, E)}{\partial E^2} \right)_{E=0} - \left( \frac{\partial^2 \bar{\pi}}{\partial E^2} \right)_{E=0} \right\} e^{-(U^{(12)}(\tau)/k_B T)} \end{aligned} \quad (2.42)$$

$$\times R^2 \sin \beta_1 \sin \beta_2 dR d\alpha_1 d\beta_1 d\gamma_1 d\alpha_2 d\beta_2 d\gamma_2.$$

As in the case of an ideal gas, the total oscillating dipole moment induced in a molecule is used to determine the refractive index of a dense gas. Now, the dipole moment of a representative molecule 1 is induced by both the oscillating

electric field  $\mathcal{E}_{0i}$  associated with the light wave, and also partly by the oscillating field  $\mathcal{F}_i^{(1)}$  and field gradient  $\mathcal{F}_{ij}^{(1)}$  arising at molecule one due to the oscillating moments of the neighbouring molecule 2. It was at this point that Couling and Graham [11, 12] made the assumption that the quadrupole and field-gradient effects would be negligibly small and therefore omitted them from further consideration. These contributions will however be retained in the present analysis. Their inclusion yields the dipole moment of molecule 1 as [3]

$$\mu_i^{(1)}(\mathcal{E}_0) = \left( \alpha_{ij}^{(1)} + \beta_{ijk}^{(1)} E_k + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l + \dots \right) \left( \mathcal{E}_{0j} + \mathcal{F}_j^{(1)} \right) + \frac{1}{3} A_{ijk}^{(1)} \left( \mathcal{E}_{0jk} + \mathcal{F}_{jk}^{(1)} \right), \quad (2.43)$$

where  $E_i$  is the strong applied static field. The oscillating quadrupole moment of molecule 1 is

$$\theta_{ij}^{(1)}(\mathcal{E}_0) = A_{kij}^{(1)} \left( \mathcal{E}_{0k} + \mathcal{F}_k^{(1)} \right) + C_{ijkl}^{(1)} \left( \mathcal{E}_{0kl} + \mathcal{F}_{kl}^{(1)} \right). \quad (2.44)$$

The relation between the dipole moment of molecule 2 and the field due to this oscillating moment measured at the origin of molecule 1 is expressed via  $T$ -tensors [3] (see appendix A.1) as

$$\mathcal{F}_i^{(1)} = T_{ij} \mu_j^{(2)} - \frac{1}{3} T_{ijk} \theta_{jk}^{(2)} \quad (2.45)$$

and

$$\mathcal{F}_{ij}^{(1)} = T_{ijk} \mu_k^{(2)} - \frac{1}{3} T_{ijkl} \theta_{kl}^{(2)}. \quad (2.46)$$

The dipole and quadrupole moments of molecule 2 are themselves modified by molecule 1's oscillating dipole moment together with the oscillating field of the light beam

$$\mu_i^{(2)}(\mathcal{E}_0) = \left( \alpha_{ij}^{(2)} + \beta_{ijk}^{(2)} E_k + \frac{1}{2} \gamma_{ijkl}^{(2)} E_k E_l + \dots \right) \left( \mathcal{E}_{0j} + \mathcal{F}_j^{(2)} \right) + \frac{1}{3} A_{ijk}^{(2)} \left( \mathcal{E}_{0jk} + \mathcal{F}_{jk}^{(2)} \right), \quad (2.47)$$

and

$$\theta_{ij}^{(2)}(\mathcal{E}_0) = A_{kij}^{(2)} \left( \mathcal{E}_{0k} + \mathcal{F}_k^{(2)} \right) + C_{ijkl}^{(2)} \left( \mathcal{E}_{0kl} + \mathcal{F}_{kl}^{(2)} \right). \quad (2.48)$$

The electric field arising at the origin of molecule 2 from the oscillating dipole moment of molecule 1 is

$$\mathcal{F}_i^{(2)} = T_{ijk} \mu_j^{(1)} + \frac{1}{3} T_{ijkl} \theta_{jk}^{(1)}, \quad (2.49)$$

while the field gradient is

$$\mathcal{F}_{ij}^{(2)} = -T_{ijk} \mu_k^{(1)} - \frac{1}{3} T_{ijkl} \theta_{kl}^{(1)}. \quad (2.50)$$

Now the field gradient of the light wave  $\mathcal{E}_{0ij}$  can be neglected since the dimensions of the molecules are extremely small in comparison to the optical wavelength. The expression for the total dipole of molecule 1 is ultimately achieved by substituting equations (2.47) to (2.50) into equations (2.45) and (2.46), followed by successive substitutions of  $\mathcal{F}_i^{(1)}$ ,  $\mathcal{F}_i^{(2)}$ ,  $\mathcal{F}_{ij}^{(1)}$  and  $\mathcal{F}_{ij}^{(2)}$ , giving rise to a lengthy series of terms which contribute to the net field  $\mathcal{F}_i^{(1)}$  and field gradient  $\mathcal{F}_{ij}^{(1)}$  in equations (2.45) and (2.46). Finally, substituting these lengthy series into equation (2.43) gives the final expression for the total oscillating dipole induced on molecule 1 by the light wave in the presence of molecule 2. This somewhat large expression is presented in Appendix A.2. The differential polarizability of a general molecule  $p$ , which is in the presence of both the static applied field  $E_i$  and a neighbouring molecule  $q$ , is determined by differentiating the expression for  $\mu_i^{(1)}$  with respect to  $\mathcal{E}_{0i}$ . The resulting equation for the differential polarizability is also presented

in Appendix A.2.

For a specific relative interaction configuration  $\tau$  of molecules  $p$  and  $q$  in the presence of the static applied field, the difference between the differential polarizabilities  $\pi_{ij}^{(p)} a_i^x a_j^x$  and  $\pi_{ij}^{(p)} a_i^y a_j^y$  is given by

$$\pi^{(p)}(\tau, E) = \pi_{ij}^{(p)} (a_i^x a_j^x - a_i^y a_j^y). \quad (2.51)$$

In the long-range limit the assumption that the interacting molecules each retain their separate identities is clearly valid. In the very short-range, when the molecules come close enough together such that the charge distributions of the interacting molecules begin to overlap, difficulties begin to arise since the molecules can no longer be unambiguously defined. For a definitive description, *ab initio* quantum-mechanical calculations are required, but these calculations are notoriously difficult to perform even for atoms [19], and are beyond the scope of this analysis. Treating the interacting molecules as if they retain their separate identities even in the short-range overlap region, the total dipole moment of the interacting pair is given by

$$\mu_i^{(12)} = \mu_i^{(1)} + \mu_i^{(2)} \quad (2.52)$$

so that the differential polarizability of the interacting pair can be written as

$$\pi_{ij}^{(12)} = \frac{\partial \mu_i^{(12)}}{\partial \mathcal{E}_0 j} = \frac{\partial (\mu_i^{(1)} + \mu_i^{(2)})}{\partial \mathcal{E}_0}. \quad (2.53)$$

For a specific relative interaction configuration  $\tau$  of an interacting pair in the presence of the static applied field, the difference between the differential polarizabilities  $\pi_{ij}^{(12)} a_i^x a_j^x$  and  $\pi_{ij}^{(12)} a_i^y a_j^y$  is given by

$$\begin{aligned}
\pi^{(12)}(\tau, E) &= \pi_{ij}^{(12)}(a_i^x a_j^x - a_i^y a_j^y) \\
&= (\pi_{ij}^{(1)} + \pi_{ij}^{(2)}) (a_i^x a_j^x - a_i^y a_j^y) \\
&= \pi^{(1)}(\tau, E) + \pi^{(2)}(\tau, E).
\end{aligned} \tag{2.54}$$

The interacting pair's potential energy in the presence of the biasing electric field is given by

$$U^{(12)}(\tau, E) = U^{(12)}(\tau, 0) - \int_0^E \mu_i^{(12)}(\tau, E) a_i^x dE, \tag{2.55}$$

where  $E_i$  has been written as  $Ea_i^x$  and  $\mu_i^{(12)}$  is the total dipole moment of the pair in the presence of  $E_i$ .

The dipole moment of the molecule  $p$  in the presence of molecule  $q$  and the static uniform applied field  $E_i$  is

$$\mu_i^{(p)} = \mu_{0i}^{(p)} + \left( a_{ij}^{(p)} + b_{ijk}^{(p)} E_k + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l + \dots \right) (E_j + F_j^{(p)}) + \frac{1}{3} A_{ijk}^{(p)} F_{jk}^{(p)} \tag{2.56}$$

and

$$\theta_{ij}^{(p)} = \theta_{0ij}^{(p)} + A_{kij}^{(p)} (E_{0k} + F_k^{(p)}) + C_{ijkl}^{(p)} F_{kl}^{(p)}, \tag{2.57}$$

where  $\mu_{0i}^{(p)}$  and  $\theta_{0ij}^{(p)}$  are the permanent dipole and quadrupole moments of the molecule respectively, while  $F_i^{(p)}$  and  $F_{ij}^{(p)}$  are the static field and field gradient arising at molecule  $p$  due to the permanent and induced dipole and quadrupole moments of molecule  $q$  as given by

$$F_i^{(p)} = T_{ij} \mu_j^{(q)} - \frac{1}{3} T_{ijk}^{(p)} \theta_{jk}^{(q)} \tag{2.58}$$

and

$$F_{ij}^{(p)} = T_{ijk}^{(p)} \mu_k^{(q)} - \frac{1}{3} T_{ijkl} \theta_{kl}^{(q)}. \quad (2.59)$$

Repeated substitutions of  $F_i^{(p)}$ ,  $F_{ij}^{(p)}$ ,  $\mu_i^{(q)}$  and  $\theta_{ij}^{(q)}$  into equation (2.56) yields an expression for  $\mu_i^{(p)}$  which is provided explicitly in Appendix A.3.

Equation (2.55) and the equation for  $\mu_i^{(p)}$  in Appendix A.3 together yield an expression for the potential energy of molecule  $p$  arising from the applied static field  $E_i$  and the fields arising from molecule  $q$ , this expression being provided in Appendix A.4. The interacting pair's potential energy becomes

$$U^{(12)}(\tau, E) = U^{(12)}(\tau, 0) + U^{(1)}(\tau, E) + U^{(2)}(\tau, E). \quad (2.60)$$

The term  $\frac{1}{2} \left( \overline{\frac{\partial^2 \pi^{(12)}(\tau, E)}{\partial E^2}} \right)_{E=0}$  in the expression for  $B_K$  given by equation (2.41) can now be evaluated. The isotropic averages in equation (2.38), namely

$$\begin{aligned} \frac{1}{2} \left( \overline{\frac{\partial^2 \pi^{(12)}(\tau, E)}{\partial E^2}} \right)_{E=0} &= \frac{1}{2} \left\langle \frac{\partial^2 \pi^{(12)}}{\partial E^2} \right\rangle - \frac{1}{2k_B T} \left\langle 2 \frac{\partial \pi^{(12)}}{\partial E} \frac{\partial U^{(12)}}{\partial E} + \pi^{(12)} \frac{\partial^2 U^{(12)}}{\partial E^2} \right\rangle \\ &\quad + \frac{1}{2(k_B T)^2} \left\langle \pi^{(12)} \left( \frac{\partial U^{(12)}}{\partial E} \right)^2 \right\rangle, \end{aligned} \quad (2.61)$$

are now evaluated. Equation (2.54), coupled with the recognition that molecule 1 and molecule 2 are identical such that the isotropic averages of their polarizabilities must be the same, gives rise to the following rearrangement:

$$\begin{aligned} \frac{1}{2} \left\langle \frac{\partial^2 \pi^{(12)}}{\partial E^2} \right\rangle &= \frac{1}{2} \left\langle \frac{\partial^2 \pi^{(1)}}{\partial E^2} \right\rangle + \frac{1}{2} \left\langle \frac{\partial^2 \pi^{(2)}}{\partial E^2} \right\rangle \\ &= \left\langle \frac{\partial^2 \pi^{(1)}}{\partial E^2} \right\rangle. \end{aligned} \quad (2.62)$$

Similar arguments, together with equation (2.61), give

$$\left\{ \begin{array}{l} \left\langle \frac{\partial \pi^{(12)}}{\partial E} \frac{\partial U^{(12)}}{\partial E} \right\rangle = \left\langle 2 \frac{\partial \pi^{(1)}}{\partial E} \frac{\partial U^{(1)}}{\partial E} \right\rangle + \left\langle 2 \frac{\partial \pi^{(1)}}{\partial E} \frac{\partial U^{(2)}}{\partial E} \right\rangle \\ \left\langle \pi^{(12)} \frac{\partial^2 U^{(12)}}{\partial E^2} \right\rangle = \left\langle 2 \pi^{(1)} \frac{\partial^2 U^{(1)}}{\partial E^2} \right\rangle + \left\langle 2 \pi^{(1)} \frac{\partial^2 U^{(2)}}{\partial E^2} \right\rangle \end{array} \right\} \quad (2.63)$$

and

$$\left\langle \pi^{(12)} \left( \frac{\partial U^{(12)}}{\partial E} \right)^2 \right\rangle = 2 \left[ \left\langle \pi^{(1)} \left( \frac{\partial U^{(1)}}{\partial E} \right)^2 \right\rangle + \left\langle 2 \pi^{(1)} \frac{\partial U^{(1)}}{\partial E} \frac{\partial U^{(2)}}{\partial E} \right\rangle + \left\langle \pi^{(1)} \left( \frac{\partial U^{(2)}}{\partial E} \right)^2 \right\rangle \right]. \quad (2.64)$$

Collecting the expressions gives

$$\begin{aligned} \frac{1}{2} \left( \frac{\partial^2 \overline{\pi^{(12)}(\tau, E)}}{\partial E^2} \right)_{E=0} &= \left\langle \frac{\partial^2 \pi^{(1)}}{\partial E^2} \right\rangle - \frac{1}{k_B T} \left\{ \left\langle 2 \frac{\partial \pi^{(1)}}{\partial E} \frac{\partial U^{(1)}}{\partial E} \right\rangle + \left\langle 2 \frac{\partial \pi^{(1)}}{\partial E} \frac{\partial U^{(2)}}{\partial E} \right\rangle \right\} \\ &\quad - \frac{1}{k_B T} \left\{ \left\langle \pi^{(1)} \frac{\partial^2 U^{(1)}}{\partial E^2} \right\rangle + \left\langle \pi^{(1)} \frac{\partial^2 U^{(2)}}{\partial E^2} \right\rangle \right\} + \\ &\quad \frac{1}{(k_B T)^2} \left\{ \left\langle \pi^{(1)} \left( \frac{\partial U^{(1)}}{\partial E} \right)^2 \right\rangle + \left\langle \pi^{(1)} \left( \frac{\partial U^{(2)}}{\partial E} \right)^2 \right\rangle + \left\langle 2 \pi^{(1)} \frac{\partial U^{(1)}}{\partial E} \frac{\partial U^{(2)}}{\partial E} \right\rangle \right\}. \end{aligned} \quad (2.65)$$

Up to this point, the analysis has been general, allowing both for dipolar and non-dipolar molecules. This will aid future investigation of the quadrupole-induced-dipole contribution for dipolar species, although it is anticipated that the

dipole-induced-dipole contribution will, in general, swamp the QID terms (possible exceptions are molecules with a small permanent dipole moment, like carbon monoxide). From this juncture, the focus is solely on non-dipolar molecules, and the surviving terms are

$$\begin{aligned} \left\{ \frac{1}{2} \left( \frac{\partial^2 \overline{\pi}^{(12)}(\tau, E)}{\partial E^2} \right)_{E=0} - \left( \frac{\partial^2 \overline{\pi}}{\partial E^2} \right)_{E=0} \right\} &= \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7 + \dots \\ &\quad + \gamma_1 \alpha_1 + \gamma_1 \alpha_2 + \dots \\ &\quad + \theta_2 \alpha_3 + \theta_2 \alpha_4 + \theta_2 \alpha_5 + \theta_2 \alpha_6 + \theta_2 \alpha_7 \dots , \end{aligned} \tag{2.66}$$

which are given explicitly below. The series of terms purely in the polarizability have previously been evaluated up to  $\alpha_5$  [11, 12], but have been extended here to include  $\alpha_6$  and  $\alpha_7$ . The reason for this was to verify that the series had converged to a meaningful numerical result: for C<sub>2</sub>H<sub>4</sub> at the lower temperatures of around 200 K,  $\alpha_6$  contributes 3.3% to  $B_K$ , which is non-negligible, while  $\alpha_7$  has diminished to 0.25% of  $B_K$ , suggesting convergence of the series has been achieved. For CO<sub>2</sub>,  $\alpha_6$  and  $\alpha_7$  contribute only 0.3% and 0.01% to  $B_K$  respectively at  $T = 200$  K, while for C<sub>2</sub>H<sub>6</sub> the respective contributions at 200 K are 1.2% and 0.06%.

The series of terms in the second hyperpolarizability term were previously found to contribute negligibly for C<sub>2</sub>H<sub>4</sub> (0.04% at 333 K) [12], so are omitted here, as are any contributions arising from the minuscule  $C$ -tensor.

Hohls [13] evaluated the terms  $\theta_2 \alpha_3$ ,  $\theta_2 \alpha_4$  and  $\theta_2 \alpha_5$ . Unfortunately, the terms for  $\theta_2 \alpha_4$  and  $\theta_2 \alpha_5$  in her thesis are missing some of the contributing expressions, and while the lowest-order  $\theta_2 \alpha_3$  term has all contributing expressions, the calculated contributions to  $B_K$  for CO<sub>2</sub>, for example, are 5 times smaller than what is achieved in this work. The algebra in this work has consequently been thor-

oughly re-checked to ensure no erroneous inputs via Mathematica, and found to be accurate.

The explicit expressions for  $\alpha_2$  to  $\theta_2\alpha_7$  are now provided.

$$\alpha_2 = \frac{1}{k_B T} \left\{ \alpha_{ab}^{(1)} a_{pq}^{(2)} \right\} \langle a_a^x a_b^x a_p^x a_q^x - a_a^y a_b^y a_p^x a_q^x \rangle, \quad (2.67)$$

$$\begin{aligned} \alpha_3 = & \frac{1}{k_B T} \left\{ \alpha_{ad}^{(1)} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} + \alpha_{ad}^{(1)} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} \right. \\ & \left. + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} a_{ps}^{(1)} + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} a_{ps}^{(2)} \right\} \\ & \times \langle a_a^x a_d^x a_p^x a_s^x - a_a^y a_d^y a_p^x a_s^x \rangle, \end{aligned} \quad (2.68)$$

$$\begin{aligned} \alpha_4 = & \frac{1}{k_B T} \left\{ \alpha_{af}^{(1)} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tu}^{(1)} + \alpha_{af}^{(1)} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{st} a_{tu}^{(2)} \right. \\ & + \alpha_{ab}^{(1)} T_{bc} \alpha_{cf}^{(2)} a_{pq}^{(1)} T_{qr} a_{ru}^{(2)} + \alpha_{ab}^{(1)} T_{bc} \alpha_{cf}^{(2)} a_{pq}^{(2)} T_{qr} a_{ru}^{(1)} \\ & \left. + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{ef}^{(1)} a_{pu}^{(1)} + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{ef}^{(1)} a_{pu}^{(2)} \right\} \\ & \times \langle a_a^x a_f^x a_p^x a_u^x - a_a^y a_f^y a_p^x a_u^x \rangle, \end{aligned} \quad (2.69)$$

$$\begin{aligned}
\alpha_5 &= \frac{1}{k_B T} \left\{ \alpha_{ah}^{(1)} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tu}^{(1)} T_{uv} a_{vw}^{(2)} \right. \\
&\quad + \alpha_{ah}^{(1)} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{st} a_{tu}^{(2)} T_{uv} a_{vw}^{(1)} \\
&\quad + \alpha_{ab}^{(1)} T_{bc} \alpha_{ch}^{(2)} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tw}^{(1)} \\
&\quad + \alpha_{ab}^{(1)} T_{bc} \alpha_{ch}^{(2)} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{st} a_{tw}^{(2)} \\
&\quad + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{eh}^{(1)} a_{pq}^{(1)} T_{qr} a_{rw}^{(2)} \\
&\quad + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{eh}^{(1)} a_{pq}^{(2)} T_{qr} a_{rw}^{(1)} \\
&\quad + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{ef}^{(1)} T_{fg} \alpha_{gh}^{(2)} a_{pw}^{(1)} \\
&\quad \left. + \alpha_{ab}^{(1)} T_{bc} \alpha_{cd}^{(2)} T_{de} \alpha_{ef}^{(1)} T_{fg} \alpha_{gh}^{(2)} a_{pw}^{(2)} \right\} \\
&\quad \times \langle a_a^x a_h^x a_p^x a_w^x - a_a^y a_h^y a_p^x a_w^x \rangle, \tag{2.70}
\end{aligned}$$

$$\begin{aligned}
\alpha_6 &= \frac{1}{k_B T} \left\{ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rv}^{(1)} \right. \\
&\quad + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\omega}^{(1)} a_{iv}^{(1)} \\
&\quad + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pv}^{(2)} \\
&\quad + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kv}^{(2)}
\end{aligned}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mv}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\omega}^{(1)} a_{iv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mv}^{(2)} \Big\}$$

$$\times \langle a_\alpha^x a_\omega^x a_i^x a_v^x - a_\alpha^y a_\omega^y a_i^x a_v^x \rangle \quad (2.71)$$

$$\alpha_7 = \frac{1}{k_B T} \left\{ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{st} a_{tv}^{(2)} \right.$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\phi}^{(1)} T_{\phi\lambda} \alpha_{\lambda\omega}^{(2)} a_{iv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\phi}^{(1)} a_{ij}^{(1)} T_{jk} a_{kv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mv}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\phi}^{(1)} T_{\phi\lambda} \alpha_{\lambda\omega}^{(2)} a_{iv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rv}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} T_{\mu\nu} \alpha_{\nu\phi}^{(1)} a_{ij}^{(2)} T_{jk} a_{kv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pv}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\mu}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mv}^{(2)} \Big\}$$

$$\times \langle a_\alpha^x a_\omega^x a_i^x a_v^x - a_\alpha^y a_\omega^y a_i^x a_v^x \rangle \quad (2.72)$$

$$\theta_2 \alpha_3 = \frac{1}{9} \frac{1}{(k_B T)^2} \left\{ \alpha_{\alpha\tau}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bch} \theta_{0ch}^{(2)} \right.$$

$$+ \alpha_{\alpha\tau}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bch} \theta_{0ch}^{(1)} \Big\}$$

$$\times \langle a_\alpha^x a_\tau^x a_a^x a_i^x - a_\alpha^y a_\tau^y a_a^x a_i^x \rangle, \quad (2.73)$$

$$\theta_2 \alpha_4 = \frac{1}{3(k_B T)^2} \left\{ \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{abc} \theta_{0ct}^{(2)} \right.$$

$$\begin{aligned}
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{det} \theta_{0et}^{(1)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \\
& +\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{abc} \theta_{0ct}^{(1)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)} \\
& -2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{abc} \theta_{0ct}^{(1)} \\
& +2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)} \\
& +2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)} \Big\} \\
& \times \langle a_\alpha^x a_\omega^x a_i^x a_a^x - a_\alpha^y a_\omega^y a_i^x a_a^x \rangle \quad (2.74) \\
\theta_2 \alpha_5 & = \frac{1}{3(kT)^2} \left\{ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{det} \theta_{0et}^{(1)} \right. \\
& +\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fgt} \theta_{0gt}^{(2)} \\
& \left. +\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \right\}
\end{aligned}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{det} \theta_{0et}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgt} \theta_{0gt}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgt} \theta_{0gt}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+ \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)} \}$$

$$\times \langle a_\alpha^x a_\omega^x a_i^x a_a^x - a_\alpha^y a_\omega^y a_i^x a_a^x \rangle \quad (2.75)$$

$$\begin{aligned}
\theta_2 \alpha_6 = & \frac{1}{3(kT)^2} \left\{ -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrv} \theta_{0rv}^{(1)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \right. \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrv} \theta_{0rv}^{(1)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fgt} \theta_{0gt}^{(2)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{det} \theta_{0et}^{(1)} \\
& + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{det} \theta_{0et}^{(1)} \\
& + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \\
& + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \\
& -\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)} \\
& + \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bct} \theta_{0ct}^{(2)} \\
& -\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hst} \theta_{0st}^{(2)}
\end{aligned}$$

$$-\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qrv} \theta_{0rv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$-\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgt} \theta_{0gt}^{(1)}$$

$$-\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hst} \theta_{0st}^{(2)}$$

$$+2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrv} \theta_{0rv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgt} \theta_{0gt}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$-2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$-2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgt} \theta_{0gt}^{(1)}$$

$$-2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$+2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{det} \theta_{0et}^{(2)}$$

$$+2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)}$$

$$\left. -2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bct} \theta_{0ct}^{(1)} \right\}$$

$$\times \langle a_\alpha^x a_\omega^x a_i^x a_a^x - a_\alpha^y a_\omega^y a_i^x a_a^x \rangle \quad (2.76)$$

$$\theta_2 \alpha_7 = \frac{1}{3(kT)^2} \left\{ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fgu} \theta_{0gu}^{(2)} \right.$$

$$+ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fg} a_{gh}^{(2)} T_{hsu} \theta_{0su}^{(1)}$$

$$+ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} \theta_{0rv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{deu} \theta_{0eu}^{(1)}$$

$$+ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fg} a_{gh}^{(2)} T_{hw} a_{wy}^{(1)} T_{yzu} \theta_{0zu}^{(2)}$$

$$+ \alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{stv} \theta_{0tv}^{(2)} a_{ab}^{(1)} T_{bcu} \theta_{0cu}^{(2)}$$

$$- \alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fg} a_{gh}^{(2)} T_{hsu} \theta_{0su}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrv} \theta_{0rv}^{(1)} a_{ab}^{(1)} T_{bcu} \theta_{0cu}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fgu} \theta_{0gu}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{deu} \theta_{0eu}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{deu} \theta_{0eu}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(1)} T_{bcu} \theta_{0cu}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bc} a_{cd}^{(2)} T_{de} a_{ef}^{(1)} T_{fgu} \theta_{0gu}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(1)} T_{bcu} \theta_{0cu}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\kappa}^{(2)} T_{\kappa\lambda} \alpha_{\lambda\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(1)} T_{bcu} \theta_{0cu}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgu} \theta_{0gu}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hsu} \theta_{0su}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qrv} \theta_{0rv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hw} a_{wy}^{(2)} T_{yzu} \theta_{0zu}^{(1)}$$

$$+\alpha_{\alpha\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{stv} \theta_{0tv}^{(1)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hsu} \theta_{0su}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{np} a_{pq}^{(1)} T_{qrv} \theta_{0rv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgu} \theta_{0gu}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgu} \theta_{0gu}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lm} a_{mn}^{(2)} T_{npv} \theta_{0pv}^{(1)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)}$$

$$-\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\kappa}^{(2)} a_{ij}^{(2)} T_{jk} a_{kl}^{(1)} T_{lmv} \theta_{0mv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)}$$

$$+\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\kappa}^{(2)} T_{\kappa\lambda} \alpha_{\lambda\omega}^{(1)} a_{ij}^{(2)} T_{jkv} \theta_{0kv}^{(1)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(2)}$$

$$-2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgu} \theta_{0gu}^{(1)}$$

$$-2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hsu} \theta_{0su}^{(2)}$$

$$-2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrv} \theta_{0rv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)}$$

$$\begin{aligned}
& -2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hw} a_{wy}^{(2)} T_{yzu} \theta_{0zu}^{(1)} \\
& -2\alpha_{\alpha\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rs}^{(1)} T_{stv} \theta_{0tv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(2)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fg} a_{gh}^{(1)} T_{hsu} \theta_{0su}^{(2)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} \theta_{0rv}^{(1)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{de} a_{ef}^{(2)} T_{fgu} \theta_{0gu}^{(1)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)} \\
& -2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\omega}^{(1)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmv} \theta_{0mv}^{(1)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0eu}^{(2)} \\
& -2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bc} a_{cd}^{(1)} T_{deu} \theta_{0gu}^{(1)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\omega}^{(2)} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npv} \theta_{0pv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)} \\
& +2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\kappa}^{(2)} T_{\kappa\lambda} \alpha_{\lambda\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)} \\
& -2\alpha_{\alpha\beta}^{(1)} T_{\beta\gamma} \alpha_{\gamma\delta}^{(2)} T_{\delta\epsilon} \alpha_{\epsilon\eta}^{(1)} T_{\eta\theta} \alpha_{\theta\kappa}^{(2)} T_{\kappa\lambda} \alpha_{\lambda\omega}^{(1)} a_{ij}^{(1)} T_{jkv} \theta_{0kv}^{(2)} a_{ab}^{(2)} T_{bcu} \theta_{0cu}^{(1)} \Big\} \\
& \times \langle a_\alpha^x a_\omega^x a_i^x a_a^x - a_\alpha^y a_\omega^y a_i^x a_a^x \rangle \tag{2.77}
\end{aligned}$$

Using equations (2.21) and (2.27), the isotropic averages can be evaluated. The procedure is illustrated by considering the term for  $\theta_2\alpha_3$  in equation (2.73):

$$\begin{aligned} \theta_2\alpha_3 = \frac{1}{270} \frac{1}{(k_B T)^2} & \left\{ -6\alpha\theta_{0ab}^{(2)} T_{abc} a_{cd}^{(1)} a_{de}^{(1)} T_{efg} \theta_{0fg}^{(2)} + 6\theta_{0ab}^{(2)} T_{abc} a_{cd}^{(1)} \alpha_{de}^{(1)} a_{ef}^{(1)} T_{fgh} \theta_{0gh}^{(2)} \right. \\ & -6\alpha\theta_{0ab}^{(1)} T_{abc} a_{cd}^{(2)} a_{de}^{(2)} T_{efg} \theta_{0fg}^{(1)} + 6\theta_{0ab}^{(1)} T_{abc} a_{cd}^{(2)} \alpha_{de}^{(1)} a_{ef}^{(2)} T_{fgh} \theta_{0gh}^{(1)} \\ & \left. -12\alpha\theta_{0ab}^{(2)} T_{abc} a_{cd}^{(1)} a_{de}^{(2)} T_{efg} \theta_{0fg}^{(1)} + 12\theta_{0ab}^{(2)} T_{abc} a_{cd}^{(1)} \alpha_{de}^{(1)} a_{ef}^{(2)} T_{fgh} \theta_{0gh}^{(1)} \right\}. \end{aligned} \quad (2.78)$$

The tensor manipulation facilities of the algebraic manipulation package Mathematica are then used to evaluate the expressions for each term: these expressions are extremely large, taking many pages to express, and so cannot be quoted here. When numerically averaged (*i.e.* integrated) over pair interaction coordinates by equation (2.42), each term's contribution to  $B_K$  is obtained. A sample Fortran program (to achieve numerical integration of the  $\theta_2\alpha_3$  term's contribution via equation (2.42), achieved by Gaussian quadrature) is contained in Appendix B. This requires the classical intermolecular potential energy  $U_{12}(\tau)$ . Couling and Graham [12] have used the classical potential

$$U_{12}(\tau) = U_{LJ} + U_{\mu,\mu} + U_{\mu,\theta} + U_{\theta,\theta} + U_{\mu,\text{ind}\mu} + U_{\theta,\text{ind}\mu} + U_{\text{shape}} \quad (2.79)$$

where  $U_{LJ}$  is the Lennard-Jones 6:12 potential,  $U_{\mu,\mu}$ ,  $U_{\mu,\theta}$  and  $U_{\theta,\theta}$  are the

dipole-dipole, dipole-quadrupole and quadrupole-quadrupole interaction energies of the two molecules, and  $U_{\mu,\text{ind}\mu}$  and  $U_{\theta,\text{ind}\mu}$  are the dipole-induced-dipole and quadrupole-induced-dipole interaction energies of the two molecules.  $U_{\text{shape}}$  accounts for the angular dependence of short-range repulsive force for non-spherical molecules. Explicit expressions for these various contributions to  $U_{12}(\tau)$  have been provided [11, 12].

In equation (2.42), the ranges of the angular variables were divided into 16 intervals each, while the intermolecular separation was given a range of 0.1 nm to 3.0 nm divided into 64 intervals. The Fortran programs were run in double precision on a dual core processor PC using the Salford F90 compiler. Program run-times were of the order of 15 minutes each.

Computation of  $B_K$  for the species  $\text{C}_2\text{H}_4$ ,  $\text{CO}_2$  and  $\text{C}_2\text{H}_6$  are now reported, together with comparison with available experimental data.

# Chapter 3

## Results and Discussion

### 3.1 Ethene

The molecular data required in the calculations of  $B_K$  for ethene ( $\text{C}_2\text{H}_4$ ) are presented in Table 3.1. Use has been made of the optimized values for the Lennard-Jones force constants  $R_0$  and  $\epsilon/k$  as well as the shape parameters  $D_1$  and  $D_2$  which were obtained by fitting the calculated second pressure virial coefficient  $B(T)$  to experimental data [20] over a range of temperature [21]. Ethene is of  $D_{2h}$  symmetry, and the previous calculations of the second light-scattering virial coefficient  $B_\rho$  have demonstrated that only when full account of the molecular symmetry is taken into consideration is agreement between measured and calculated  $B_\rho$  values achieved (to better than 3%).

Tables 3.2 to 3.6 provide the relative magnitudes of the various contributions to  $B_K$  calculated at intervals of temperature spanning 202.4 K and 363.7 K (chosen because the measured data fall within these limits). At  $T = 202.4$  K, the pure polarizability terms  $\sum_{n=2}^7 \alpha_n$  contribute 53% to  $B_K$ , while the quadrupole series of terms  $\sum_{n=3}^7 \theta_2 \alpha_n$  account for 47%. As the temperature increases, the quadrupole terms begin to gradually diminish, contributing only 11.5% to  $B_K$  at  $T = 363.7$  K.

Table 3.1: Molecular properties of ethene used in the calculation of  $B_K^{theory}(T)$ .

Properties	Value	Reference
$R_0(\text{nm})$	0.4232	[11, 21, 22]
$\varepsilon/k(\text{K})$	190.0	[11, 21, 22]
$D_1$	0.22965	[11, 21, 22]
$D_2$	0.21383	[11, 21, 22]
$10^{40}\theta_{11} (\text{Cm}^2)$	5.370	[23]
$10^{40}\theta_{22} (\text{Cm}^2)$	-10.92	[23]
$10^{40}\theta_{33} (\text{Cm}^2)$	5.549	[23]
$10^{40}\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	4.7124	[11, 21, 24, 25]
$10^{40}\Delta\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	2.0215	[11, 21, 24, 25]
$10^{40}\alpha_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.305	[11, 21, 24, 25]
$10^{40}\alpha_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	3.804	[11, 21, 24, 25]
$10^{40}\alpha_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	6.029	[11, 21, 24, 25]
$10^{40}a (\text{C}^2\text{m}^2\text{J}^{-1})$	4.571	[11, 21, 26]
$10^{40}\Delta a (\text{C}^2\text{m}^2\text{J}^{-1})$	1.914	[11, 21, 26]
$10^{40}a_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.245	[11, 21, 26]
$10^{40}a_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	3.666	[11, 21, 26]
$10^{40}a_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	5.803	[11, 21, 26]

Table 3.2: The relative magnitudes of the various contributions to  $B_K$  for ethene calculated at  $T = 202.4$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	25.885	49.703
$\alpha_3$	-57.240	-109.909
$\alpha_4$	54.733	105.095
$\alpha_5$	2.536	4.869
$\alpha_6$	1.699	3.262
$\alpha_7$	0.128	0.246
$\theta_2\alpha_3$	-3.806	-7.308
$\theta_2\alpha_4$	17.141	32.913
$\theta_2\alpha_5$	7.154	13.737
$\theta_2\alpha_6$	3.073	5.901
$\theta_2\alpha_7$	0.776	1.490
$\sum_n a_n$	27.741	53.004
$\sum_n \theta_2 a_n$	24.339	46.996
$B_k$	52.080	100

Table 3.3: The relative magnitudes of the various contributions to  $B_K$  for ethene calculated at  $T = 250.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	7.852	30.982
$\alpha_3$	-19.836	-78.269
$\alpha_4$	28.712	113.292
$\alpha_5$	1.514	5.974
$\alpha_6$	0.611	2.411
$\alpha_7$	0.047	0.185
$\theta_2\alpha_3$	-0.066	-0.260
$\theta_2\alpha_4$	4.147	16.363
$\theta_2\alpha_5$	1.598	6.305
$\theta_2\alpha_6$	0.617	2.435
$\theta_2\alpha_7$	0.148	0.584
$\sum_n a_n$	18.900	74.577
$\sum_n \theta_2 a_n$	6.443	25.423
$B_k$	25.343	100

Table 3.4: The relative magnitudes of the various contributions to  $B_K$  for ethene calculated at  $T = 300.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	3.427	19.526
$\alpha_3$	-9.937	-56.617
$\alpha_4$	19.718	112.344
$\alpha_5$	1.098	6.256
$\alpha_6$	0.345	1.966
$\alpha_7$	0.027	0.154
$\theta_2\alpha_3$	0.330	1.880
$\theta_2\alpha_4$	1.681	9.578
$\theta_2\alpha_5$	0.607	3.458
$\theta_2\alpha_6$	0.210	1.196
$\theta_2\alpha_7$	0.047	0.270
$\sum_n a_n$	14.677	83.617
$\sum_n \theta_2 a_n$	2.876	16.383
$B_k$	17.552	100

Table 3.5: The relative magnitudes of the various contributions to  $B_K$  for ethene calculated at  $T = 333.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	2.264	15.217
$\alpha_3$	-7.117	-47.835
$\alpha_4$	16.515	111.001
$\alpha_5$	0.938	6.304
$\alpha_6$	0.270	1.815
$\alpha_7$	0.021	0.141
$\theta_2\alpha_3$	0.339	2.278
$\theta_2\alpha_4$	1.105	7.427
$\theta_2\alpha_5$	0.388	2.608
$\theta_2\alpha_6$	0.127	0.854
$\theta_2\alpha_7$	0.028	0.188
$\sum_n a_n$	12.892	86.649
$\sum_n \theta_2 a_n$	1.986	13.351
$B_k$	14.878	100

Table 3.6: The relative magnitudes of the various contributions to  $B_K$  for ethene calculated at  $T = 363.7$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	1.639	12.490
$\alpha_3$	-5.507	-41.965
$\alpha_4$	14.411	109.817
$\alpha_5$	0.830	6.325
$\alpha_6$	0.226	1.722
$\alpha_7$	0.018	0.137
$\theta_2\alpha_3$	0.314	2.393
$\theta_2\alpha_4$	0.807	6.150
$\theta_2\alpha_5$	0.279	2.126
$\theta_2\alpha_6$	0.087	0.663
$\theta_2\alpha_7$	0.018	0.137
$\sum_n a_n$	11.618	88.532
$\sum_n \theta_2 a_n$	1.505	11.468
$B_k$	13.123	100

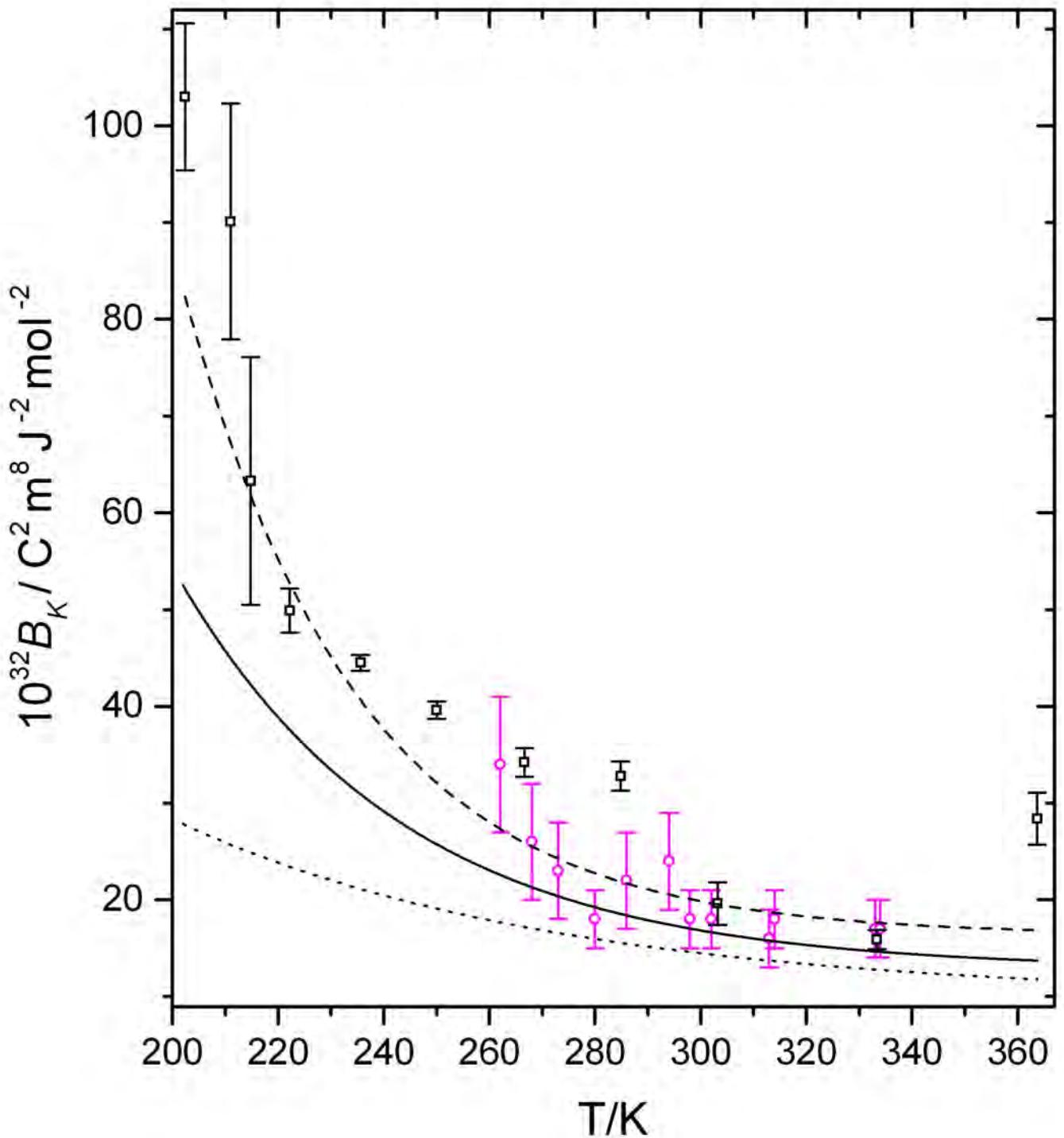


Figure 3.1: Temperature dependence of the calculated and measured second Kerr-effect virial coefficients of ethene. The dotted curve is for the pure polarizability terms, while the solid curve also includes quadrupole contributions, both curves being for the molecular parameter set in Table 3.1. The dashed curve is for the alternative force constants discussed in the text. Circles are the experimental data of Buckingham *et al.*[27] while squares are the measured data of Tammer and Hüttner [25].

Figure 3.1 contains a plot of the available measured  $B_K$  data together with the computed  $B_K$  curves both of the pure polarizability terms (dotted line) as well as with inclusion of the quadrupole terms (solid line). Note that the collision-induced  $\theta_2\alpha_4$  term makes the dominant contribution to the quadrupole series for all temperatures examined, and that the series converges quite rapidly by the  $\theta_2\alpha_7$  term, which contributes 1.5% to  $B_K$  at 202.4 K, but only 0.14% at  $T = 363.7$  K. It is especially at the lower temperatures that the higher-order terms require inclusion,  $\theta_2\alpha_6$  contributing 6% to  $B_K$  at 202.4 K, although only contributing 0.7% at 363.7 K.

The experimental data are of limited precision, often with considerable error bars, and the accuracy is questionable, with large scatter in the points. At the lower temperatures, the measured data span a small range of pressure, so that the extracted  $B_K$  values are rendered especially imprecise and inaccurate.

To explore the effect of a change in force constants on the calculated  $B_K$  curves, calculations were performed for  $R_0 = 0.41$  nm,  $\epsilon/k = 195$  K and  $D_1 = 0.22874$ ,  $D_2 = 0.21298$ . The shape factors were obtained by optimizing the calculated second pressure virial coefficients to the measured data, although the fit was 5% more discrepant than for the carefully-optimized force constants in Table 3.1. The dashed  $B_K$  curve in Figure 3.1 is obtained, which more closely matches the low-temperature  $B_K$  measured data, although more precise re-measurements would be useful to decide on the accuracy of these points. These new force constants yield a second light-scattering virial coefficient at room temperature that is 15% away from the measured data, suggesting that these force constants are not optimal.

Hohls' calculated  $B_K$  terms are sometimes almost an order of magnitude in error [13], and after a thorough and careful investigation of the present work, we conclude that something has gone awry in her analysis.

Tammer and Hüttner performed calculations of  $B_K$  for  $\text{C}_2\text{H}_4$  using DID theory but approximating the molecule to be of axial symmetry [27]. At  $T = 202.4$  K, for example, their computed  $B_K$  is some 21% lower than our pure polarizability term contributions, further indicating the necessity of taking full molecular symmetry into account. They have neglected QID contributions altogether.

## 3.2 Carbon Dioxide

Table 3.7 contains the molecular properties required for the calculations of  $B_K$  for the axially-symmetric carbon dioxide ( $\text{CO}_2$ ) molecule. Again, the same optimized force constants established from earlier work on second light-scattering virial coefficients [11] are used. Like  $\text{C}_2\text{H}_4$ ,  $\text{CO}_2$  has a relatively large quadrupole moment and polarizability anisotropy, and the quadrupole series of terms are found to dominate  $B_K$  at the lower temperatures (67% of  $B_K$  at  $T = 200$  K and 56% at 380 K). Even at 490 K, as the quadrupole contribution diminishes, the pure polarizability terms are only contributing almost equally to  $B_K$  as the quadrupole terms. Here it is the  $\theta_2\alpha_3$  term which dominates the quadrupole series. Tables 3.8 to 3.11 present the relative magnitudes of the various contributions to  $B_K$  over a range of temperature spanning 200 to 290 K. Figure 3.2 makes a comparison with the measured  $B_K$  data of Buckingham *et al.* [26] and of Gentle *et al.* [28]

Table 3.7: Molecular properties of carbon dioxide used in the calculation of  $B_K^{theory}(T)$ .

Properties	Value	Reference
$R_0(\text{nm})$	0.400	[11]
$\varepsilon/k(\text{K})$	190.0	[11]
$D_1$	0.250	[11]
$D_2$	0.000	[11]
$10^{40}\theta_{11} (\text{Cm}^2)$	7.50	[11]
$10^{40}\theta_{22} (\text{Cm}^2)$	7.50	[11]
$10^{40}\theta_{33} (\text{Cm}^2)$	-15.0	[11]
$10^{40}\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	2.9314	[11]
$10^{40}\Delta\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	2.349	[11]
$10^{40}\alpha_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	2.149	[11]
$10^{40}\alpha_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	2.149	[11]
$10^{40}\alpha_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.497	[11]
$10^{40}a (\text{C}^2\text{m}^2\text{J}^{-1})$	2.885	[11]
$10^{40}\Delta a (\text{C}^2\text{m}^2\text{J}^{-1})$	2.252	[11]
$10^{40}a_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	2.134	[11]
$10^{40}a_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	2.134	[11]
$10^{40}a_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.387	[11]

Table 3.8: The relative magnitudes of the various contributions to  $B_K$  for carbon dioxide calculated at  $T = 200.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	3.080	19.941
$\alpha_3$	-5.075	-27.916
$\alpha_4$	7.632	41.983
$\alpha_5$	0.266	1.465
$\alpha_6$	0.050	0.273
$\alpha_7$	0.002	0.013
$\theta_2\alpha_3$	10.288	56.593
$\theta_2\alpha_4$	1.571	8.642
$\theta_2\alpha_5$	0.318	1.750
$\theta_2\alpha_6$	0.041	0.228
$\theta_2\alpha_7$	0.005	0.030
$\sum_n a_n$	5.955	32.757
$\sum_n \theta_2 a_n$	12.224	67.243
$B_k$	18.179	100

Table 3.9: The relative magnitudes of the various contributions to  $B_K$  for carbon dioxide calculated at  $T = 270.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	1.204	14.836
$\alpha_3$	-2.982	-36.742
$\alpha_4$	4.601	56.698
$\alpha_5$	0.155	1.913
$\alpha_6$	0.030	0.368
$\alpha_7$	0.001	0.017
$\theta_2\alpha_3$	4.352	53.616
$\theta_2\alpha_4$	0.600	7.398
$\theta_2\alpha_5$	0.135	1.659
$\theta_2\alpha_6$	0.016	0.217
$\theta_2\alpha_7$	0.002	0.030
$\sum_n a_n$	3.010	37.081
$\sum_n \theta_2 a_n$	5.107	62.919
$B_k$	8.116	100

Table 3.10: The relative magnitudes of the various contributions to  $B_K$  for carbon dioxide calculated at  $T = 380.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.480	12.304
$\alpha_3$	-1.717	-43.975
$\alpha_4$	2.856	73.165
$\alpha_5$	0.096	2.459
$\alpha_6$	0.019	0.491
$\alpha_7$	0.001	0.024
$\theta_2\alpha_3$	1.864	47.747
$\theta_2\alpha_4$	0.235	6.019
$\theta_2\alpha_5$	0.060	1.531
$\theta_2\alpha_6$	0.008	0.205
$\theta_2\alpha_7$	0.001	0.031
$\sum_n a_n$	1.736	44.468
$\sum_n \theta_2 a_n$	2.168	55.532
$B_k$	3.904	100

Table 3.11: The relative magnitudes of the various contributions to  $B_K$  for carbon dioxide calculated at  $T = 490.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.260	10.426
$\alpha_3$	-1.165	-46.715
$\alpha_4$	2.094	83.945
$\alpha_5$	0.071	2.866
$\alpha_6$	0.015	0.588
$\alpha_7$	0.001	0.030
$\theta_2\alpha_3$	1.051	42.135
$\theta_2\alpha_4$	0.127	5.083
$\theta_2\alpha_5$	0.035	1.418
$\theta_2\alpha_6$	0.005	0.194
$\theta_2\alpha_7$	0.001	0.031
$\sum_n a_n$	1.276	51.139
$\sum_n \theta_2 a_n$	1.219	48.861
$B_k$	2.494	100

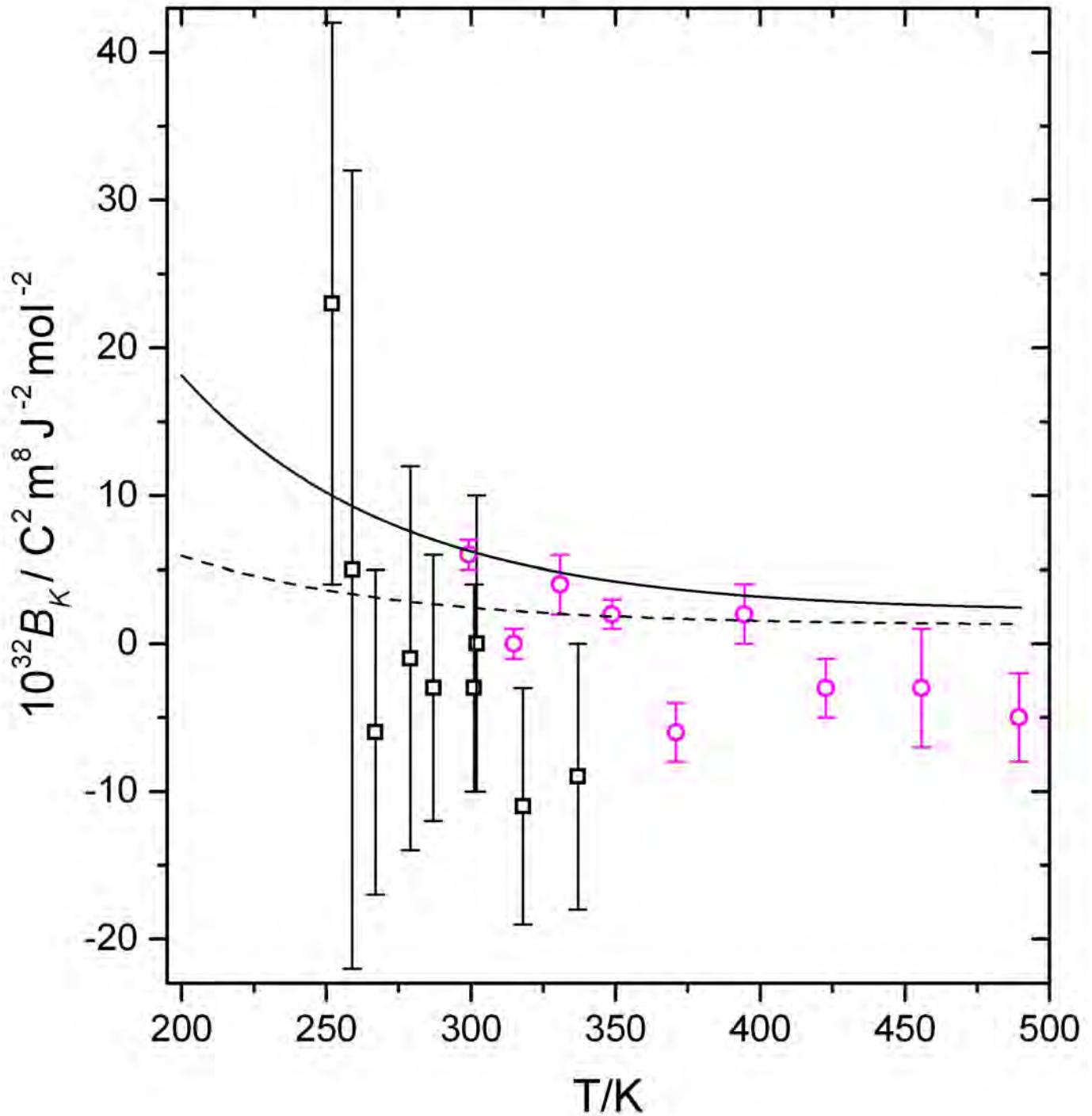


Figure 3.2: Temperature dependence of the calculated and measured second Kerr-effect virial coefficients of CO<sub>2</sub>. The dashed curve is for the pure polarizability terms, while the solid curve includes quadrupole contributions, both for the molecular parameter set in Table 3.7. Squares are the experimental data of Buckingham *et al.*[27] while circles are the measured data of Gentle *et al.* [26].

For CO<sub>2</sub>, the  $\theta_2\alpha_3$  term makes the dominant contribution to the quadrupole series over the range of experimental temperature, the series rapidly converging by the  $\theta_2\alpha_6$  term. The magnitude and sign of the various collision-induced terms depends in part on the intermolecular potential, and hence on the permanent electric quadrupole moment as well as the polarizability and induced dipole and quadrupole moments. At 200 K, the terms in the polarizability contribute only 33% to  $B_K$ , the new QID terms accounting for the other 67%. Unfortunately, the precision and accuracy of the measured  $B_K$  data are rather poor, so that a future goal will be to revisit the experimental measurement of the Kerr effect for this species.

### 3.3 Ethane

Table 3.12 contains the molecular data required in the calculation of  $B_K$  of ethane (C<sub>2</sub>H<sub>6</sub>). Here, the relatively tiny quadrupole moment and polarizability anisotropy of the molecule sees the quadrupole series contributing 0.5% or less to the overall  $B_K$  values. The experimental data span 255 to 318 K [29], and Tables 3.13 to 3.16 present the relative magnitudes of the various contributions to  $B_K$  over the temperature range 200 to 320 K.

Table 3.12: Molecular properties of ethane used in the calculation of  $B_K^{theory}(T)$ .

Properties	Value	Reference
$R_0(\text{nm})$	0.4418	[11]
$\varepsilon/k(\text{K})$	230.0	[11]
$D_1$	0.200	[11]
$D_2$	0.000	[11]
$10^{40}\theta_{11} (\text{Cm}^2)$	1.67	[11]
$10^{40}\theta_{22} (\text{Cm}^2)$	1.67	[11]
$10^{40}\theta_{33} (\text{Cm}^2)$	-3.34	[11]
$10^{40}\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	4.9680	[11]
$10^{40}\Delta\alpha (\text{C}^2\text{m}^2\text{J}^{-1})$	0.743	[11]
$10^{40}\alpha_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.720	[11]
$10^{40}\alpha_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.720	[11]
$10^{40}\alpha_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	5.464	[11]
$10^{40}a (\text{C}^2\text{m}^2\text{J}^{-1})$	4.870	[11]
$10^{40}\Delta a (\text{C}^2\text{m}^2\text{J}^{-1})$	0.638	[11]
$10^{40}a_{11} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.657	[11]
$10^{40}a_{22} (\text{C}^2\text{m}^2\text{J}^{-1})$	4.657	[11]
$10^{40}a_{33} (\text{C}^2\text{m}^2\text{J}^{-1})$	5.295	[11]

Table 3.13: The relative magnitudes of the various contributions to  $B_K$  for ethane calculated at  $T = 200.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.303	1.000
$\alpha_3$	-7.633	-25.230
$\alpha_4$	34.906	115.371
$\alpha_5$	2.112	6.980
$\alpha_6$	0.358	1.182
$\alpha_7$	0.026	0.057
$\theta_2\alpha_3$	0.049	0.162
$\theta_2\alpha_4$	0.096	0.318
$\theta_2\alpha_5$	0.032	0.107
$\theta_2\alpha_6$	0.006	0.019
$\theta_2\alpha_7$	0.001	0.002
$\sum_n a_n$	30.071	99.391
$\sum_n \theta_2 a_n$	0.037	0.122
$B_k$	30.255	100

Table 3.14: The relative magnitudes of the various contributions to  $B_K$  for ethane calculated at  $T = 240.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.171	0.752
$\alpha_3$	-4.734	-20.829
$\alpha_4$	25.428	111.646
$\alpha_5$	1.526	6.698
$\alpha_6$	0.259	1.137
$\alpha_7$	0.019	0.085
$\theta_2\alpha_3$	0.031	0.136
$\theta_2\alpha_4$	0.061	0.266
$\theta_2\alpha_5$	0.020	0.089
$\theta_2\alpha_6$	0.004	0.016
$\theta_2\alpha_7$	0.001	0.002
$\sum_n a_n$	22.660	99.491
$\sum_n \theta_2 a_n$	0.116	0.509
$B_k$	22.776	100

Table 3.15: The relative magnitudes of the various contributions to  $B_K$  for ethane calculated at  $T = 280.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.110	0.603
$\alpha_3$	-3.278	-17.951
$\alpha_4$	19.938	109.182
$\alpha_5$	1.192	6.527
$\alpha_6$	0.203	1.114
$\alpha_7$	0.015	0.085
$\theta_2\alpha_3$	0.021	0.117
$\theta_2\alpha_4$	0.042	0.230
$\theta_2\alpha_5$	0.014	0.077
$\theta_2\alpha_6$	0.003	0.014
$\theta_2\alpha_7$	0.001	0.002
$\sum_n a_n$	18.203	99.678
$\sum_n \theta_2 a_n$	0.080	0.440
$B_k$	18.262	100

Table 3.16: The relative magnitudes of the various contributions to  $B_K$  for ethane calculated at  $T = 320.0$  K.

Contributing Term	$\frac{10^{32} \times \text{Value}}{\text{C}^2 \text{m}^8 \text{J}^{-2} \text{mol}^{-2}}$	% Contribution to $B_K$
$\alpha_2$	0.077	0.500
$\alpha_3$	-2.430	-15.800
$\alpha_4$	16.393	106.606
$\alpha_5$	0.980	6.370
$\alpha_6$	0.168	1.095
$\alpha_7$	0.130	0.843
$\theta_2\alpha_3$	0.016	0.103
$\theta_2\alpha_4$	0.031	0.201
$\theta_2\alpha_5$	0.010	0.068
$\theta_2\alpha_6$	0.002	0.0124
$\theta_2\alpha_7$	0.001	0.002
$\sum_n a_n$	15.318	99.614
$\sum_n \theta_2 a_n$	0.059	0.386
$B_k$	15.377	100

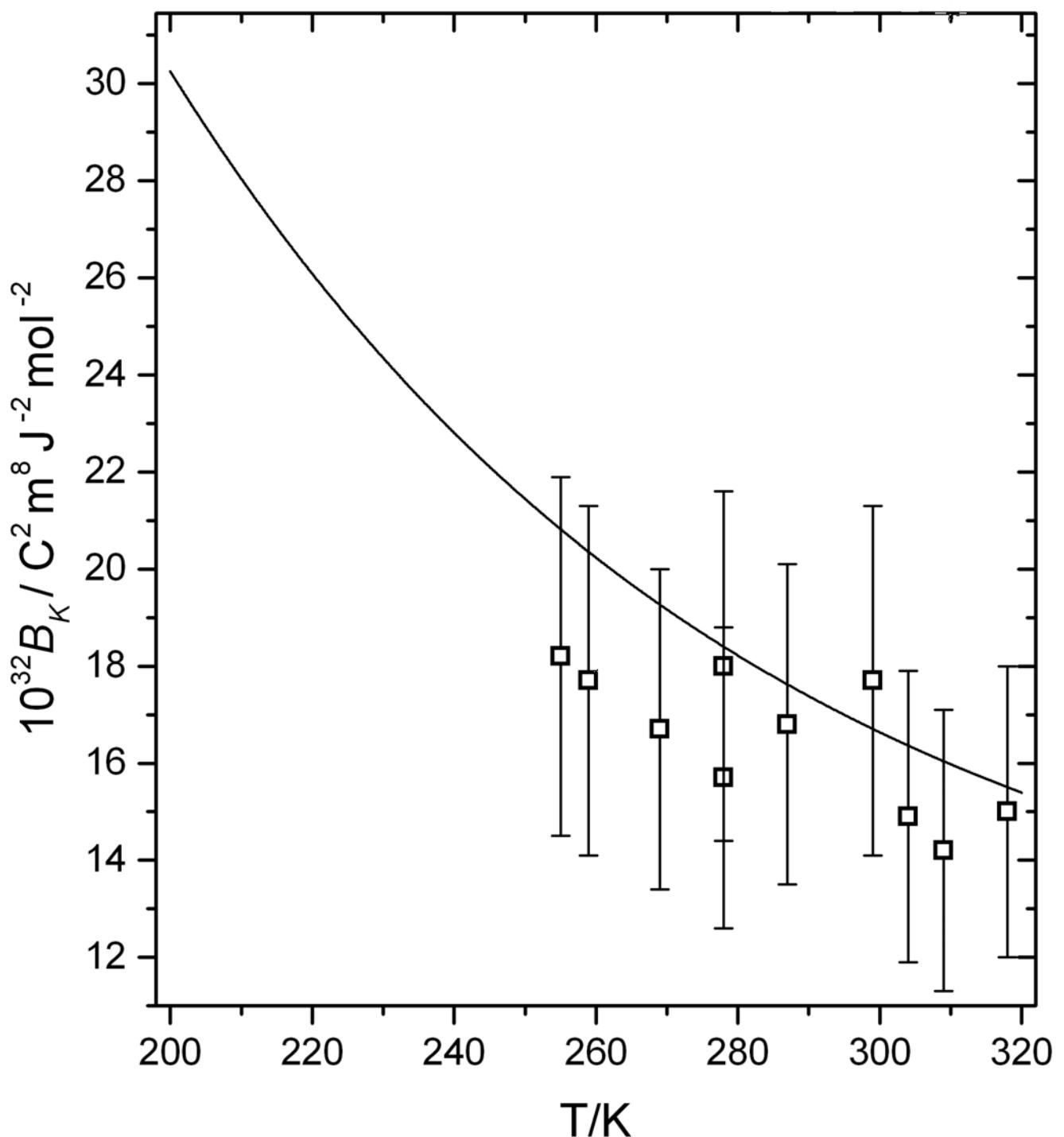


Figure 3.3: Temperature dependence of the calculated and measured second Kerr-effect virial coefficients of ethane. The solid curve includes quadrupole contributions, though more than 99.5% of  $B_K$  arises from the pure polarizability terms. Squares are the measured data of Buckingham [27].

### 3.4 Concluding Remarks

This project has seen the extension of the existing molecular-tensor theory of  $B_K$  to include contributions arising from the molecular electric quadrupole moment. For non-dipolar molecules which possess a relatively large permanent quadrupole moment and polarizability anisotropy, these new terms are seen to make a considerable contribution to  $B_K$ , often in excess of 50%. The calculated  $B_K$  values for C<sub>2</sub>H<sub>4</sub> and CO<sub>2</sub> are seen to be in reasonable agreement with the existing experimental data, though the poor precision and accuracy of the measured data would suggest that more refined experimental measurements are warranted. A new Kerr-effect apparatus is under development [30], and will hopefully soon yield more precise  $B_K$  measurements, which should provide a more stringent test of the molecular-tensor theory presented here.

# Appendix A

## A.1 The Euler angles and the $T$ -tensors.

The relative orientation of an interacting pair of modules under the influence of a static applied electric field  $E_i$  is shown in figure A.1.1 below

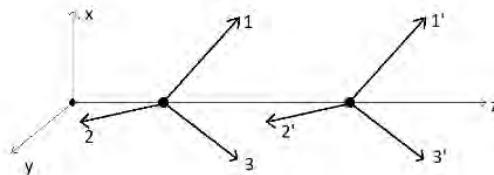


Figure A.1: Molecule-fixed axes  $O(1, 2, 3)$  and  $O(1', 2', 3')$  of the interacting pair of molecules 1 and 2 respectively. The space-fixed axes are  $O(x, y, z)$ .

The space-fixed axes are defined by the direction of the applied uniform electric field, which is  $E_x$ . The molar Kerr-constant determinations are performed in the space-fixed axes, while to exploit the symmetry of the molecule its physical property tensors must be referred to a system of molecule-fixed axes. Since the molecules are tumbling around in space, their molecule-fixed axes are continually changing with respect to the space-fixed axes. The average projection of a

molecule's tensor properties in the space-fixed axes is then obtained by referring the molecular-property tensors to molecule-fixed axes, and then projecting them into the space-fixed axes and averaging the projection over the orientational motion of the molecule.

As before, the Greek tensor subscripts are used to denote the tensor in the space-fixed axes while  $i,j,k$  and  $i',j',k'$  denote the tensors for molecules 1 and 2 respectively, expressed in their own system of molecule-fixed axes as illustrated in figure A.1.1. Nine direction cosines  $a_i^\alpha$  are required to describe the relative orientation of each set of molecule-fixed axes and the space-fixed axes. Euler angles are used to describe an arbitrary rotation of a system of Cartesian axes about its origin. For molecule 1, the nine direction cosines  $a_i^\alpha$  can be expressed as functions of three Euler angles  $\alpha_1, \beta_1$  and  $\gamma_1$  as follows

$$\begin{aligned}
l_i^\alpha &= \begin{bmatrix} \cos\gamma_1 & \sin\gamma_1 & 0 \\ -\sin\gamma_1 & \cos\gamma_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\beta_1 & 0 & -\sin\beta_1 \\ 0 & 1 & 0 \\ \sin\beta_1 & 0 & \cos\beta_1 \end{bmatrix} \begin{bmatrix} \cos\alpha_1 & \sin\alpha_1 & 0 \\ -\sin\alpha_1 & \cos\alpha_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} \cos\alpha_1\cos\beta_1\cos\gamma_1 - \sin\alpha_1\sin\gamma_1 & \sin\alpha_1\cos\beta_1\cos\gamma_1 + \cos\alpha_1\sin\alpha_1\gamma_1 & -\sin\beta_1\cos\gamma_1 \\ -\cos\alpha_1\cos\beta_1\sin\gamma_1 - \sin\alpha_1\cos\gamma_1 & -\sin\alpha_1\cos\beta_1\sin\gamma_1 + \cos\alpha_1\cos\gamma_1 & \sin\beta_1\sin\gamma_1 \\ \cos\alpha_1\sin\beta_1 & \sin\alpha_1\sin\beta_1 & \cos\beta_1 \end{bmatrix} \quad (\text{A.1})
\end{aligned}$$

For molecule 2, the relation between the Euler angles and direction cosines is given as

$$\begin{aligned}
a_{i'}^\alpha &= \begin{bmatrix} \cos\gamma_2 & \sin\gamma_2 & 0 \\ -\sin\gamma_2 & \cos\gamma_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\beta_2 & 0 & -\sin\beta_2 \\ 0 & 1 & 0 \\ \sin\beta_2 & 0 & \cos\beta_2 \end{bmatrix} \begin{bmatrix} \cos\alpha_2 & \sin\alpha_2 & 0 \\ -\sin\alpha_2 & \cos\alpha_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} \cos\alpha_2\cos\beta_2\cos\gamma_2 - \sin\alpha_2\sin\gamma_2 & \sin\alpha_2\cos\beta_2\cos\gamma_2 + \cos\alpha_2\sin\alpha_2\gamma_2 & -\sin\beta_2\cos\gamma_2 \\ -\cos\alpha_2\cos\beta_2\sin\gamma_2 - \sin\alpha_2\cos\gamma_2 & -\sin\alpha_2\cos\beta_2\sin\gamma_2 + \cos\alpha_2\cos\gamma_2 & \sin\beta_2\sin\gamma_2 \\ \cos\alpha_2\sin\beta_2 & \sin\alpha_2\sin\beta_2 & \cos\beta_2 \end{bmatrix} \quad (\text{A.2})
\end{aligned}$$

where

$$\left\{ \begin{array}{l} 0 \leq \alpha \leq 2\pi \\ 0 \leq \beta \leq \pi \\ 0 \leq \gamma \leq 2\pi \end{array} \right\}. \quad (\text{A.3})$$

The six Euler angle above, together with the  $R$  parameter (which gives the inter-molecular separation), are sufficient to fully describe the relative configuration of the two interacting molecules.

The general form of the  $T$ -tensors is

$$T^{(1)} = (-1)^n T^{(2)} \quad (\text{A.4})$$

where  $n$  is the order of the  $T$ -tensor. The second-rank  $T$ -tensor is given as

$$T_{\alpha\beta}^{(1)} = \frac{1}{4\pi\varepsilon_0} \nabla_\alpha \nabla_\beta R^{-1} = \frac{1}{4\pi\varepsilon_0} (3R_\alpha R_\beta - R^2 \delta_{\alpha\beta}) R^{-5} \quad (\text{A.5})$$

where  $R$  is the relative separation of the interacting molecules measured from their respective origins. The third-rank  $T$ -tensor is given as [3]

$$T_{\alpha\beta\gamma}^{(1)} = -\frac{1}{4\pi\varepsilon_0} \nabla_\alpha \nabla_\beta \nabla_\gamma R^{-1} = \frac{3}{4\pi\varepsilon_0} [5R_\alpha R_\beta R_\gamma - R^2(R_\alpha \delta_{\beta\gamma} + R_\beta \delta_{\gamma\alpha} + R_\gamma \delta_{\alpha\beta})] R^{-7}. \quad (\text{A.6})$$

## A.2 The Total Oscillating Dipole Moment of Molecule 1 in the presence of Molecule 2

The total electric dipole moment induced on a representative molecule 1 in terms of molecular-property tensors is given below. The inducing electric field is that of the light beam  $\mathcal{E}$  as well as the field due to the oscillating multipole moments of the neighbouring molecule 2.

$$\begin{aligned} \mu_i^{(1)}(\mathcal{E}_0) &= \alpha_{iw}^{(1)} \mathcal{E}_{ow} + \alpha_{ij}^{(1)} T_{jk} \alpha_{kw}^{(2)} \mathcal{E}_{ow} - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{nw}^{(1)} \mathcal{E}_{ow} \\ &\quad + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pw} \mathcal{E}_{ow} + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mw}^{(1)} \mathcal{E}_{ow} \\ &\quad + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mw}^{(2)} \mathcal{E}_{ow} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qw}^{(2)} \mathcal{E}_{ow} \\ &\quad + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\ &\quad + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qw}^{(2)} \mathcal{E}_{ow} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq} T_{qr} \alpha_{rw} \mathcal{E}_{ow} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \alpha_{qw}^{(2)} \alpha_{ij}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \alpha_{sw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} C_{pqr}^{(2)} T_{rst} \alpha_{tw}^{(1)} \mathcal{E}_{ow} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \alpha_{rw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\
& + \beta_{iwj}^{(1)} E_j + \alpha_{ij}^{(1)} T_{jk} \beta_{kwl}^{(2)} E_l + \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lw}^{(2)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \beta_{nwp}^{(1)} E_p \mathcal{E}_{ow} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pw}^{(1)} \mathcal{E}_{ow} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \beta_{pwq}^{(1)} E_q \mathcal{E}_{ow}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} C_{lmnp}^{(2)} T_{pq} \alpha_{qw}^{(1)} \mathcal{E}_{ow} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mwn}^{(1)} E_n + \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{nw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{nw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mwn}^{(2)} E_n + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \beta_{qwr}^{(2)} E_r \mathcal{E}_{ow} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \beta_{rws}^{(2)} E_s \mathcal{E}_{ow} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \beta_{qwr}^{(2)} E_r \mathcal{E}_{ow} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \beta_{npq}^{(1)} E_q T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \beta_{rws}^{(2)} E_s \mathcal{E}_{ow}
\end{aligned}$$

$$+\frac{1}{3}\beta_{ijk}^{(1)}E_k T_{jlm} C_{lmnp}^{(2)} T_{npq} \alpha_{qr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \beta_{pqr}^{(1)} E_r T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \beta_{pwq}^{(2)} E_q \mathcal{E}_{ow}$$

$$+\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nq} \alpha_{qw}^{(2)} \mathcal{E}_{ow}$$

$$+\beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \beta_{qwr}^{(2)} E_r \mathcal{E}_{ow}$$

$$+\frac{1}{3}\beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} A_{npq}^{(1)} T_{pqr} \alpha_{rw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} A_{npq}^{(1)} T_{pqr} \alpha_{rw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \beta_{pwq}^{(1)} E_q \mathcal{E}_{ow}$$

$$+\frac{1}{3}A_{ijk}^{(1)} T_{klm} \beta_{mnp}^{(2)} E_p T_{nq} \alpha_{qw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \beta_{swt}^{(1)} E_t \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \beta_{qrs}^{(2)} E_s T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{3}\alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} A_{qnp}^{(1)} T_{qr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$\begin{aligned}
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \beta_{twu}^{(1)} E_u \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \beta_{rst}^{(2)} E_t T_{su} \alpha_{uw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} C_{npqr}^{(1)} T_{qrs} \alpha_{st}^{(2)} T_{su} \alpha_{uw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} \alpha_{st}^{(2)} T_{su} \alpha_{uw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{ln} \alpha_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nqr} C_{pqr}^{(2)} T_{rst} \beta_{twu}^{(1)} E_u \mathcal{E}_{ow} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nqr} C_{qrs}^{(2)} T_{stu} \alpha_{uw}^{(1)} \mathcal{E}_{ow} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pqr} C_{qrs}^{(2)} T_{stu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}
\end{aligned}$$

$$+\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \beta_{rws}^{(1)} E_s \mathcal{E}_{ow}$$

$$+\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \beta_{pqr}^{(2)} E_p T_{qs} \alpha_{sw}^{(1)} \mathcal{E}_{ow}$$

$$+\alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} \mathcal{E}_{ow}$$

$$+\alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} \mathcal{E}_{ow}$$

$$+\beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mnp}^{(2)} E_p T_{nq} \alpha_{qr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \beta_{pqr}^{(1)} E_r T_{qs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \beta_{rws}^{(2)} E_s \mathcal{E}_{ow}$$

$$+\frac{1}{2} \gamma_{iwlk}^{(1)} E_j E_k + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{kwlm}^{(2)} E_l E_m$$

$$+\frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{nwp}^{(1)} E_p E_q$$

$$-\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{qw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pwqr}^{(1)} E_q E_r \mathcal{E}_{ow}$$

$$\begin{aligned}
& -\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} C_{mnpq}^{(2)} T_{qr} \alpha_{rw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mwnp}^{(1)} E_n E_p \mathcal{E}_{ow} \\
& + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pw}^{(1)} \mathcal{E}_{ow} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{pw}^{(1)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mwnp}^{(2)} E_n E_p \mathcal{E}_{ow} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r E_s \mathcal{E}_{ow} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rwst}^{(2)} E_s E_t \mathcal{E}_{ow} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \mathcal{E}_{ow} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r E_s \mathcal{E}_{ow} \\
& - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{pr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{npqr}^{(1)} E_q E_r T_{rs} \alpha_{sw}^{(2)} \mathcal{E}_{ow} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s E_t \mathcal{E}_{ow}
\end{aligned}$$

$$+\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} C_{mnpq}^{(2)} T_{pqr} \alpha_{rs}^{(1)} T_{st} \alpha_{tw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pqrs}^{(1)} E_r E_s T_{st} \alpha_{tw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pwqr}^{(2)} E_q E_r \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nr} \alpha_{rw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \gamma_{qwrs}^{(2)} E_r E_s \mathcal{E}_{ow}$$

$$+\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klm}^{(2)} E_m E_n T_{lp} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pwqr}^{(1)} E_q E_r \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p E_q T_{nr} \alpha_{rw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t E_u \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qrst}^{(2)} E_s E_t T_{tu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \gamma_{twuv}^{(1)} E_u E_v \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rstu}^{(2)} E_t E_u T_{sv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t E_u \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} \gamma_{twuv}^{(1)} E_u E_v \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$-\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \gamma_{rwst}^{(1)} E_s E_t \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pqrs}^{(2)} E_r E_s T_{qt} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{qp}^{(1)} T_{rq} \alpha_{sr}^{(2)} T_{st} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{sr}^{(2)} T_{ts} \alpha_{tw}^{(1)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p E_q T_{nr} \alpha_{sr}^{(1)} T_{st} \alpha_{tw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pqrs}^{(1)} E_r E_s T_{qt} \alpha_{tw}^{(2)} \mathcal{E}_{ow}$$

$$+\frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s E_t \mathcal{E}_{ow}$$

The differential polarizability of molecule 1 in the presence of both the applied static field and a neighbouring molecule 2 is given as  $\pi_{ij}^{(1)} = \frac{\partial \mu_{ij}^{(1)}}{\partial \mathcal{E}_{0j}}$ . Applying this on the above equation gives

$$\begin{aligned} \pi_{iw}^{(1)} &= \alpha_{iw}^{(1)} + \alpha_{ij}^{(1)} T_{jk} \alpha_{kw}^{(2)} - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{nw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pw} \\ &\quad + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mw}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qw}^{(2)} \\ &\quad + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qw}^{(2)} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq} T_{qr} \alpha_{rw} + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pw}^{(2)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \alpha_{qw}^{(2)} \alpha_{ij}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pw}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{pmnq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \alpha_{sw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} \alpha_{tw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \alpha_{rw}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \beta_{iwl}^{(1)} E_j + \alpha_{ij}^{(1)} T_{jk} \beta_{kwl}^{(2)} E_l + \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lw}^{(2)} - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \beta_{nwp}^{(1)} E_p \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \beta_{pwq}^{(1)} E_q + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} C_{lmnp}^{(2)} T_{pq} \alpha_{qw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mwn}^{(1)} E_n + \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{nw}^{(1)} + \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{nw}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mwn}^{(2)} E_n + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \beta_{qwr}^{(2)} E_r \\
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \beta_{rws}^{(2)} E_s \\
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{lnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \beta_{qwr}^{(2)} E_r - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jkl} A_{mkl}^{(2)} \text{T}_{mn} \beta_{npq}^{(1)} \text{E}_q \text{T}_{qr} \alpha_{rw}^{(2)} + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} \alpha_{pq}^{(1)} \text{T}_{qr} \beta_{rws}^{(2)} \text{E}_s \\
& + \frac{1}{3}\beta_{ijk}^{(1)} \text{E}_k \text{T}_{jlm} C_{lmnp}^{(2)} \text{T}_{npq} \alpha_{qr}^{(1)} \text{T}_{rs} \alpha_{sw}^{(2)} + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} \beta_{pqr}^{(1)} \text{E}_r \text{T}_{rs} \alpha_{sw}^{(2)} \\
& + \alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lm} \alpha_{mn}^{(1)} \text{T}_{np} \beta_{pwq}^{(2)} \text{E}_q + \alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lm} \beta_{mnp}^{(1)} \text{E}_p \text{T}_{nq} \alpha_{qw}^{(2)} \\
& + \alpha_{ij}^{(1)} \text{T}_{jk} \beta_{klm}^{(2)} \text{E}_m \text{T}_{ln} \alpha_{np}^{(1)} \text{T}_{pq} \alpha_{qw}^{(2)} + \beta_{ijk}^{(1)} \text{E}_k \text{T}_{jl} \alpha_{lm}^{(2)} \text{T}_{mn} \alpha_{np}^{(1)} \text{T}_{pq} \alpha_{qw}^{(2)} \\
& + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lm} A_{mnp}^{(1)} \text{T}_{npq} \beta_{qwr}^{(2)} \text{E}_r + \frac{1}{3}\beta_{ijk}^{(1)} \text{E}_k \text{T}_{jl} \alpha_{lm}^{(2)} \text{T}_{mn} A_{npq}^{(1)} \text{T}_{pqr} \alpha_{rw}^{(2)} \\
& + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \beta_{klm}^{(2)} \text{E}_m \text{T}_{ln} A_{npq}^{(1)} \text{T}_{pqr} \alpha_{rw}^{(2)} + \frac{1}{3}A_{ijk}^{(1)} \text{T}_{klm} \alpha_{mn}^{(2)} \text{T}_{np} \beta_{pwq}^{(1)} \text{E}_q \\
& + \frac{1}{3}A_{ijk}^{(1)} \text{T}_{klm} \beta_{mnp}^{(2)} \text{E}_p \text{T}_{nq} \alpha_{qw}^{(1)} + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lmn} A_{pmn}^{(1)} \text{T}_{pq} \alpha_{qr}^{(2)} \text{T}_{rs} \beta_{swt}^{(1)} \text{E}_t \\
& + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lmn} A_{pmn}^{(1)} \text{T}_{pq} \beta_{qrs}^{(2)} \text{E}_s \text{T}_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{3}\beta_{ijk}^{(1)} \text{E}_k \text{T}_{jl} \alpha_{lm}^{(2)} \text{T}_{mnp} A_{qnp}^{(1)} \text{T}_{qr} \alpha_{rs}^{(2)} \text{T}_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lmn} C_{mnpq}^{(1)} \text{T}_{pqr} \alpha_{rs}^{(2)} \text{T}_{st} \beta_{twu}^{(1)} \text{E}_u \\
& + \frac{1}{3}\alpha_{ij}^{(1)} \text{T}_{jk} \alpha_{kl}^{(2)} \text{T}_{lmn} C_{mnpq}^{(1)} \text{T}_{pqr} \beta_{rst}^{(2)} \text{E}_t \text{T}_{su} \alpha_{uw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} \alpha_{st}^{(2)} T_{su} \alpha_{uw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{nlp} A_{rpq}^{(2)} T_{rs} \beta_{swt}^{(1)} E_t \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{ln} \alpha_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{nlp} C_{pqrs}^{(2)} T_{rst} \beta_{twu}^{(1)} E_u \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pqr} C_{qrst}^{(2)} T_{stu} \alpha_{uw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pqr} C_{qrst}^{(2)} T_{stu} \alpha_{uw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \beta_{rws}^{(1)} E_s + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \beta_{pqr}^{(2)} E_r T_{qs} \alpha_{sw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} E_p T_{nq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} + \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} E_m T_{ln} \alpha_{np}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} \\
& + \beta_{ijk}^{(1)} E_k T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \alpha_{sw}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mnp}^{(2)} E_p T_{nq} \alpha_{qr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \beta_{pqr}^{(1)} E_r T_{qs} \alpha_{sw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \beta_{rws}^{(2)} E_s
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \gamma_{ijk}^{(1)} E_j E_k + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{kwl}^{(2)} E_l E_m + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{nwp}^{(1)} E_p E_q - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{qw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pwqr}^{(1)} E_q E_r - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} C_{mnpq}^{(2)} T_{qr} \alpha_{rw}^{(1)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mwnp}^{(1)} E_n E_p \\
& + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pw}^{(1)} + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{pw}^{(1)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mwnp}^{(2)} E_n E_p \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r E_s + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rwst}^{(2)} E_s E_t \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r E_s - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{pr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{npqr}^{(1)} E_q E_r T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s E_t \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jmn} C_{mnpq}^{(2)} T_{pqr} \alpha_{rs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pqrs}^{(1)} E_r E_s T_{st} \alpha_{tw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pwqr}^{(2)} E_q E_r + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nr} \alpha_{rw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \gamma_{qwrs}^{(2)} E_r E_s + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klm}^{(2)} E_m E_n T_{lp} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pwqr}^{(1)} E_q E_r \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p E_q T_{nr} \alpha_{rw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t E_r \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qrst}^{(2)} E_s E_t T_{tu} \alpha_{uw}^{(1)} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \gamma_{twuv}^{(1)} E_u E_v \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rstu}^{(2)} E_t E_u T_{sv} \alpha_{vw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lpq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t E_u \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{6} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& -\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} \gamma_{twuv}^{(1)} E_u E_v \\
& -\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p E_q T_{nrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& -\frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& +\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \gamma_{rwst}^{(1)} E_s E_t \\
& +\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pqrs}^{(2)} E_r E_s T_{qt} \alpha_{tw}^{(1)} \\
& +\frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m E_n T_{lp} \alpha_{qp}^{(1)} T_{rq} \alpha_{sr}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& +\frac{1}{2} \gamma_{ijkl}^{(1)} E_k E_l T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{sr}^{(2)} T_{ts} \alpha_{tw}^{(1)} \\
& +\frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p E_q T_{nr} \alpha_{sr}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& +\frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pqrs}^{(1)} E_r E_s T_{qt} \alpha_{tw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s E_t
\end{aligned}$$

The first derivative of the differential polarizability of molecule 1 in the pres-

ence of both the applied static field and a neighbouring molecule 2 with respect to the electric field  $E$  is given as

$$\begin{aligned}
\frac{\partial \pi_{iw}^{(1)}}{\partial E} = & +\beta_{iwj}^{(1)} + \alpha_{ij}^{(1)} T_{jk} \beta_{kwl}^{(2)} + \beta_{ijk}^{(1)} T_{jl} \alpha_{lw}^{(2)} - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \beta_{nwp}^{(1)} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \beta_{pwq}^{(1)} + \frac{1}{3} \beta_{ijk}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{pq} \alpha_{qw}^{(1)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mwn}^{(1)} + \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{nw}^{(1)} + \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{ln} \alpha_{nw}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mwn}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \beta_{qwr}^{(2)} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \beta_{rws}^{(2)} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \beta_{qwr}^{(2)} - \frac{1}{3} \beta_{ijk}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \beta_{npq}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \beta_{rws}^{(2)} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} \alpha_{qr}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \beta_{pqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \beta_{pwq}^{(2)} + \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \beta_{mnp}^{(1)} T_{nq} \alpha_{qw}^{(2)} \\
& + \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{ln} \alpha_{np}^{(1)} T_{pq} \alpha_{qw}^{(2)} + \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \alpha_{qw}^{(2)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \beta_{qwr}^{(2)} + \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mn} A_{npq}^{(1)} T_{pqr} \alpha_{rw}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{ln} A_{npq}^{(1)} T_{pqr} \alpha_{rw}^{(2)} + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \beta_{pwq}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{klm} \beta_{mnp}^{(2)} T_{nq} \alpha_{qw}^{(1)} + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \beta_{swt}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \beta_{qrs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \beta_{twu}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \beta_{rst}^{(2)} T_{su} \alpha_{uw}^{(1)} \\
& + \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \beta_{klm}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrs} \alpha_{st}^{(2)} T_{su} \alpha_{uw}^{(1)} \\
& + \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} \alpha_{st}^{(2)} T_{su} \alpha_{uw}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \beta_{swt}^{(1)} \\
& - \frac{1}{3} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{ln} \beta_{mnp}^{(1)} T_{nqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& - \frac{1}{3} \beta_{ijk}^{(1)} T_{jl} \alpha_{lm}^{(2)} T_{ln} \alpha_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{st} \alpha_{tw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3}\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\alpha_{mn}^{(1)}T_{npq}C_{pqrs}^{(2)}T_{rst}\beta_{twu}^{(1)} \\
& -\frac{1}{3}\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\beta_{mnp}^{(1)}T_{nqr}C_{qrst}^{(2)}T_{stu}\alpha_{uw}^{(1)} \\
& -\frac{1}{3}\alpha_{ij}^{(1)}T_{jk}\beta_{klm}^{(2)}T_{ln}\alpha_{np}^{(1)}T_{pqr}C_{qrst}^{(2)}T_{stu}\alpha_{uw}^{(1)} \\
& +\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\alpha_{mn}^{(1)}T_{np}\alpha_{pq}^{(2)}T_{qr}\beta_{rws}^{(1)}+\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\alpha_{mn}^{(1)}T_{np}\beta_{pqr}^{(2)}T_{qs}\alpha_{sw}^{(1)} \\
& +\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\beta_{mnp}^{(1)}T_{nq}\alpha_{qr}^{(2)}T_{rs}\alpha_{sw}^{(1)}+\alpha_{ij}^{(1)}T_{jk}\beta_{klm}^{(2)}T_{ln}\alpha_{np}^{(1)}T_{pq}\alpha_{qr}^{(2)}T_{rs}\alpha_{sw}^{(1)} \\
& +\beta_{ijk}^{(1)}T_{jl}\alpha_{lm}^{(2)}T_{mn}\alpha_{np}^{(1)}T_{pq}\alpha_{qr}^{(2)}T_{rs}\alpha_{sw}^{(1)}+\frac{1}{3}A_{ijk}^{(1)}T_{klm}\beta_{mnp}^{(2)}T_{nq}\alpha_{qr}^{(1)}T_{rs}\alpha_{sw}^{(2)} \\
& +\frac{1}{3}A_{ijk}^{(1)}T_{klm}\alpha_{mn}^{(2)}T_{np}\beta_{pqr}^{(1)}T_{qs}\alpha_{sw}^{(2)}+\frac{1}{6}A_{ijk}^{(1)}T_{klm}\alpha_{mn}^{(2)}T_{np}\alpha_{pq}^{(1)}T_{qr}\beta_{rws}^{(2)} \\
& +\frac{1}{2}\gamma_{iwljk}^{(1)}E_j+\frac{1}{2}\alpha_{ij}^{(1)}T_{jk}\gamma_{kwlml}^{(2)}E_l+\frac{1}{2}\gamma_{ijkl}^{(1)}E_kT_{jm}\alpha_{mw}^{(1)} \\
& -\frac{1}{6}\alpha_{ij}^{(1)}T_{jkl}A_{mkl}^{(2)}T_{mn}\gamma_{nwp}^{(1)}E_p-\frac{1}{6}\gamma_{ijkl}^{(1)}E_kT_{jmn}A_{pmn}^{(2)}T_{pq}\alpha_{qw}^{(1)} \\
& -\frac{1}{6}\alpha_{ij}^{(1)}T_{jkl}C_{klmn}^{(2)}T_{mnp}\gamma_{pwqr}^{(1)}E_q-\frac{1}{6}\gamma_{ijkl}^{(1)}E_kT_{jmn}C_{mnpq}^{(2)}T_{qr}\alpha_{rw}^{(1)} \\
& +\frac{1}{2}\alpha_{ij}^{(1)}T_{jk}\alpha_{kl}^{(2)}T_{lm}\gamma_{mwnp}^{(1)}E_n \\
& +\frac{1}{2}\gamma_{ijkl}^{(1)}E_kT_{jm}\alpha_{mn}^{(2)}T_{np}\alpha_{pw}^{(1)}+\frac{1}{2}\alpha_{ij}^{(1)}T_{jk}\gamma_{klmn}^{(2)}E_mT_{lp}\alpha_{pw}^{(1)}+\frac{1}{6}A_{ijk}^{(1)}T_{klm}\gamma_{mwnp}^{(2)}E_n
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rwst}^{(2)} E_s \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lpq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \gamma_{qwrs}^{(2)} E_r - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} A_{pmn}^{(2)} T_{pq} \alpha_{pr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{npqr}^{(1)} E_q T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} C_{mnpq}^{(2)} T_{pqr} \alpha_{rs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pqrs}^{(1)} E_r T_{st} \alpha_{tw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pwqr}^{(2)} E_q + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p T_{nr} \alpha_{rw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lp} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \gamma_{qwrs}^{(2)} E_r + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{np} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klm}^{(2)} E_m T_{lp} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pwqr}^{(1)} E_q \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p T_{nr} \alpha_{rw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qrst}^{(2)} E_s T_{tu} \alpha_{uw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \gamma_{twuv}^{(1)} E_u \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rstu}^{(2)} E_t T_{sv} \alpha_{vw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lpq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \gamma_{swtu}^{(1)} E_t \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p T_{nrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lp} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p T_{nrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} E_m T_{lp} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \gamma_{rwst}^{(1)} E_s \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pqrs}^{(2)} E_r T_{qt} \alpha_{tw}^{(1)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} E_p T_{nr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{2} \gamma_{ijkl}^{(1)} E_k T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{sr}^{(2)} T_{ts} \alpha_{tw}^{(1)} \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} E_p T_{nr} \alpha_{sr}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pqrs}^{(1)} E_r T_{qt} \alpha_{tw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} E_s
\end{aligned}$$

The second derivative of the differential polarizability of molecule 1 in the presence of both the applied static field and a neighbouring molecule 2 with respect to the electric field  $E$  is given as

$$\begin{aligned}
\frac{\partial^2 \pi_{iw}^{(1)}}{\partial E^2} = & + \frac{1}{2} \gamma_{iwjk}^{(1)} + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{kwlm}^{(2)} + \frac{1}{2} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{nwp}^{(1)} - \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{qw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pwqr}^{(1)} - \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jmn} C_{mnpq}^{(2)} T_{qr} \alpha_{rw}^{(1)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mwnp}^{(1)} \\
& + \frac{1}{2} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pw}^{(1)} + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lp} \alpha_{pw}^{(1)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mwnp}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qwr}^{(2)} + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lpq} A_{rpq}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rwst}^{(2)} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lpq} C_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \alpha_{np}^{(1)} T_{pq} \gamma_{qwr}^{(2)} - \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jmn} A_{pmn}^{(2)} T_{pq} \alpha_{pr}^{(1)} T_{rs} \alpha_{sw}^{(2)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \gamma_{npqr}^{(1)} T_{rs} \alpha_{sw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jmn} C_{mnpq}^{(2)} T_{pqr} \alpha_{rs}^{(1)} T_{st} \alpha_{tw}^{(2)} + \frac{1}{6} \alpha_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \gamma_{pqrs}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pwqr}^{(2)} + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} T_{nr} \alpha_{rw}^{(2)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lp} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} + \frac{1}{2} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{rw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} A_{mnp}^{(1)} T_{npq} \gamma_{qwr}^{(2)} + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klm}^{(2)} T_{lp} A_{pqr}^{(1)} T_{qrs} \alpha_{sw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pwqr}^{(1)} \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} T_{nr} \alpha_{rw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \alpha_{qr}^{(2)} T_{rs} \gamma_{swtu}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \gamma_{qrst}^{(2)} T_{tu} \alpha_{uw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{npq} A_{rpq}^{(1)} T_{rs} \alpha_{st}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \alpha_{rs}^{(2)} T_{st} \gamma_{twuv}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} \gamma_{rstu}^{(2)} T_{sv} \alpha_{vw}^{(1)} \\
& + \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lpq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \\
& + \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{npq} C_{pqrs}^{(1)} T_{rst} \alpha_{tu}^{(2)} T_{uv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} \gamma_{swtu}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} T_{nrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lp} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} A_{trs}^{(2)} T_{tu} \alpha_{uw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} T_{nrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \alpha_{ij}^{(1)} T_{jk} \gamma_{klmn}^{(2)} T_{lp} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)} \\
& - \frac{1}{6} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qrs} C_{rstu}^{(2)} T_{tuv} \alpha_{vw}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \alpha_{pq}^{(2)} T_{qr} \gamma_{rwst}^{(1)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \alpha_{mn}^{(1)} T_{np} \gamma_{pqrs}^{(2)} T_{qt} \alpha_{tw}^{(1)} \\
& + \frac{1}{2} \alpha_{ij}^{(1)} T_{jk} \alpha_{kl}^{(2)} T_{lm} \gamma_{mnpq}^{(1)} T_{nr} \alpha_{rs}^{(2)} T_{st} \alpha_{tw}^{(1)} \\
& + \frac{1}{2} \gamma_{ijkl}^{(1)} T_{jm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \alpha_{sr}^{(2)} T_{ts} \alpha_{tw}^{(1)} \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \gamma_{mnpq}^{(2)} T_{nr} \alpha_{sr}^{(1)} T_{st} \alpha_{tw}^{(2)} \\
& + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \gamma_{pqrs}^{(1)} T_{qt} \alpha_{tw}^{(2)} + \frac{1}{6} A_{ijk}^{(1)} T_{klm} \alpha_{mn}^{(2)} T_{np} \alpha_{pq}^{(1)} T_{qr} \gamma_{rwst}^{(2)}
\end{aligned}$$

### A.3 The Total Static Dipole Moment of Molecule $p$ in the presence of Molecule $q$

The terms contributing to the static dipole moment are given below:

$$\begin{aligned}
u_i^{(p)} &= \mu_{oi}^{(p)} + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} \mu_{ol}^{(q)} - \frac{1}{9} A_{ijk}^{(p)} T_{jklm} \theta_{olm}^{(q)} + a_{ij}^{(p)} E_j \\
& + a_{ij}^{(p)} T_{jk} \mu_{ok}^{(q)} + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} E_l \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} E_m - \frac{1}{3} a_{ij}^{(p)} T_{jkl} \theta_{okl}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} E_m \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} \mu_{om}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} A_{jkl}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} \mu_{om}^{(p)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} \mu_{on}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} \mu_{on}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} E_n + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} E_p \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} E_p \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} E_p + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} \mu_{op}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} E_q \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} \theta_{omn}^{(p)} + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mnp} \theta_{onp}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mnp} \theta_{onp}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mnp} \theta_{onp}^{(p)} + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnpq} \theta_{opq}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} E_p + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} \mu_{op}^{(q)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} \mu_{oq}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} \mu_{oq}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} \mu_{oq}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} \mu_{or}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} \mu_{oq}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} A_{mnp}^{(p)} T_{npq} \mu_{oq}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} \mu_{or}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} \theta_{opq}^{(q)} \\
& - \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} - \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pqr} \theta_{oqr}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} A_{mnp}^{(p)} T_{npqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} \theta_{ors}^{(q)} + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} E_q \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} E_r - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} E_r \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} E_r + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} E_r + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} E_r \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} E_s - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} E_r \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} \mu_{or}^{(p)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{os}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} \mu_{os}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} a_{rs}^{(p)} E_s \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} a_{st}^{(p)} E_t \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} a_{st}^{(p)} E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{rst} a_{tu}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qrs} \theta_{ors}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + b_{ijk}^{(p)} E_j E_k + b_{ijk}^{(p)} E_k T_{jl} \mu_{ol}^{(q)} + b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} E_m + a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m E_l \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n E_m - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} \theta_{olm}^{(q)} - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} E_n
\end{aligned}$$

$$\begin{aligned}
& + b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} \mu_{on}^{(p)} + a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} \mu_{on}^{(p)} \\
& + \frac{1}{3} A_{jkl}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} \mu_{op}^{(p)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} \mu_{op}^{(p)} + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{mnp} \mu_{op}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p E_n + b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} E_p \\
& + a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} E_p + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q E_p \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} E_q - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q E_p \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} E_q + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} \mu_{oq}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqr}^{(p)} E_r E_q + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} E_r \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} \theta_{onp}^{(p)} + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} \theta_{onp}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mpq} \theta_{opq}^{(p)} - \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{mnpq} \theta_{opq}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{mnpq} \theta_{opq}^{(p)} + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npqr} \theta_{oqr}^{(p)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} E_q + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} E_q \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nq} \mu_{oq}^{(q)} + b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{qp} \mu_{oq}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pq} \mu_{oq}^{(q)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} \mu_{or}^{(q)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} \mu_{or}^{(q)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npq}^{(p)} E_q T_{pr} \mu_{or}^{(q)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{lml}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqr}^{(p)} E_r T_{qs} \mu_{os}^{(q)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} \mu_{os}^{(q)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} \mu_{or}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} C_{npqr}^{(p)} T_{qrs} \mu_{os}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} C_{npqr}^{(p)} T_{qrs} \mu_{os}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{prs} \theta_{ors}^{(q)} \\
& - \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{prs} \theta_{ors}^{(q)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{prs} \theta_{ors}^{(q)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npq}^{(p)} E_q T_{prs} \theta_{ors}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqr}^{(p)} E_r T_{qst} \theta_{ost}^{(q)} \\
& - \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} T_{qrs} \theta_{ors}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{9} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(p)} T_{mnp} A_{qnp}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& -\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} A_{npq}^{(p)} T_{pqrs} \theta_{ors}^{(q)} \\
& -\frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(p)} T_{mn} A_{npq}^{(p)} T_{pqrs} \theta_{ors}^{(q)} \\
& -\frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} C_{npqr}^{(p)} T_{qrst} \theta_{ost}^{(q)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} b_{pqr}^{(q)} E_r E_q \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nq} a_{qr}^{(q)} E_r \\
& + a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} E_r \\
& + b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} E_r \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s E_r \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s E_r \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} E_s
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s E_r \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} b_{rst}^{(q)} E_t E_s \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npg} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} b_{qrs}^{(q)} E_s E_r \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npg} b_{qrs}^{(q)} E_s E_r \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} E_s \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} E_s
\end{aligned}$$

$$+\frac{1}{3} a_{ij}^{(p)} \text{T}_{jk} a_{kl}^{(q)} \text{T}_{lmn} C_{mnpq}^{(p)} \text{T}_{pqr} b_{rst}^{(q)} \text{E}_t \text{E}_s$$

$$+\frac{1}{3} a_{ij}^{(p)} \text{T}_{jk} b_{klm}^{(q)} \text{E}_m \text{T}_{lnp} C_{npqr}^{(p)} \text{T}_{qrs} a_{st}^{(q)} \text{E}_t$$

$$+\frac{1}{3} a_{ij}^{(p)} \text{T}_{jk} b_{klm}^{(q)} \text{E}_m \text{T}_{lnp} C_{npqr}^{(p)} \text{T}_{qrs} a_{st}^{(q)} \text{E}_t$$

$$-\frac{1}{3} a_{ij}^{(p)} \text{T}_{jk} a_{kl}^{(q)} \text{T}_{lm} b_{mnp}^{(p)} \text{E}_p \text{T}_{nqr} A_{sqr}^{(q)} \text{E}_s$$

$$-\frac{1}{3} a_{ij}^{(p)} \text{T}_{jk} b_{klm}^{(p)} \text{E}_m \text{T}_{ln} a_{np}^{(p)} \text{T}_{pqr} A_{sqr}^{(q)} \text{E}_s$$

$$-\frac{1}{3} b_{ijk}^{(p)} \text{E}_k \text{T}_{jl} a_{lm}^{(q)} \text{T}_{mn} a_{np}^{(p)} \text{T}_{pqr} A_{sqr}^{(q)} \text{E}_s$$

$$+a_{ij}^{(p)} \text{T}_{jk} a_{kl}^{(q)} \text{T}_{lm} a_{mn}^{(p)} \text{T}_{np} b_{pqr}^{(q)} \text{E}_r \text{T}_{qs} \mu_{os}^{(p)}$$

$$+a_{ij}^{(p)} \text{T}_{jk} a_{kl}^{(q)} \text{T}_{lm} b_{mnp}^{(p)} \text{E}_p \text{T}_{nq} a_{qr}^{(q)} \text{T}_{rs} \mu_{os}^{(p)}$$

$$+b_{ijk}^{(p)} \text{E}_k \text{T}_{jl} a_{lm}^{(q)} \text{T}_{mn} a_{np}^{(p)} \text{T}_{pq} a_{qr}^{(q)} \text{T}_{rs} \mu_{os}^{(p)}$$

$$+\frac{1}{3} A_{ijk}^{(p)} \text{T}_{jkl} a_{lm}^{(q)} \text{T}_{mn} a_{np}^{(p)} \text{T}_{pq} b_{qrs}^{(q)} \text{E}_s \text{T}_r \mu_{ot}^{(p)}$$

$$+\frac{1}{3} A_{ijk}^{(p)} \text{T}_{jkl} a_{lm}^{(q)} \text{T}_{mn} b_{npq}^{(p)} \text{E}_q \text{T}_{pr} a_{rs}^{(q)} \text{T}_{st} \mu_{ot}^{(p)}$$

$$+\frac{1}{3} A_{ijk}^{(p)} \text{T}_{jkl} b_{lmn}^{(q)} \text{E}_n \text{T}_{mp} a_{pq}^{(p)} \text{T}_{qr} a_{rs}^{(q)} \text{T}_{st} \mu_{ot}^{(p)}$$

$$-\frac{1}{3} a_{ij}^{(p)} \text{T}_{jkl} A_{mkl}^{(q)} \text{T}_{mn} a_{np}^{(p)} \text{T}_{pq} b_{qrs}^{(q)} \text{E}_s \text{T}_{st} \mu_{ot}^{(p)}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& -\frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{lmm}^{(q)} T_{lmn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} b_{rst}^{(q)} E_t T_{su} \mu_{ou}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmm}^{(q)} T_{mnp} b_{pqr}^{(p)} E_r T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{rt} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} b_{qrs}^{(q)} E_s T_{rt} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{npq}^{(p)} T_{nqr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{lnp} A_{npq}^{(p)} T_{nqr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpn}^{(p)} T_{pqr} b_{rst}^{(q)} E_t T_{su} \mu_{ou}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} A_{sqr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{nqr} A_{sqr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{nqr} A_{qrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{nqr} A_{qrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{nqr} A_{qrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} C_{qrst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{nqr} C_{qrst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} b_{rst}^{(p)} E_t E_s
\end{aligned}$$

$$+a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} B_{pqr}^{(q)} E_r T_{qs} a_{st}^{(p)} E_t$$

$$+a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t$$

$$+a_{ij}^{(p)} T_{jk} B_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t$$

$$+b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{st}^{(p)} E_t$$

$$+\frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} b_{stu}^{(p)} E_u E_t$$

$$+\frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(p)} E_s T_{rt} a_{tu}^{(p)} E_u$$

$$+\frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u$$

$$+\frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u$$

$$-\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} b_{stu}^{(p)} E_u E_t$$

$$-\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(p)} E_s T_{rt} a_{tu}^{(p)} E_u$$

$$-\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u$$

$$-\frac{1}{3} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_t$$

$$+\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} b_{stu}^{(p)} E_u E_t$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}A_{klm}^{(q)}T_{lmn}a_{np}^{(p)}T_{pq}b_{qrs}^{(p)}E_sT_{rt}a_{tu}^{(p)}E_u$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}A_{klm}^{(q)}T_{lmn}b_{npq}^{(p)}E_qT_{pr}a_{rs}^{(q)}T_{st}a_{tu}^{(p)}E_u$$

$$+\frac{1}{3}b_{ijk}^{(p)}E_kT_{jlm}A_{lmn}^{(q)}T_{mnp}a_{pq}^{(p)}T_{qr}a_{rs}^{(q)}T_{st}a_{tu}^{(p)}E_t$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}A_{klm}^{(q)}T_{lmn}a_{np}^{(p)}T_{pq}a_{qr}^{(q)}T_{rs}b_{stu}^{(p)}E_uE_t$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}A_{klm}^{(q)}T_{lmn}b_{npq}^{(p)}E_qT_{pr}a_{rs}^{(q)}T_{st}a_{tu}^{(p)}E_u$$

$$+\frac{1}{3}b_{ijk}^{(p)}E_kT_{jlm}A_{lmn}^{(q)}T_{mnp}a_{pq}^{(p)}T_{qr}a_{rs}^{(q)}T_{st}a_{tu}^{(p)}E_t$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}C_{klmn}^{(q)}T_{mnp}a_{pq}^{(p)}T_{qr}a_{rs}^{(q)}T_{st}b_{tuv}^{(p)}E_vE_u$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}C_{klmn}^{(q)}T_{mnp}a_{pq}^{(p)}T_{qr}b_{rst}^{(p)}E_tT_{su}a_{uv}^{(p)}E_v$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jkl}C_{klmn}^{(q)}T_{mnp}b_{pqr}^{(p)}E_rT_{qs}a_{st}^{(q)}T_{tu}a_{uv}^{(p)}E_v$$

$$+\frac{1}{3}b_{ijk}^{(p)}E_kT_{jlm}C_{lmnp}^{(q)}T_{npq}a_{qr}^{(p)}T_{rs}a_{st}^{(q)}T_{tu}a_{uv}^{(p)}E_v$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jk}a_{kl}^{(q)}T_{lmn}A_{pmn}^{(p)}T_{pq}a_{qr}^{(q)}T_{rs}b_{stu}^{(p)}E_uE_t$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jk}a_{kl}^{(q)}T_{lmn}A_{pmn}^{(p)}T_{pq}b_{qrs}^{(p)}E_sT_{rt}a_{tu}^{(p)}E_u$$

$$+\frac{1}{3}a_{ij}^{(p)}T_{jk}b_{klm}^{(q)}E_mT_{lnp}A_{qnp}^{(p)}T_{qr}a_{rs}^{(q)}T_{st}a_{tu}^{(p)}E_u$$

$$\begin{aligned}
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rs} b_{stu}^{(p)} E_u E_t \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} b_{qrs}^{(p)} E_s T_{rt} a_{tu}^{(p)} E_u \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} b_{tuv}^{(p)} E_v E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} b_{rst}^{(p)} E_t T_{su} a_{uv}^{(p)} E_v \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} b_{stu}^{(p)} E_u E_t \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} A_{sqr}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{st} a_{tu}^{(p)} E_u
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} b_{stu}^{(p)} E_u E_t \\
& -\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} A_{qrs}^{(q)} T_{rst} a_{tu}^{(p)} E_u \\
& -\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pqr} A_{qrs}^{(q)} T_{rst} a_{tu}^{(p)} E_u \\
& -\frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} A_{qrs}^{(q)} T_{rst} a_{tu}^{(p)} E_u \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{qrst} b_{tuv}^{(p)} E_v E_u \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} C_{qrs}^{(q)} T_{stu} a_{uv}^{(p)} E_v \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pqr} C_{qrs}^{(q)} T_{stu} a_{uv}^{(p)} E_v \\
& +\frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} C_{qrs}^{(q)} T_{stu} a_{uv}^{(p)} E_v \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} b_{pqr}^{(q)} E_r T_{qst} \theta_{ost}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& +\frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& +\frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{stu} \theta_{otu}^{(p)} \\
& +\frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmn}^{(q)} E_n T_{mp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{stu} \theta_{otu}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npq}^{(p)} E_q T_{pr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} A_{lmn}^{(q)} T_{lnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} b_{rst}^{(q)} E_t T_{suv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqr}^{(p)} E_r T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} b_{qrs}^{(q)} E_s T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} b_{qrs}^{(q)} E_s T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} b_{rst}^{(q)} E_t T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nqr} A_{sqr}^{(q)} T_{stu} \theta_{otu} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(p)} E_m T_{ln} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{stu} \theta_{otu} \\
& - \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{stu} \theta_{otu} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} b_{pqr}^{(q)} E_r T_{qst} A_{ust}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnp}^{(p)} E_p T_{nq} a_{qr}^{(q)} T_{rst} A_{ust}^{(p)} E_u \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klm}^{(q)} E_m T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} A_{ust}^{(p)} E_u \\
& + \frac{1}{3} b_{ijk}^{(p)} E_k T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} A_{ust}^{(p)} E_u \\
& + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l E_j + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} \mu_{om}^{(q)} + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} E_n
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n E_l \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p E_m - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} \theta_{omn}^{(q)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} E_p \\
& + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} \mu_{op}^{(p)} + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} \mu_{op}^{(p)} \\
& + \frac{1}{6} A_{jkl}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} \mu_{oq}^{(p)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} \mu_{oq}^{(p)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} \mu_{oq}^{(p)} \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q E_n \\
& + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} E_q \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} E_q \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r E_p \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} a_{qr}^{(p)} E_r \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r E_p \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} E_r
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} \mu_{or}^{(p)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s E_q \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} E_s \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} \theta_{opq}^{(p)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} \theta_{opq}^{(p)} \\
& + \frac{1}{18} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mqr} \theta_{oqr}^{(p)} \\
& - \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{npqr} \theta_{oqr}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npqr} \theta_{oqr}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqrs} \theta_{ors}^{(p)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} E_r \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} E_r \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nr} \mu_{or}^{(q)} \\
& + \frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} \mu_{os}^{(q)} \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} a_{qr}^{(p)} T_{rs} \mu_{os}^{(q)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{rs} \mu_{os}^{(q)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rs} \mu_{os}^{(q)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{rs} \mu_{os}^{(q)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} \mu_{os}^{(q)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{st} \mu_{ot}^{(q)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{st} \mu_{ot}^{(q)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} T_{rs} \mu_{os}^{(q)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{pqr}^{(p)} T_{qrs} \mu_{os}^{(q)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{pqr}^{(p)} T_{qrs} \mu_{os}^{(q)} \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} C_{pqrs}^{(p)} T_{rst} \mu_{ot}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} \mu_{ot}^{(q)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} \theta_{ors}^{(q)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{prs} \theta_{ors}^{(q)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& - \frac{1}{18} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{rst} \theta_{ost}^{(q)} \\
& - \frac{1}{18} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} a_{qr}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{rst} \theta_{ost}^{(q)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{pst} \theta_{ost}^{(q)} \\
& - \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& - \frac{1}{18} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{qtu} \theta_{otu}^{(q)} \\
& - \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{stu} \theta_{otu}^{(q)} \\
& - \frac{1}{18} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} T_{rst} \theta_{ost}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& -\frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} A_{pqr}^{(p)} T_{qrst} \theta_{ost}^{(q)} \\
& -\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(p)} T_{np} A_{pqr}^{(p)} T_{qrst} \theta_{ost}^{(q)} \\
& -\frac{1}{18} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rstu} \theta_{otu}^{(q)} \\
& +\frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} g_{pqrs}^{(q)} E_r E_s E_q \\
& +\frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nr} a_{rs}^{(q)} E_s \\
& +\frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& +\frac{1}{2} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} E_s \\
& +\frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t E_r \\
& +\frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{rs} a_{st}^{(q)} E_t \\
& -\frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t E_r \\
& -\frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{rs} a_{st}^{(q)} E_t
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t E_r \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} g_{rstu}^{(q)} E_t E_u E_s \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{qt} a_{tu}^{(q)} E_u \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{st} a_{tu}^{(q)} E_u \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t E_r \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} g_{qrst}^{(q)} E_s E_t E_r \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} E_t \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} E_t
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} g_{rstu}^{(q)} E_t E_u E_s \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} E_u \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} E_u \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} A_{trs}^{(q)} E_t \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(p)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} E_t \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} E_t \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{ru} \mu_{ou}^{(p)} \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{ru} \mu_{ou}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& -\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{ts} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} g_{rstu}^{(q)} E_t E_u T_{sv} \mu_{ov}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmm}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{st} a_{tu}^{(q)} T_{uv} \mu_{ov}^{(p)} \\
& +\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{st} a_{tu}^{(q)} T_{uv} \mu_{ov}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{ru} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} g_{qrst}^{(q)} E_s E_t T_{ru} \mu_{ou}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpn}^{(p)} T_{pqr} g_{rstu}^{(q)} E_t E_u T_{sv} \mu_{ov}^{(p)} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} T_{uv} \mu_{ov}^{(p)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} T_{uv} \mu_{ov}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} A_{trs}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{lp} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{qrs} A_{rst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qrs} A_{rst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qrs} A_{rst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} C_{rstu}^{(q)} T_{tuv} \mu_{ov}^{(p)} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{qp}^{(p)} T_{qrs} C_{rstu}^{(q)} T_{tuv} \mu_{ov}^{(p)} \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} g_{rstu}^{(p)} E_t E_u E_s
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} g_{pqrs}^{(q)} E_r E_s T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{2} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tu}^{(p)} E_u \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(p)} E_s E_t T_{ru} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_{uv} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} g_{qrst}^{(p)} E_s E_t T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} g_{tuvw}^{(p)} E_v E_w E_u \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} g_{rstu}^{(p)} E_t E_u T_{sv} a_{vw}^{(p)} E_w \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{qt} a_{tu}^{(q)} T_{uv} a_{vw}^{(p)} E_w \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{st} a_{tu}^{(q)} T_{uv} a_{vw}^{(p)} E_w \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} g_{qrst}^{(p)} E_s E_t T_{ru} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} g_{qrst}^{(p)} E_s E_t T_{rt} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} g_{tuvw}^{(p)} E_v E_w E_u \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} g_{rstu}^{(p)} E_t E_u T_{uv} a_{vw}^{(p)} E_w \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} T_{uv} a_{vw}^{(p)} E_w \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} T_{uv} a_{vw}^{(p)} E_w \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} g_{stuv}^{(p)} E_u E_v E_t \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} A_{trs}^{(q)} T_{tu} a_{uv}^{(p)} E_v \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} T_{tu} a_{uv}^{(p)} E_v
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} g_{stuv}^{(p)} E_u E_v E_t \\
& -\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} A_{rst}^{(q)} T_{stu} a_{uv}^{(p)} E_v \\
& -\frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qrs} A_{rst}^{(q)} T_{stu} a_{uv}^{(p)} E_v \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{qrst} g_{tuvw}^{(p)} E_v E_w E_u \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} C_{rstu}^{(q)} T_{tuv} a_{vw}^{(p)} E_w \\
& +\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qrs} C_{rstu}^{(q)} T_{tuv} a_{vw}^{(p)} E_w \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} g_{pqrs}^{(q)} E_r E_s T_{qtu} \theta_{otu}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& +\frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& +\frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& +\frac{1}{18} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{suv} \theta_{ouv}^{(p)} \\
& +\frac{1}{18} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{18} A_{ijk}^{(p)} T_{jkl} g_{lmnp}^{(q)} E_n E_p T_{mq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& - \frac{1}{18} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{suv} \theta_{ouv}^{(p)} \\
& - \frac{1}{18} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} g_{npqr}^{(p)} E_q E_r T_{ps} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{pmn}^{(q)} T_{pq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{suv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} A_{mnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} g_{rstu}^{(q)} E_t E_u T_{svw} \theta_{ovw}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} g_{pqrs}^{(p)} E_r E_s T_{rt} a_{tu}^{(q)} T_{uvw} \theta_{ovw}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jmn} C_{mnpq}^{(q)} T_{pqr} a_{rs}^{(p)} T_{st} a_{tu}^{(q)} T_{uvw} \theta_{ovw}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} g_{qrst}^{(q)} E_s E_t T_{suv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{rpq}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{owv}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} g_{qrst}^{(q)} E_s E_t T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{npq} A_{pqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} g_{rstu}^{(q)} E_t E_u T_{tvw} \theta_{ovw}^{(p)} \\
& + \frac{1}{18} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lpq} C_{pqrs}^{(p)} T_{rst} a_{tu}^{(q)} T_{uvw} \theta_{ovw}^{(p)} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{nrs} A_{trs}^{(q)} T_{tuv} \theta_{ouv} \\
& - \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(p)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} T_{tuv} \theta_{ouv} \\
& - \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qrs} A_{trs}^{(q)} T_{tuv} \theta_{ouv} \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} g_{pqrs}^{(q)} E_r E_s T_{qtu} A_{vtu}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} g_{mnpq}^{(p)} E_p E_q T_{qr} a_{rs}^{(q)} T_{stu} A_{vtu}^{(p)} E_v \\
& + \frac{1}{6} a_{ij}^{(p)} T_{jk} g_{klmn}^{(q)} E_m E_n T_{lp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} A_{vtu}^{(p)} E_v \\
& + \frac{1}{6} g_{ijkl}^{(p)} E_k E_l T_{jm} a_{mn}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} A_{vtu}^{(p)} E_v
\end{aligned}$$

## A.4 The Potential Energy of a Representative Molecule $p$ .

The potential energy of an interacting molecule  $p$  under the influence of the static electric field  $E_i$  may be written as

$$\begin{aligned}
U^{(p)}(\tau, E) = & - \left( \mu_{ov}^{(p)} + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} \mu_{ov}^{(q)} - \frac{1}{9} A_{ijk}^{(p)} T_{jklm} \theta_{olv}^{(q)} + a_{ij}^{(p)} T_{jk} \mu_{ov}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} \theta_{okv}^{(q)} \right. \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} \mu_{ov}^{(p)} + \frac{1}{3} A_{jkl}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} \mu_{ov}^{(p)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} \mu_{ov}^{(p)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} \theta_{omv}^{(p)} + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mnp} \theta_{onv}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mnp} \theta_{onv}^{(p)} + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mnp} \theta_{onv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnpq} \theta_{opv}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} \mu_{ov}^{(q)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} \mu_{ov}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} \mu_{ov}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} \mu_{ov}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} \mu_{ov}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} \mu_{ov}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} A_{mnp}^{(p)} T_{npq} \mu_{ov}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} \mu_{ov}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} \theta_{opv}^{(q)} \\
& - \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqv}^{(q)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqv}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqv}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qrs} \theta_{orv}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pqr} \theta_{oqv}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} A_{mnp}^{(p)} T_{npqr} \theta_{oqv}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqrs} \theta_{orv}^{(q)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} \mu_{ov}^{(p)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{ov}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{ov}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} \mu_{ov}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} \mu_{ov}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} \mu_{ov}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qrs} \theta_{orv}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{osv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{rst} \mu_{ov}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{osv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{osv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otv}^{(p)}
\end{aligned}$$

$$+\frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{osv}^{(p)}$$

$$+\frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qr}^{(q)} T_{rst} \theta_{osv}^{(p)}$$

$$+\frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otv}^{(p)} \right) E a_i^x$$

$$-\frac{1}{2} \left( a_{iv}^{(p)} + a_{ij}^{(p)} T_{jk} a_{kv}^{(q)} + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lv}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{vkl}^{(q)}$$

$$+ a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mv}^{(p)} + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{nv}^{(p)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{nv}^{(p)}$$

$$+ \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{nv}^{(p)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pv}^{(p)}$$

$$+ \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{vmn}^{(p)} + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pv}^{(q)}$$

$$+ \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qv}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qv}^{(q)}$$

$$+ \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qv}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rv}^{(q)}$$

$$+ \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} a_{qv}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} a_{qv}^{(q)}$$

$$+ a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rv}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{vpq}^{(q)}$$

$$+ a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qr} a_{rv}^{(p)}$$

$$+ \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{sv}^{(p)}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{sv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} a_{tv}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} a_{sv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{npq} a_{qr}^{(q)} T_{rs} a_{sv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{st} a_{tv}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{rpq}^{(q)} T_{rs} a_{sv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} A_{pqr}^{(q)} T_{qrs} a_{sv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{npq} C_{pqrs}^{(q)} T_{rst} a_{tv}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} a_{pq}^{(q)} T_{qrs} A_{trv}^{(p)} \\
& + b_{ijv}^{(p)} T_{jl} \mu_{ol}^{(q)} - \frac{1}{3} b_{ijv}^{(p)} T_{jlm} \theta_{olm}^{(q)} + b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} \mu_{on}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} \mu_{on}^{(p)} + \frac{1}{3} A_{jkl}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mp} \mu_{op}^{(p)} \\
& - \frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{nlm}^{(q)} T_{np} \mu_{op}^{(p)} + \frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{lmn}^{(q)} T_{mnp} \mu_{op}^{(p)} \\
& + \frac{1}{3} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npq} \mu_{oq}^{(p)} + \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} \theta_{onp}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} \theta_{onp}^{(p)} + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mpq} \theta_{opq}^{(p)} \\
& - \frac{1}{9} b_{ijv}^{(p)} T_{jlm} A_{nlm}^{(q)} T_{mnpq} \theta_{opq}^{(p)} + \frac{1}{9} b_{ijv}^{(p)} T_{jlm} A_{lmn}^{(q)} T_{mnpq} \theta_{opq}^{(p)} \\
& + \frac{1}{9} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npqr} \theta_{oqr}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nq} \mu_{oq}^{(q)} + b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{qp} \mu_{oq}^{(q)} \\
& + a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{pq} \mu_{oq}^{(q)} + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} \mu_{or}^{(q)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mp} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} \mu_{or}^{(q)} \\
& - \frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npv}^{(p)} T_{pr} \mu_{or}^{(q)} \\
& \frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} \mu_{or}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqv}^{(p)} T_{qs} \mu_{os}^{(q)} \\
& + \frac{1}{3} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} \mu_{os}^{(q)} + \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} \mu_{or}^{(q)} + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qr} \mu_{or}^{(q)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} C_{npqr}^{(p)} T_{qrs} \mu_{os}^{(q)} - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nqr} \theta_{oqr}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)} - \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} \theta_{oqr}^{(q)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npv}^{(p)} T_{prs} \theta_{ors}^{(q)} - \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mp} a_{pq}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npv}^{(p)} T_{prs} \theta_{ors}^{(q)} + \frac{1}{9} b_{ijv}^{(p)} T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{prs} \theta_{ors}^{(q)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npv}^{(p)} T_{prs} \theta_{ors}^{(q)} + \frac{1}{9} b_{ijv}^{(p)} T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{prs} \theta_{ors}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqv}^{(p)} T_{qst} \theta_{ost}^{(q)} - \frac{1}{9} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rst} \theta_{ost}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qrs} \theta_{ors}^{(q)} - \frac{1}{9} b_{ijv}^{(p)} T_{jl} a_{lm}^{(p)} T_{mnp} A_{qnp}^{(p)} T_{qrs} \theta_{ors}^{(q)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} A_{npq}^{(p)} T_{pqrs} \theta_{ors}^{(q)} - \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(p)} T_{mn} A_{npq}^{(p)} T_{pqrs} \theta_{ors}^{(q)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} C_{npqr}^{(p)} T_{qrst} \theta_{ost}^{(q)} - \frac{1}{9} b_{ijv}^{(p)} T_{jl} a_{lm}^{(p)} T_{mnp} C_{npqr}^{(p)} T_{qrst} \theta_{ost}^{(q)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} b_{pqv}^{(q)} T_{qs} \mu_{os}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rs} \mu_{os}^{(p)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_r \mu_{ot}^{(p)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{3} A_{ijk}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& -\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& -\frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{nlm}^{(q)} T_{np} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} b_{ijv}^{(p)} T_{jlm} A_{lmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} b_{rs}^{(q)} T_{su} \mu_{ou}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jkl} C_{klmm}^{(q)} T_{mnp} b_{pqv}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{3} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} b_{qr}^{(q)} T_{rt} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& +\frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} b_{qr}^{(q)} T_{rt} \mu_{ot}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{npq}^{(p)} T_{nqr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{lnp} A_{npq}^{(p)} T_{nqr} a_{rs}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpn}^{(p)} T_{pqr} b_{rsv}^{(q)} T_{su} \mu_{ou}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& + \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{lnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tu} \mu_{ou}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nqr} A_{sqr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{nqr} A_{sqr}^{(q)} T_{st} \mu_{ot}^{(p)} \\
& - \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{nqr} A_{sqr}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nqr} A_{qrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{nqr} A_{qrs}^{(q)} T_{rst} \mu_{ot}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nqr} C_{qrst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{nqr} C_{qrst}^{(q)} T_{stu} \mu_{ou}^{(p)} \\
& - \frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{nqr} C_{qrst}^{(q)} T_{stu} \mu_{ou}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} a_{mn}^{(p)} T_{np} b_{pqv}^{(q)} T_{qst} \theta_{ost}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{ln} a_{np}^{(p)} T_{pq} a_{qr}^{(q)} T_{rst} \theta_{ost}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} a_{lm}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} A_{ijk}^{(p)} T_{jkl} b_{lmv}^{(q)} T_{mp} a_{pq}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& - \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{mkl}^{(q)} T_{mn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} a_{np}^{(p)} T_{pq} b_{qr}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} A_{klm}^{(q)} T_{lmn} b_{npv}^{(p)} T_{pr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} a_{pq}^{(p)} T_{qr} b_{rs}^{(q)} T_{suv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jkl} C_{klmn}^{(q)} T_{mnp} b_{pqv}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} b_{ijv}^{(p)} T_{jlm} C_{lmnp}^{(q)} T_{npq} a_{qr}^{(p)} T_{rs} a_{st}^{(q)} T_{tuv} \theta_{ouv}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{pmn}^{(p)} T_{pq} b_{qr}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} A_{qnp}^{(p)} T_{qr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} A_{mnp}^{(p)} T_{npq} b_{qr}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} b_{klv}^{(q)} T_{lnp} A_{npq}^{(p)} T_{pqr} a_{rs}^{(q)} T_{stu} \theta_{otu}^{(p)} \\
& + \frac{1}{9} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lmn} C_{mnpq}^{(p)} T_{pqr} b_{rs}^{(q)} T_{tuw} \theta_{ouw}^{(p)} \\
& + \frac{1}{9} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mnp} C_{npqr}^{(p)} T_{qrs} a_{st}^{(q)} T_{tuw} \theta_{ouw}^{(p)} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} a_{kl}^{(q)} T_{lm} b_{mnv}^{(p)} T_{nqr} A_{sqr}^{(q)} T_{stu} \theta_{otu} \\
& - \frac{1}{3} a_{ij}^{(p)} T_{jk} b_{klv}^{(p)} T_{ln} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{stu} \theta_{otu}
\end{aligned}$$

$$-\frac{1}{3} b_{ijv}^{(p)} T_{jl} a_{lm}^{(q)} T_{mn} a_{np}^{(p)} T_{pqr} A_{sqr}^{(q)} T_{stu} \theta_{otu} \Big) E^2 a_i^x a_v^x$$

The first derivative of the potential with respect to the static electric field is given by

$$\begin{aligned} \frac{\partial U^{(1)}(\tau, E)}{\partial E} = & - \left( \mu_{ov}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} \mu_{ov}^{(2)} - \frac{1}{9} A_{ijk}^{(1)} T_{jklm} \theta_{olv}^{(2)} + a_{ij}^{(1)} T_{jk} \mu_{ov}^{(2)} \right. \\ & - \frac{1}{3} a_{ij}^{(1)} T_{jkl} \theta_{okv}^{(2)} + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} \mu_{ov}^{(1)} + \frac{1}{3} A_{jkl}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} \mu_{ov}^{(1)} \\ & - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} \mu_{ov}^{(1)} + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} \mu_{ov}^{(1)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} \mu_{ov}^{(1)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} \theta_{omv}^{(1)} + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mnp} \theta_{onv}^{(1)} \\ & - \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mnp} \theta_{onv}^{(1)} + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mnp} \theta_{onv}^{(1)} \\ & + \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnpq} \theta_{opv}^{(1)} \\ & + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} \mu_{ov}^{(2)} \\ & + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} \mu_{ov}^{(2)} \\ & - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} \mu_{ov}^{(2)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} \mu_{ov}^{(2)} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} \mu_{ov}^{(2)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} \mu_{ov}^{(2)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} \mu_{ov}^{(2)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} \theta_{opv}^{(2)} \\
& - \frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} \theta_{oqv}^{(2)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} \theta_{oqv}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} \theta_{oqv}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qrs} \theta_{orv}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pqr} \theta_{oqv}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npqr} \theta_{oqv}^{(2)} \\
& + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} \mu_{ov}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{ov}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{ov}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{ov}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ov}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{ov}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} a_{qr}^{(2)} T_{rs} \mu_{ov}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{rqp}^{(2)} T_{rs} \mu_{ov}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{pqr}^{(2)} T_{qrs} \mu_{ov}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} a_{pq}^{(2)} T_{qrs} \theta_{orv}^{(1)} \\
& + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} a_{qr}^{(2)} T_{rst} \theta_{osv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} \mu_{ov}^{(1)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rst} \theta_{osv}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rst} \theta_{osv}^{(1)}
\end{aligned}$$

$$+\frac{1}{9} a_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} a_{pq}^{(1)} \text{T}_{qr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otv}^{(1)}$$

$$+\frac{1}{9} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} A_{pmn}^{(1)} \text{T}_{pq} a_{qr}^{(2)} \text{T}_{rst} \theta_{osv}^{(1)}$$

$$+\frac{1}{9} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} A_{mnp}^{(1)} \text{T}_{npq} a_{qr}^{(2)} \text{T}_{rst} \theta_{osv}^{(1)}$$

$$+\frac{1}{9} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} C_{mnpq}^{(1)} \text{T}_{pqr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otv}^{(1)} \Big) \text{ a}_i^x$$

$$-\left( a_{iv}^{(1)} + a_{ij}^{(1)} \text{T}_{jk} a_{kv}^{(2)} + \frac{1}{3} A_{ijk}^{(1)} \text{T}_{jkl} a_{lv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{vkl}^{(2)} \right.$$

$$+a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} a_{mv}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} \text{T}_{jkl} a_{lm}^{(2)} \text{T}_{mn} a_{nv}^{(1)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{mkl}^{(2)} \text{T}_{mn} a_{nv}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{klm}^{(2)} \text{T}_{lmn} a_{nv}^{(1)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} a_{pv}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} A_{vmn}^{(1)} + a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} a_{mn}^{(1)} \text{T}_{np} a_{pv}^{(2)}$$

$$+\frac{1}{3} A_{ijk}^{(1)} \text{T}_{jkl} a_{lm}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{pq} a_{qv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{mkl}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{pq} a_{qv}^{(2)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{klm}^{(2)} \text{T}_{lmn} a_{np}^{(1)} \text{T}_{pq} a_{qv}^{(2)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} a_{pq}^{(1)} \text{T}_{qr} a_{rv}^{(2)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} A_{pmn}^{(1)} \text{T}_{pq} a_{qv}^{(2)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} A_{mnp}^{(1)} \text{T}_{npq} a_{qv}^{(2)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lmn} C_{mnpq}^{(1)} \text{T}_{pqr} a_{rv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} a_{mn}^{(1)} \text{T}_{npq} A_{vpq}^{(2)}$$

$$+a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} a_{mn}^{(1)} \text{T}_{np} a_{pq}^{(2)} \text{T}_{qr} a_{rv}^{(1)}$$

$$\begin{aligned}
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tv}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{st} a_{tv}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} a_{sv}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{pqr}^{(2)} T_{qrs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} a_{tv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrs} A_{trv}^{(1)} \\
& + b_{ijv}^{(1)} T_{jl} \mu_{ol}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jlm} \theta_{olm}^{(2)} + b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} \mu_{on}^{(1)} \\
& + a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} \mu_{on}^{(1)} + \frac{1}{3} A_{jkl}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} \mu_{op}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} A_{nlm}^{(2)} \text{T}_{np} \mu_{op}^{(1)} + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} A_{lmn}^{(2)} \text{T}_{mnp} \mu_{op}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} C_{lmnp}^{(2)} \text{T}_{npq} \mu_{oq}^{(1)} + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mnp} \theta_{onp}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{lnp} \theta_{onp}^{(1)} + \frac{1}{9} A_{ijk}^{(1)} \text{T}_{jkl} b_{lmv}^{(2)} \text{T}_{mpq} \theta_{opq}^{(1)} \\
& - \frac{1}{9} b_{ijv}^{(1)} \text{T}_{jlm} A_{nlm}^{(2)} \text{T}_{mnpq} \theta_{opq}^{(1)} + \frac{1}{9} b_{ijv}^{(1)} \text{T}_{jlm} A_{lmn}^{(2)} \text{T}_{mnpq} \theta_{opq}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} \text{T}_{jlm} C_{lmnp}^{(2)} \text{T}_{npqr} \theta_{oqr}^{(1)} \\
& + a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} b_{mnv}^{(1)} \text{T}_{nq} \mu_{oq}^{(2)} + b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{qp} \mu_{oq}^{(2)} \\
& + a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{ln} a_{np}^{(1)} \text{T}_{pq} \mu_{oq}^{(2)} + \frac{1}{3} A_{ijk}^{(1)} \text{T}_{jkl} a_{lm}^{(2)} \text{T}_{mn} b_{npv}^{(1)} \text{T}_{pr} \mu_{or}^{(2)} \\
& + \frac{1}{3} A_{ijk}^{(1)} \text{T}_{jkl} b_{lmv}^{(2)} \text{T}_{mp} a_{pq}^{(1)} \text{T}_{qr} \mu_{or}^{(2)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{mkl}^{(2)} \text{T}_{mn} b_{npv}^{(1)} \text{T}_{pr} \mu_{or}^{(2)} \\
& - \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} A_{nlm}^{(2)} \text{T}_{np} a_{pq}^{(1)} \text{T}_{qr} \mu_{or}^{(2)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} A_{klm}^{(2)} \text{T}_{lmn} b_{npv}^{(1)} \text{T}_{pr} \mu_{or}^{(2)} \\
& \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} A_{lmn}^{(2)} \text{T}_{mnp} a_{pq}^{(1)} \text{T}_{qr} \mu_{or}^{(2)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jkl} C_{klmn}^{(2)} \text{T}_{mnp} b_{pqv}^{(1)} \text{T}_{qs} \mu_{os}^{(2)} \\
& + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jlm} C_{lmnp}^{(2)} \text{T}_{npq} a_{qr}^{(1)} \text{T}_{rs} \mu_{os}^{(2)} + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mnp} A_{qnp}^{(1)} \text{T}_{qr} \mu_{or}^{(2)} \\
& + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mnp} A_{npq}^{(1)} \text{T}_{pqr} \mu_{or}^{(2)} + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{lnp} A_{qnp}^{(1)} \text{T}_{qr} \mu_{or}^{(2)} \\
& + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{lnp} A_{npq}^{(1)} \text{T}_{pqr} \mu_{or}^{(2)} + \frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mnp} C_{npqr}^{(1)} \text{T}_{qrs} \mu_{os}^{(2)} \\
& + \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{lnp} C_{npqr}^{(1)} \text{T}_{qrs} \mu_{os}^{(2)} - \frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} b_{mnv}^{(1)} \text{T}_{nqr} \theta_{oqr}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pqr} \theta_{oqr}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} \theta_{oqr}^{(2)} \\
& -\frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} - \frac{1}{9} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qrs} \theta_{ors}^{(2)} \\
& +\frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{prs} \theta_{ors}^{(2)} \\
& +\frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{prs} \theta_{ors}^{(2)} \\
& -\frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{qst} \theta_{ost}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} a_{qr}^{(1)} T_{rst} \theta_{ost}^{(2)} \\
& -\frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qrs} \theta_{ors}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mnp} A_{qnp}^{(1)} T_{qrs} \theta_{ors}^{(2)} \\
& -\frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} A_{npq}^{(1)} T_{pqrs} \theta_{ors}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mn} A_{npq}^{(1)} T_{pqrs} \theta_{ors}^{(2)} \\
& -\frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrst} \theta_{ost}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mnp} C_{npqr}^{(1)} T_{qrst} \theta_{ost}^{(2)} \\
& +a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} b_{pqv}^{(2)} T_{qs} \mu_{os}^{(1)} \\
& +a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mnv}^{(1)} T_{nq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} \\
& +a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} \\
& +b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} \\
& +\frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_r \mu_{ot}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} b_{rs}^{(2)} T_{su} \mu_{ou}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmm}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{rs} a_{st}^{(2)} T_{tu} \mu_{ou}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} a_{qr}^{(1)} T_{rs} a_{st}^{(2)} T_{tu} \mu_{ou}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} b_{qrv}^{(2)} T_{rt} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} b_{qr}^{(2)} T_{rt} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npq}^{(1)} T_{nqr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{lnp} A_{npq}^{(1)} T_{nqr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpn}^{(1)} T_{pqr} b_{rs}^{(2)} T_{su} \mu_{ou}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tu} \mu_{ou}^{(1)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tu} \mu_{ou}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{nqr} A_{sqr}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{nqr} A_{sqr}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mnv}^{(1)} T_{nqr} A_{qrs}^{(2)} T_{rst} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{nqr} A_{qrs}^{(2)} T_{rst} \mu_{ot}^{(1)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{nqr} A_{qrs}^{(2)} T_{rst} \mu_{ot}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{ln} a_{np}^{(1)} \text{T}_{nqr} C_{qrst}^{(2)} \text{T}_{stu} \mu_{ou}^{(1)} \\
& -\frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{nqr} C_{qrst}^{(2)} \text{T}_{stu} \mu_{ou}^{(1)} \\
& +\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} a_{kl}^{(2)} \text{T}_{lm} a_{mn}^{(1)} \text{T}_{np} b_{pqv}^{(2)} \text{T}_{qst} \theta_{ost}^{(1)} \\
& +\frac{1}{3} a_{ij}^{(1)} \text{T}_{jk} b_{klv}^{(2)} \text{T}_{ln} a_{np}^{(1)} \text{T}_{pq} a_{qr}^{(2)} \text{T}_{rst} \theta_{ost}^{(1)} \\
& +\frac{1}{3} b_{ijv}^{(1)} \text{T}_{jl} a_{lm}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{pq} a_{qr}^{(2)} \text{T}_{rst} \theta_{ost}^{(1)} \\
& +\frac{1}{9} A_{ijk}^{(1)} \text{T}_{jkl} a_{lm}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{pq} b_{qr}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)} \\
& +\frac{1}{9} A_{ijk}^{(1)} \text{T}_{jkl} b_{lmv}^{(2)} \text{T}_{mp} a_{pq}^{(1)} \text{T}_{qr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)} \\
& -\frac{1}{9} a_{ij}^{(1)} \text{T}_{jkl} A_{mkl}^{(2)} \text{T}_{mn} a_{np}^{(1)} \text{T}_{pq} b_{qr}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)} \\
& -\frac{1}{9} b_{ijv}^{(1)} \text{T}_{jlm} A_{nlm}^{(2)} \text{T}_{np} a_{pq}^{(1)} \text{T}_{qr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)} \\
& +\frac{1}{9} a_{ij}^{(1)} \text{T}_{jkl} A_{klm}^{(2)} \text{T}_{lmn} b_{npv}^{(1)} \text{T}_{pr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)} \\
& +\frac{1}{9} a_{ij}^{(1)} \text{T}_{jkl} A_{klm}^{(2)} \text{T}_{lmn} b_{npv}^{(1)} \text{T}_{pr} a_{rs}^{(2)} \text{T}_{stu} \theta_{otu}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{lnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} b_{rs}^{(2)} T_{suv} \theta_{ouv}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{rs} a_{st}^{(2)} T_{tuv} \theta_{ouv}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} a_{qr}^{(1)} T_{rs} a_{st}^{(2)} T_{tuv} \theta_{ouv}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{npq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} b_{rs}^{(2)} T_{tuw} \theta_{ouw}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tuw} \theta_{ouw}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tuw} \theta_{ouw}^{(1)}
\end{aligned}$$

$$-\frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mn}^{(1)} T_{nqr} A_{sqr}^{(2)} T_{stu} \theta_{otu}$$

$$-\frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(1)} T_{ln} a_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{stu} \theta_{otu}$$

$$-\frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{stu} \theta_{otu} \Big) E a_i^x a_v^x$$

The second derivative with respect to the static electric field is given by

$$\begin{aligned} \frac{\partial U^2(1)(\tau, E)}{\partial E^2} = & - \left( a_{iv}^{(1)} + a_{ij}^{(1)} T_{jk} a_{kv}^{(2)} + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{vkl}^{(2)} \right. \\ & + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mv}^{(1)} + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{nv}^{(1)} - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{nv}^{(1)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{nv}^{(1)} + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pv}^{(1)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{vmn}^{(1)} + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pv}^{(2)} \\ & + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qv}^{(2)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} a_{qv}^{(2)} + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rv}^{(2)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} a_{qv}^{(2)} + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} a_{qv}^{(2)} \\ & + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} a_{rv}^{(2)} - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{vpq}^{(2)} \\ & + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qr} a_{rv}^{(1)} \\ & + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} a_{tv}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} a_{qr}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{st} a_{tv}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{rpq}^{(2)} T_{rs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} A_{pqr}^{(2)} T_{qrs} a_{sv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{npq} C_{pqrs}^{(2)} T_{rst} a_{tv}^{(1)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} a_{pq}^{(2)} T_{qrs} A_{trv}^{(1)} \\
& + b_{ijv}^{(1)} T_{jl} \mu_{ol}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jlm} \theta_{olm}^{(2)} + b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} \mu_{on}^{(1)} \\
& + a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} \mu_{on}^{(1)} + \frac{1}{3} A_{jkl}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} \mu_{op}^{(1)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} \mu_{op}^{(1)} + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} \mu_{op}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} \mu_{oq}^{(1)} + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} \theta_{onp}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} \theta_{onp}^{(1)} + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mpq} \theta_{opq}^{(1)} \\
& - \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{mnpq} \theta_{opq}^{(1)} + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnpq} \theta_{opq}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npqr} \theta_{oqr}^{(1)} \\
& + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mnv}^{(1)} T_{nq} \mu_{oq}^{(2)} + b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{qp} \mu_{oq}^{(2)} \\
& + a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pq} \mu_{oq}^{(2)} + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} \mu_{or}^{(2)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qr} \mu_{or}^{(2)} - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} \mu_{or}^{(2)} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} \mu_{or}^{(2)} + \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{pr} \mu_{or}^{(2)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} \mu_{os}^{(2)} + \frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{qs} \mu_{os}^{(2)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} a_{qr}^{(1)} T_{rs} \mu_{os}^{(2)} + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} \mu_{or}^{(2)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{npq}^{(1)} T_{pqr} \mu_{or}^{(2)} + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} \mu_{or}^{(2)} \\
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npq}^{(1)} T_{pqr} \mu_{os}^{(2)} + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} \mu_{os}^{(2)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pqr} \theta_{oqr}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} \theta_{oqr}^{(2)}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} - \frac{1}{9} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qrs} \theta_{ors}^{(2)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{prs} \theta_{ors}^{(2)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{prs} \theta_{ors}^{(2)} + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{prs} \theta_{ors}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{qst} \theta_{ost}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{nnp} a_{qr}^{(1)} T_{rst} \theta_{ost}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qrs} \theta_{ors}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mnp} A_{qnp}^{(1)} T_{qrs} \theta_{ors}^{(2)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npq}^{(1)} T_{pqrs} \theta_{ors}^{(2)} - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mnp} C_{npq}^{(1)} T_{pqrs} \theta_{ors}^{(2)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrst} \theta_{ost}^{(2)} - \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(1)} T_{mnp} C_{npqr}^{(1)} T_{qrst} \theta_{ost}^{(2)} \\
& + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} a_{mn}^{(1)} T_{np} b_{pqv}^{(2)} T_{qs} \mu_{os}^{(1)} + a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mnv}^{(1)} T_{nq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} \\
& + a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} + b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rs} \mu_{os}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qr}^{(2)} T_{r} \mu_{ot}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& + \frac{1}{3} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qr}^{(2)} T_{st} \mu_{ot}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}
\end{aligned}$$

$$-\frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} b_{rsv}^{(2)} T_{su} \mu_{ou}^{(1)}$$

$$+\frac{1}{3} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npg} a_{qr}^{(1)} T_{rs} a_{st}^{(2)} T_{tu} \mu_{ou}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jkl} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} b_{qrv}^{(2)} T_{rt} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npg} b_{qrv}^{(2)} T_{rt} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npg}^{(1)} T_{nqr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{lnp} A_{npg}^{(1)} T_{nqr} a_{rs}^{(2)} T_{st} \mu_{ot}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lmn} C_{mnpn}^{(1)} \mathbf{T}_{pqr} b_{rsu}^{(2)} \mathbf{T}_{su} \mu_{ou}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} b_{klv}^{(2)} \mathbf{T}_{lnp} C_{npqr}^{(1)} \mathbf{T}_{qrs} a_{st}^{(2)} \mathbf{T}_{tu} \mu_{ou}^{(1)}$$

$$+\frac{1}{3} b_{ijv}^{(1)} \mathbf{T}_{jl} a_{lm}^{(2)} \mathbf{T}_{lnp} C_{npqr}^{(1)} \mathbf{T}_{qrs} a_{st}^{(2)} \mathbf{T}_{tu} \mu_{ou}^{(1)}$$

$$-\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lm} b_{mnv}^{(1)} \mathbf{T}_{nqr} A_{sqr}^{(2)} \mathbf{T}_{st} \mu_{ot}^{(1)}$$

$$-\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} b_{klv}^{(2)} \mathbf{T}_{ln} a_{np}^{(1)} \mathbf{T}_{nqr} A_{sqr}^{(2)} \mathbf{T}_{st} \mu_{ot}^{(1)}$$

$$-\frac{1}{3} b_{ijv}^{(1)} \mathbf{T}_{jl} a_{lm}^{(2)} \mathbf{T}_{mn} a_{np}^{(1)} \mathbf{T}_{nqr} A_{sqr}^{(2)} \mathbf{T}_{st} \mu_{ot}^{(1)}$$

$$-\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lm} b_{mnv}^{(1)} \mathbf{T}_{nqr} A_{sqr}^{(2)} \mathbf{T}_{rst} \mu_{ot}^{(1)}$$

$$-\frac{1}{3} b_{ijv}^{(1)} \mathbf{T}_{jl} a_{lm}^{(2)} \mathbf{T}_{mn} a_{np}^{(1)} \mathbf{T}_{nqr} A_{sqr}^{(2)} \mathbf{T}_{rst} \mu_{ot}^{(1)}$$

$$-\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lm} b_{mnv}^{(1)} \mathbf{T}_{nqr} C_{qrst}^{(2)} \mathbf{T}_{stu} \mu_{ou}^{(1)}$$

$$-\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} b_{klv}^{(2)} \mathbf{T}_{ln} a_{np}^{(1)} \mathbf{T}_{nqr} C_{qrst}^{(2)} \mathbf{T}_{stu} \mu_{ou}^{(1)}$$

$$-\frac{1}{3} b_{ijv}^{(1)} \mathbf{T}_{jl} a_{lm}^{(2)} \mathbf{T}_{mn} a_{np}^{(1)} \mathbf{T}_{nqr} C_{qrst}^{(2)} \mathbf{T}_{stu} \mu_{ou}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lm} a_{mn}^{(1)} \mathbf{T}_{np} b_{pqv}^{(2)} \mathbf{T}_{qst} \theta_{ost}^{(1)}$$

$$+\frac{1}{3} a_{ij}^{(1)} \mathbf{T}_{jk} a_{kl}^{(2)} \mathbf{T}_{lm} b_{mnv}^{(1)} \mathbf{T}_{nq} a_{qr}^{(2)} \mathbf{T}_{rst} \theta_{ost}^{(1)}$$

$$\begin{aligned}
& + \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{ln} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rst} \theta_{ost}^{(1)} \\
& + \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} a_{qr}^{(2)} T_{rst} \theta_{ost}^{(1)} \\
& + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} a_{lm}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} A_{ijk}^{(1)} T_{jkl} b_{lmv}^{(2)} T_{mp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} a_{np}^{(1)} T_{pq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& - \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{mkl}^{(2)} T_{mn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& - \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{nlm}^{(2)} T_{np} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} A_{klm}^{(2)} T_{lmn} b_{npv}^{(1)} T_{pr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} A_{lmn}^{(2)} T_{lnp} a_{pq}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} a_{pq}^{(1)} T_{qr} b_{rsv}^{(2)} T_{suv} \theta_{ouv}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jkl} C_{klmn}^{(2)} T_{mnp} b_{pqv}^{(1)} T_{rs} a_{st}^{(2)} T_{tuv} \theta_{ouv}^{(1)}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{9} b_{ijv}^{(1)} T_{jlm} C_{lmnp}^{(2)} T_{npq} a_{qr}^{(1)} T_{rs} a_{st}^{(2)} T_{tuv} \theta_{ouw}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{pmn}^{(1)} T_{pq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{qnp}^{(1)} T_{qr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} A_{mnp}^{(1)} T_{npq} b_{qrv}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} A_{npq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} A_{npq}^{(1)} T_{pqr} a_{rs}^{(2)} T_{stu} \theta_{otu}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lmn} C_{mnpq}^{(1)} T_{pqr} b_{rs}^{(2)} T_{tuw} \theta_{ouw}^{(1)} \\
& + \frac{1}{9} a_{ij}^{(1)} T_{jk} b_{klv}^{(2)} T_{lnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tuw} \theta_{ouw}^{(1)} \\
& + \frac{1}{9} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mnp} C_{npqr}^{(1)} T_{qrs} a_{st}^{(2)} T_{tuw} \theta_{ouw}^{(1)} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} a_{kl}^{(2)} T_{lm} b_{mnv}^{(1)} T_{nqr} A_{sqr}^{(2)} T_{stu} \theta_{otu} \\
& - \frac{1}{3} a_{ij}^{(1)} T_{jk} b_{klv}^{(1)} T_{ln} a_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{stu} \theta_{otu} \\
& - \frac{1}{3} b_{ijv}^{(1)} T_{jl} a_{lm}^{(2)} T_{mn} a_{np}^{(1)} T_{pqr} A_{sqr}^{(2)} T_{stu} \theta_{otu} \Big) a_i^x a_v^x
\end{aligned}$$

# Appendix B

## B.1 Fortran code used to calculate the $\theta_2\alpha_3$ contribution to the second Kerr virial coefficient.

```
PROGRAM KERR_Q2A3
```

```
C
```

```
C 2 September 2016
```

```
C PROGRAM TO CALCULATE TERM Q2A3 FOR C2H4 USING GAUSSIAN INTEGRATION WITH  
C 64 INTERVALS FOR THE RANGE, AND 16 INTERVALS FOR ALL ANGULAR VARIABLES  
C (I.E. ALPHA1, BETA1, GAMMA1, ALPHA2, BETA2 AND GAMMA2).
```

```
C DOUBLE PRECISION IS USED THROUGHOUT.
```

```
C
```

```
C -----
```

```
C SYSTEM INITIALIZATION:
```

```
C -----
```

```
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
```

```
COMMON COEF1,DCTC
```

```
DIMENSION COEF2(64,2),COEF1(16,2),SEP(64),AL1(16),BE1(16),GA1(16)
```

```
+ ,AL2(16),BE2(16),GA2(16),DCTC(9,16,16,16),FI(16,16,16,16,16),D1(6
+ 4),E1(16,16,16,16,16),F1(16,16,16,16,16),SE3(64),SE4(64),SE5(64),
+ SE6(64),SE8(64),SE12(64),G1(16,16,16),DDP(16,16,16,16,16),DQP(16,
+ 16,16,16,16),DIDP(16,16,16,16,16)

INTEGER X1,X2,X3,X4,X5,X6,X7
```

C

C MOLECULAR DATA FOR ethene (632.8 nm)

C

```
SS1=0.000000
SS2=0.000000
SS3=0.000000
SS4=0.000000
SS5=0.000000
SS6=0.000000
SS7=0.000000
DIP=0.000
A11=4.305
A22=3.804
A33=6.029
ALDYN=(A11+A22+A33)/3
V11=4.245
V22=3.666
V33=5.803
ALSTAT=(V11+V22+V33)/3
Q1=5.370
Q2=-10.92
AMIN1=0.1000
```

```
AMAX1=3.0000
```

```
C
```

```
C READ THE GAUSSIAN COEFFICIENTS FROM THE DATAFILE GAUSS64.DAT:
```

```
C
```

```
OPEN(UNIT=10,FILE='GAUSS64.DAT')  
DO 10 ICTR1=1,64  
    DO 20 ICTR2=1,2  
        READ(10,1010,END=11)COEF2(ICTR1,ICTR2)  
1010      FORMAT(F18.15)  
20        CONTINUE  
10        CONTINUE  
11        CLOSE(UNIT=10)
```

```
C
```

```
C CALCULATE THE INTEGRATION POINTS FOR THE RANGE:
```

```
C
```

```
SEP1=(AMAX1-AMIN1)/2  
SEP2=(AMAX1+AMIN1)/2  
DO 30 INDX=1,64  
    SEP(INDX)=SEP1*COEF2(INDX,1)+SEP2  
30        CONTINUE
```

```
C
```

```
C READ THE GAUSSIAN COEFFICIENTS FROM THE DATAFILE GAUSS16.DAT:
```

```
C
```

```
OPEN(UNIT=11,FILE='GAUSS16.DAT')  
DO 100 ICTR1=1,16  
    DO 110 ICTR2=1,2
```

```
      READ(11,6000,END=12)COEF1(ICTR1,ICTR2)
6000      FORMAT(F18.15)
110      CONTINUE
100      CONTINUE
12      CLOSE(UNIT=11)
```

C

C CALCULATE THE INTEGRATION POINTS FOR ALPHA1:

C

AMIN=0.0

AMAX=2.\*3.14159265358979323846

AL11=(AMAX-AMIN)/2.

AL12=(AMAX+AMIN)/2.

DO 120 INDX=1,16

AL1(INDX)=AL11\*COEF1(INDX,1)+AL12

120 CONTINUE

C

C CALCULATE THE INTEGRATION POINTS FOR BETA1:

C

AMIN=0.0

AMAX=3.14159265358979323846

BE11=(AMAX-AMIN)/2.

BE12=(AMAX+AMIN)/2.

DO 121 INDX=1,16

BE1(INDX)=BE11\*COEF1(INDX,1)+BE12

121 CONTINUE

C

C CALCULATE THE INTEGRATION POINTS FOR GAMMA1:

C

AMIN=0.0

AMAX=2.\*3.14159265358979323846

GA11=(AMAX-AMIN)/2.

GA12=(AMAX+AMIN)/2.

DO 122 INDX=1,16

GA1(INDX)=GA11\*COEF1(INDX,1)+GA12

122 CONTINUE

C

C CALCULATE THE INTEGRATION POINTS FOR ALPHA2:

C

AMIN=0.0

AMAX=2.\*3.14159265358979323846

AL21=(AMAX-AMIN)/2.

AL22=(AMAX+AMIN)/2.

DO 123 INDX=1,16

AL2(INDX)=AL21\*COEF1(INDX,1)+AL22

123 CONTINUE

C

C CALCULATE THE INTEGRATION POINTS FOR BETA2:

C

AMIN=0.0

AMAX=3.14159265358979323846

BE21=(AMAX-AMIN)/2.

BE22=(AMAX+AMIN)/2.

```
DO 124 INDX=1,16
      BE2(INDX)=BE21*COEF1(INDX,1)+BE22
124      CONTINUE

C
C CALCULATE THE INTEGRATION POINTS FOR GAMMA2:
C
AMIN=0.0
AMAX=2.*3.14159265358979323846

GA21=(AMAX-AMIN)/2.
GA22=(AMAX+AMIN)/2.
DO 125 INDX=1,16
      GA2(INDX)=GA21*COEF1(INDX,1)+GA22
125      CONTINUE

C -----
C MAIN PROGRAM:
C -----
OPEN(UNIT=4,FILE='kt2a3_202K')

C
C MOLECULAR PARAMETERS:
C
TEMP=202.4
TEMPK=TEMP*1.380622E-23
```

R=0.4232

PARAM2=190.0

SHAPE1=0.22965

SHAPE2=0.21383

C

C CALCULATION OF THE LENNARD-JONES 6:12 POTENTIAL & STORAGE OF THE  
C VALUES IN AN ARRAY:

C

DO 61 X1=1,64

D1(X1)=4.\*PARAM2\*1.380622E-23\*((R/SEP(X1))\*\*12-(R/SEP(X1))\*\*6)  
SE12(X1)=SEP(X1)\*\*12  
SE5(X1)=SEP(X1)\*\*5  
SE8(X1)=SEP(X1)\*\*8  
SE3(X1)=SEP(X1)\*\*3  
SE4(X1)=SEP(X1)\*\*4  
SE6(X1)=SEP(X1)\*\*6

61       CONTINUE

C

C THE DIRECTION COSINE TENSOR COMPONENTS ARE STORED IN AN ARRAY:

C

```

DO 66 X4=1,16
DO 77 X3=1,16
DO 88 X2=1,16

C
C DIRECTION COSINE TENSOR COMPONENTS:
C

A1=COS(AL1(X2))*COS(BE1(X3))*COS(GA1(X4))-1.*SIN(AL1(X2))*SIN(GA1
+ (X4))
A2=SIN(AL1(X2))*COS(BE1(X3))*COS(GA1(X4))+COS(AL1(X2))*SIN(GA1(X4
+ ))
A3=-1.*SIN(BE1(X3))*COS(GA1(X4))
A4=-1.*COS(AL1(X2))*COS(BE1(X3))*SIN(GA1(X4))-1.*SIN(AL1(X2))*COS
+ (GA1(X4))
A5=-1.*SIN(AL1(X2))*COS(BE1(X3))*SIN(GA1(X4))+COS(AL1(X2))*COS(GA
+ 1(X4))
A6=SIN(BE1(X3))*SIN(GA1(X4))
A7=COS(AL1(X2))*SIN(BE1(X3))
A8=SIN(AL1(X2))*SIN(BE1(X3))
A9=COS(BE1(X3))

DCTC(1,X2,X3,X4)=A1
DCTC(2,X2,X3,X4)=A2
DCTC(3,X2,X3,X4)=A3
DCTC(4,X2,X3,X4)=A4
DCTC(5,X2,X3,X4)=A5
DCTC(6,X2,X3,X4)=A6
DCTC(7,X2,X3,X4)=A7
DCTC(8,X2,X3,X4)=A8
DCTC(9,X2,X3,X4)=A9

```

88 CONTINUE

77 CONTINUE

66 CONTINUE

C

C THE MULTIPOLE INTERACTION ENERGIES ARE CALCULATED AND STORED

C IN ARRAYS:

C

DO 939 X7=1,16

WRITE(4,1000)X7

1000 FORMAT (1X, 'INDEX (IN RANGE 1 TO 16) IS CURRENTLY ',I2 )

WRITE(6,1111)X7

1111 FORMAT (1X, 'Index (in range 1 to 16) is currently ',I2 )

DO 40 X6=1,16

DO 50 X5=1,16

C

C MOLECULE 2'S DIRECTION COSINE TENSOR COMPONENTS:

C

B1=DCTC(1,X5,X6,X7)

B2=DCTC(2,X5,X6,X7)

B3=DCTC(3,X5,X6,X7)

B4=DCTC(4,X5,X6,X7)

B5=DCTC(5,X5,X6,X7)

B6=DCTC(6,X5,X6,X7)

B7=DCTC(7,X5,X6,X7)

```
B8=DCTC(8,X5,X6,X7)  
B9=DCTC(9,X5,X6,X7)
```

```
DO 60 X4=1,16  
    DO 70 X3=1,16  
        DO 80 X2=1,16
```

C

C MOLECULE 1'S DIRECTION COSINE TENSOR COMPONENTS:

C

```
A1=DCTC(1,X2,X3,X4)  
A2=DCTC(2,X2,X3,X4)  
A3=DCTC(3,X2,X3,X4)  
A4=DCTC(4,X2,X3,X4)  
A5=DCTC(5,X2,X3,X4)  
A6=DCTC(6,X2,X3,X4)  
A7=DCTC(7,X2,X3,X4)  
A8=DCTC(8,X2,X3,X4)  
A9=DCTC(9,X2,X3,X4)
```

C

C CALCULATION OF THE DIPOLE-DIPOLE POTENTIAL:

C

```
DDP(X2,X3,X4,X5,X6)=8.98758E-24*DIP**2*(-2*A9*B9+A6*B6+A3*B3)
```

C

C CALCULATION OF THE DIPOLE-QUADRUPOLE POTENTIAL:

C

```
DQP(X2,X3,X4,X5,X6)=8.98758E-25*DIP*(Q2*(-2*A9*B9**2+(2*A6*B6+2*A
```

```

+ 3*B3+2*A9**2-2*A8**2-A6**2+A5**2-A3**2+A2**2)*B9+2*A9*B8**2+(-2*A
+ 6*B5-2*A3*B2)*B8+A9*B6**2+(2*A5*A8-2*A6*A9)*B6-A9*B5**2+A9*B3**2+
+ (2*A2*A8-2*A3*A9)*B3-A9*B2**2)+Q1*(-2*A9*B9**2+(2*A6*B6+2*A3*B3+2
+ *A9**2-2*A7**2-A6**2+A4**2-A3**2+A1**2)*B9+2*A9*B7**2+(-2*A6*B4-2
+ *A3*B1)*B7+A9*B6**2+(2*A4*A7-2*A6*A9)*B6-A9*B4**2+A9*B3**2+(2*A1*
+ A7-2*A3*A9)*B3-A9*B1**2))

```

C

C CALCULATION OF THE DIPOLE-INDUCED DIPOLE POTENTIAL:

C

```

DIDP(X2,X3,X4,X5,X6)=-0.50*ALSTAT*8.07765E-27*DIP**2*(3*B9**2
+ +3*A9**2-2)

```

C

C CALCULATION OF THE QUADRUPOLE-QUADRUPOLE POTENTIAL:

C

```

quad1=-16.*(a6*a9-a5*a8)*(b6*b9-b5*b8)-16.*(a3*a9-a2*a8)*(b3*b9-b
+ 2*b8)+4.*(2.*a9**2-2.*a8**2-a6**2+a5**2-a3**2+a2**2)*(b9-b8)*(b9+
+ b8)+(-4.*a9**2+4.*a8**2+3.*a6**2-3.*a5**2+a3**2-a2**2)*(b6**2-b5*
+ *2)+4.*(a3*a6-a2*a5)*(b3*b6-b2*b5)+(-4.*a9**2+4.*a8**2+a6**2-a5**2
+ 2+3.*a3**2-3.*a2**2)*(b3**2-b2**2)

```

```

quad2=-16.*(a6*a9-a4*a7)*(b6*b9-b4*b7)-16.*(a3*a9-a1*a7)*(b3*b9-b
+ 1*b7)+4.*(2.*a9**2-2.*a7**2-a6**2+a4**2-a3**2+a1**2)*(b9-b7)*(b9+
+ b7)+(-4.*a9**2+4.*a7**2+3.*a6**2-3.*a4**2+a3**2-a1**2)*(b6**2-b4*
+ *2)+4.*(a3*a6-a1*a4)*(b3*b6-b1*b4)+(-4.*a9**2+4.*a7**2+a6**2-a4**2
+ 2+3.*a3**2-3.*a1**2)*(b3**2-b1**2)

```

```

quad3=4.*(4.*A9**2-2.* (A8**2+A7**2+A6**2+A3**2)+A5**2+A4**2+A2**2
+ +A1**2)*B9**2-16.* (2.*A6*A9-A5*A8-A4*A7)*B6*B9-16*(2.*A3*A9-A2*A8

```

```

+ -A1*A7)*B3*B9-4.*(2.*A9**2-2.*A7**2-A6**2+A4**2-A3**2+A1**2)*B8**
+ 2+16.*(A6*A9-A4*A7)*B5*B8+16.*(A3*A9-A1*A7)*B2*B8-4.*(2.*A9**2-2.
+ *A8**2-A6**2+A5**2-A3**2+A2**2)*B7**2+16.*(A6*A9-A5*A8)*B4*B7+16.
+ *(A3*A9-A2*A8)*B1*B7+(-8.*A9**2+4.*A8**2+A7**2)+6.*A6**2-3.*(A5*
+ *2+A4**2)+2*A3**2-A2**2-A1**2)*B6**2+4.*(2.*A3*A6-A2*A5-A1*A4)*B3
+ *B6+(4.*A9**2-4.*A7**2-3.*A6**2+3.*A4**2-A3**2+A1**2)*B5**2-4.*(A
+ 3*A6-A1*A4)*B2*B5+(4.*A9**2-4.*A8**2-3.*A6**2+3.*A5**2-A3**2+A2**
+ 2)*B4**2-4.*(A3*A6-A2*A5)*B1*B4+(-8.*A9**2+4.*A8**2+A7**2)+2.*A6
+ **2-A5**2-A4**2+6.*A3**2-3.*A2**2+A1**2)*B3**2+(4.*A9**2-4.*A7*
+ *2-A6**2+A4**2-3.*A3**2+3.*A1**2)*B2**2+(4.*A9**2-4.*A8**2-A6**2+
+ A5**2-3.*A3**2+3.*A2**2)*B1**2

```

```

E1(X2,X3,X4,X5,X6)=8.98758E-26*(1./3.)*(Q2**2*QUAD1+Q1**2*QUAD
+ 2+Q1*Q2*QUAD3)

```

C

C CALCULATION OF THE QUADRUPOLE-INDUCED DIPOLE POTENTIAL:

C

```

QID1=Q2**2*(4.*A9**4+(-8.*A8**2+4.*A5**2+4.*A2**2)*A9**2+(-8.*A5*
+ A6-8.*A2*A3)*A8*A9+4.*A8**4+(4.*A6**2+4.*A3**2)*A8**2+A6**4+(-2.*
+ A5**2+2.*A3**2-2.*A2**2)*A6**2+A5**4+(2.*A2**2-2.*A3**2)*A5**2+A3
+ **4-2.*A2**2*A3**2+A2**4)+Q1**2*(4.*A9**4+(-8.*A7**2+4.*A4**2+4.*
+ A1**2)*A9**2+(-8.*A4*A6-8.*A1*A3)*A7*A9+4.*A7**4+(4.*A6**2+4.*A3*
+ *2)*A7**2+A6**4+(-2.*A4**2+2.*A3**2-2.*A1**2)*A6**2+A4**4+(2.*A1*
+ *2-2.*A3**2)*A4**2+A3**4-2.*A1**2*A3**2+A1**4)+Q1*Q2*(8.*A9**4+(-
+ 8.*A8**2-8.*A7**2+4.*A5**2+4.*A4**2+4.*A2**2+4.*A1**2)*A9**2+((-8
+ .*A5*A6-8.*A2*A3)*A8+(-8.*A4*A6-8.*A1*A3)*A7)*A9+(8.*A7**2+4.*A6*
+ *2-4.*A4**2+4.*A3**2-4.*A1**2)*A8**2+(8.*A4*A5+8.*A1*A2)*A7*A8+(4
+ .*A6**2-4.*A5**2+4.*A3**2-4.*A2**2)*A7**2+2.*A6**4+(-2.*A5**2-2.*

```

```

+ A4**2+4.*A3**2-2.*A2**2-2.*A1**2)*A6**2+(2.*A4**2-2.*A3**2+2.*A1*
+ *2)*A5**2+(2.*A2**2-2.*A3**2)*A4**2+2.*A3**4+(-2.*A2**2-2.*A1**2)
+ *A3**2+2.*A1**2*A2**2)

QID2=Q2**2*(4.*B9**4+(-8.*B8**2+4.*B5**2+4.*B2**2))*B9**2+(-8.*B5*
+ B6-8.*B2*B3)*B8*B9+4.*B8**4+(4.*B6**2+4.*B3**2)*B8**2+B6**4+(-2.*
+ B5**2+2.*B3**2-2.*B2**2)*B6**2+B5**4+(2.*B2**2-2.*B3**2)*B5**2+B3
+ **4-2.*B2**2*B3**2+B2**4)+Q1**2*(4.*B9**4+(-8.*B7**2+4.*B4**2+4.*
+ B1**2)*B9**2+(-8.*B4*B6-8.*B1*B3)*B7*B9+4.*B7**4+(4.*B6**2+4.*B3*
+ *2)*B7**2+B6**4+(-2.*B4**2+2.*B3**2-2.*B1**2)*B6**2+B4**4+(2.*B1*
+ *2-2.*B3**2)*B4**2+B3**4-2.*B1**2*B3**2+B1**4)+Q1*Q2*(8.*B9**4+(-
+ 8.*B8**2-8.*B7**2+4.*B5**2+4.*B4**2+4.*B2**2+4.*B1**2)*B9**2+((-8
+ .*B5*B6-8.*B2*B3)*B8+(-8.*B4*B6-8.*B1*B3)*B7)*B9+(8.*B7**2+4.*B6*
+ *2-4.*B4**2+4.*B3**2-4.*B1**2)*B8**2+(8.*B4*B5+8.*B1*B2)*B7*B8+(4
+ .*B6**2-4.*B5**2+4.*B3**2-4.*B2**2)*B7**2+2.*B6**4+(-2.*B5**2-2.*
+ B4**2+4.*B3**2-2.*B2**2-2.*B1**2)*B6**2+(2.*B4**2-2.*B3**2+2.*B1*
+ *2)*B5**2+(2.*B2**2-2.*B3**2)*B4**2+2.*B3**4+(-2.*B2**2-2.*B1**2)
+ *B3**2+2.*B1**2*B2**2)

```

$$F1(X2, X3, X4, X5, X6) = -0.5 * 8.07765E-29 * ALSTAT * (QID1 + QID2)$$

C

C CALCULATION OF THE INTEGRATION ARGUMENT:

C

C

C 2nd Rank T-Tensor:

C

```

T11=2.*A7**2-A4**2-A1**2
T22=2.*A8**2-A5**2-A2**2
T33=2.*A9**2-A6**2-A3**2
T12=2.*A7*A8-A4*A5-A1*A2
T13=2.*A7*A9-A4*A6-A1*A3
T23=2.*A8*A9-A5*A6-A2*A3

```

C

C 3rd Rand T-Tensor:

C

```

T111=2*A7**3-3*A4**2*A7-3*A1**2*A7
T222=2*A8**3-3*A5**2*A8-3*A2**2*A8
T333=2*A9**3-3*A6**2*A9-3*A3**2*A9
T112=2*A7**2*A8-A4**2*A8-A1**2*A8-2*A4*A5*A7-2*A1*A2*A7
T122=2*A7*A8**2-2*A4*A5*A8-2*A1*A2*A8-A5**2*A7-A2**2*A7
T133=2*A7*A9**2-2*A4*A6*A9-2*A1*A3*A9-A6**2*A7-A3**2*A7
T233=2*A8*A9**2-2*A5*A6*A9-2*A2*A3*A9-A6**2*A8-A3**2*A8
T113=2*A7**2*A9-A4**2*A9-A1**2*A9-2*A4*A6*A7-2*A1*A3*A7
T223=2*A8**2*A9-A5**2*A9-A2**2*A9-2*A5*A6*A8-2*A2*A3*A8
T123=2*A7*A8*A9-A4*A5*A9-A1*A2*A9-A4*A6*A8-A1*A3*A8-A5*A6*A7-A2*A
+      3*A7

```

C

C Dynamic Polarizability of molecule 2 in

C molecule-fixed axes of molecule 1:

C

$$\begin{aligned}
Z11 = & A33 * (A7**2*B9**2 + (2*A4*A7*B6 + 2*A1*A7*B3) * B9 + A4**2*B6**2 + 2*A \\
+ & 1*A4*B3*B6 + A1**2*B3**2) + A22 * (A7**2*B8**2 + (2*A4*A7*B5 + 2*A1*A7*B2 \\
+ & ) * B8 + A4**2*B5**2 + 2*A1*A4*B2*B5 + A1**2*B2**2) + A11 * (A7**2*B7**2 + (2 \\
+ & *A4*A7*B4 + 2*A1*A7*B1) * B7 + A4**2*B4**2 + 2*A1*A4*B1*B4 + A1**2*B1**2)
\end{aligned}$$

$$\begin{aligned}
Z22 = & A33 * (A8**2*B9**2 + (2*A5*A8*B6 + 2*A2*A8*B3) * B9 + A5**2*B6**2 + 2*A \\
+ & 2*A5*B3*B6 + A2**2*B3**2) + A22 * (A8**2*B8**2 + (2*A5*A8*B5 + 2*A2*A8*B2 \\
+ & ) * B8 + A5**2*B5**2 + 2*A2*A5*B2*B5 + A2**2*B2**2) + A11 * (A8**2*B7**2 + (2 \\
+ & *A5*A8*B4 + 2*A2*A8*B1) * B7 + A5**2*B4**2 + 2*A2*A5*B1*B4 + A2**2*B1**2)
\end{aligned}$$

$$\begin{aligned}
Z33 = & A33 * (A9**2*B9**2 + (2*A6*A9*B6 + 2*A3*A9*B3) * B9 + A6**2*B6**2 + 2*A \\
+ & 3*A6*B3*B6 + A3**2*B3**2) + A22 * (A9**2*B8**2 + (2*A6*A9*B5 + 2*A3*A9*B2 \\
+ & ) * B8 + A6**2*B5**2 + 2*A3*A6*B2*B5 + A3**2*B2**2) + A11 * (A9**2*B7**2 + (2 \\
+ & *A6*A9*B4 + 2*A3*A9*B1) * B7 + A6**2*B4**2 + 2*A3*A6*B1*B4 + A3**2*B1**2)
\end{aligned}$$

$$\begin{aligned}
Z12 = & A33 * (A7*A8*B9**2 + ((A4*A8+A5*A7)*B6 + (A1*A8+A2*A7)*B3) * B9 + A4* \\
+ & A5*B6**2 + (A1*A5+A2*A4)*B3*B6 + A1*A2*B3**2) + A22 * (A7*A8*B8**2 + ((A4 \\
+ & *A8+A5*A7)*B5 + (A1*A8+A2*A7)*B2) * B8 + A4*A5*B5**2 + (A1*A5+A2*A4)*B2 \\
+ & *B5 + A1*A2*B2**2) + A11 * (A7*A8*B7**2 + ((A4*A8+A5*A7)*B4 + (A1*A8+A2*A \\
+ & 7)*B1) * B7 + A4*A5*B4**2 + (A1*A5+A2*A4)*B1*B4 + A1*A2*B1**2)
\end{aligned}$$

$$\begin{aligned}
Z13 = & A33 * (A7*A9*B9**2 + ((A4*A9+A6*A7)*B6 + (A1*A9+A3*A7)*B3) * B9 + A4* \\
+ & A6*B6**2 + (A1*A6+A3*A4)*B3*B6 + A1*A3*B3**2) + A22 * (A7*A9*B8**2 + ((A4 \\
+ & *A9+A6*A7)*B5 + (A1*A9+A3*A7)*B2) * B8 + A4*A6*B5**2 + (A1*A6+A3*A4)*B2 \\
+ & *B5 + A1*A3*B2**2) + A11 * (A7*A9*B7**2 + ((A4*A9+A6*A7)*B4 + (A1*A9+A3*A \\
+ & 7)*B1) * B7 + A4*A6*B4**2 + (A1*A6+A3*A4)*B1*B4 + A1*A3*B1**2)
\end{aligned}$$

$$\begin{aligned}
Z23 = & A33 * (A8*A9*B9**2 + ((A5*A9+A6*A8)*B6 + (A2*A9+A3*A8)*B3) * B9 + A5* \\
+ & A6*B6**2 + (A2*A6+A3*A5)*B3*B6 + A2*A3*B3**2) + A22 * (A8*A9*B8**2 + ((A5
\end{aligned}$$

```

+      *A9+A6*A8)*B5+(A2*A9+A3*A8)*B2)*B8+A5*A6*B5**2+(A2*A6+A3*A5)*B2
+
+      *B5+A2*A3*B2**2)+A11*(A8*A9*B7**2+((A5*A9+A6*A8)*B4+(A2*A9+A3*A
+
+      8)*B1)*B7+A5*A6*B4**2+(A2*A6+A3*A5)*B1*B4+A2*A3*B1**2)

```

C

C Static Polarizability of molecule 2 in

C molecule-fixed axes of molecule 1:

C

```

W11 = V33*(A7**2*B9**2+(2*A4*A7*B6+2*A1*A7*B3)*B9+A4**2*B6**2+2*A
+
+      1*A4*B3*B6+A1**2*B3**2)+V22*(A7**2*B8**2+(2*A4*A7*B5+2*A1*A7*B2
+
+      )*B8+A4**2*B5**2+2*A1*A4*B2*B5+A1**2*B2**2)+V11*(A7**2*B7**2+(2
+
+      *A4*A7*B4+2*A1*A7*B1)*B7+A4**2*B4**2+2*A1*A4*B1*B4+A1**2*B1**2)

```

```

W22 = V33*(A8**2*B9**2+(2*A5*A8*B6+2*A2*A8*B3)*B9+A5**2*B6**2+2*A
+
+      2*A5*B3*B6+A2**2*B3**2)+V22*(A8**2*B8**2+(2*A5*A8*B5+2*A2*A8*B2
+
+      )*B8+A5**2*B5**2+2*A2*A5*B2*B5+A2**2*B2**2)+V11*(A8**2*B7**2+(2
+
+      *A5*A8*B4+2*A2*A8*B1)*B7+A5**2*B4**2+2*A2*A5*B1*B4+A2**2*B1**2)

```

```

W33 = V33*(A9**2*B9**2+(2*A6*A9*B6+2*A3*A9*B3)*B9+A6**2*B6**2+2*A
+
+      3*A6*B3*B6+A3**2*B3**2)+V22*(A9**2*B8**2+(2*A6*A9*B5+2*A3*A9*B2
+
+      )*B8+A6**2*B5**2+2*A3*A6*B2*B5+A3**2*B2**2)+V11*(A9**2*B7**2+(2
+
+      *A6*A9*B4+2*A3*A9*B1)*B7+A6**2*B4**2+2*A3*A6*B1*B4+A3**2*B1**2)

```

```

W12 = V33*(A7*A8*B9**2+((A4*A8+A5*A7)*B6+(A1*A8+A2*A7)*B3)*B9+A4*
+
+      A5*B6**2+(A1*A5+A2*A4)*B3*B6+A1*A2*B3**2)+V22*(A7*A8*B8**2+((A4
+
+      *A8+A5*A7)*B5+(A1*A8+A2*A7)*B2)*B8+A4*A5*B5**2+(A1*A5+A2*A4)*B2
+
+      )*B5+A1*A2*B2**2)+V11*(A7*A8*B7**2+((A4*A8+A5*A7)*B4+(A1*A8+A2*A
+
+      7)*B1)*B7+A4*A5*B4**2+(A1*A5+A2*A4)*B1*B4+A1*A2*B1**2)

```

$$\begin{aligned}
W_{13} = & V_{33} * (A_7 * A_9 * B_9 ** 2 + ((A_4 * A_9 + A_6 * A_7) * B_6 + (A_1 * A_9 + A_3 * A_7) * B_3) * B_9 + A_4 * \\
& + A_6 * B_6 ** 2 + (A_1 * A_6 + A_3 * A_4) * B_3 * B_6 + A_1 * A_3 * B_3 ** 2) + V_{22} * (A_7 * A_9 * B_8 ** 2 + ((A_4 \\
& + A_9 + A_6 * A_7) * B_5 + (A_1 * A_9 + A_3 * A_7) * B_2) * B_8 + A_4 * A_6 * B_5 ** 2 + (A_1 * A_6 + A_3 * A_4) * B_2 \\
& + * B_5 + A_1 * A_3 * B_2 ** 2) + V_{11} * (A_7 * A_9 * B_7 ** 2 + ((A_4 * A_9 + A_6 * A_7) * B_4 + (A_1 * A_9 + A_3 * A \\
& + 7) * B_1) * B_7 + A_4 * A_6 * B_4 ** 2 + (A_1 * A_6 + A_3 * A_4) * B_1 * B_4 + A_1 * A_3 * B_1 ** 2)
\end{aligned}$$

$$\begin{aligned}
W_{23} = & V_{33} * (A_8 * A_9 * B_9 ** 2 + ((A_5 * A_9 + A_6 * A_8) * B_6 + (A_2 * A_9 + A_3 * A_8) * B_3) * B_9 + A_5 * \\
& + A_6 * B_6 ** 2 + (A_2 * A_6 + A_3 * A_5) * B_3 * B_6 + A_2 * A_3 * B_3 ** 2) + V_{22} * (A_8 * A_9 * B_8 ** 2 + ((A_5 \\
& + A_9 + A_6 * A_8) * B_5 + (A_2 * A_9 + A_3 * A_8) * B_2) * B_8 + A_5 * A_6 * B_5 ** 2 + (A_2 * A_6 + A_3 * A_5) * B_2 \\
& + * B_5 + A_2 * A_3 * B_2 ** 2) + V_{11} * (A_8 * A_9 * B_7 ** 2 + ((A_5 * A_9 + A_6 * A_8) * B_4 + (A_2 * A_9 + A_3 * A \\
& + 8) * B_1) * B_7 + A_5 * A_6 * B_4 ** 2 + (A_2 * A_6 + A_3 * A_5) * B_1 * B_4 + A_2 * A_3 * B_1 ** 2)
\end{aligned}$$

C

C Quadrupole Moment of molecule 2 in  
 C molecule-fixed axes of molecule 1:  
 C

$$\begin{aligned}
Q_{11} = & A_7 ** 2 * B_8 ** 2 * Q_2 + 2 * A_4 * A_7 * B_5 * B_8 * Q_2 + 2 * A_1 * A_7 * B_2 * B_8 * Q_2 + A_4 ** 2 * B_5 \\
1 & ** 2 * Q_2 + 2 * A_1 * A_4 * B_2 * B_5 * Q_2 + A_1 ** 2 * B_2 ** 2 * Q_2 + A_7 ** 2 * B_9 ** 2 * (-Q_2 - Q_1) + 2 \\
2 & * A_4 * A_7 * B_6 * B_9 * (-Q_2 - Q_1) + 2 * A_1 * A_7 * B_3 * B_9 * (-Q_2 - Q_1) + A_4 ** 2 * B_6 ** 2 * (-Q_2 \\
3 & - Q_1) + 2 * A_1 * A_4 * B_3 * B_6 * (-Q_2 - Q_1) + A_1 ** 2 * B_3 ** 2 * (-Q_2 - Q_1) + A_7 ** 2 * B_7 ** 2 * \\
4 & Q_1 + 2 * A_4 * A_7 * B_4 * B_7 * Q_1 + 2 * A_1 * A_7 * B_1 * B_7 * Q_1 + A_4 ** 2 * B_4 ** 2 * Q_1 + 2 * A_1 * A_4 * B \\
5 & 1 * B_4 * Q_1 + A_1 ** 2 * B_1 ** 2 * Q_1
\end{aligned}$$

$$\begin{aligned}
Q_{22} = & A_8 ** 2 * B_8 ** 2 * Q_2 + 2 * A_5 * A_8 * B_5 * B_8 * Q_2 + 2 * A_2 * A_8 * B_2 * B_8 * Q_2 + A_5 ** 2 * B_5 \\
1 & ** 2 * Q_2 + 2 * A_2 * A_5 * B_2 * B_5 * Q_2 + A_2 ** 2 * B_2 ** 2 * Q_2 + A_8 ** 2 * B_9 ** 2 * (-Q_2 - Q_1) + 2 \\
2 & * A_5 * A_8 * B_6 * B_9 * (-Q_2 - Q_1) + 2 * A_2 * A_8 * B_3 * B_9 * (-Q_2 - Q_1) + A_5 ** 2 * B_6 ** 2 * (-Q_2
\end{aligned}$$

```

3   -Q1)+2*A2*A5*B3*B6*(-Q2-Q1)+A2**2*B3**2*(-Q2-Q1)+A8**2*B7**2*
4   Q1+2*A5*A8*B4*B7*Q1+2*A2*A8*B1*B7*Q1+A5**2*B4**2*Q1+2*A2*A5*B
5   1*B4*Q1+A2**2*B1**2*Q1

```

```

Q33 = A9**2*B8**2*Q2+2*A6*A9*B5*B8*Q2+2*A3*A9*B2*B8*Q2+A6**2*B5
1   **2*Q2+2*A3*A6*B2*B5*Q2+A3**2*B2**2*Q2+A9**2*B9**2*(-Q2-Q1)+2
2   *A6*A9*B6*B9*(-Q2-Q1)+2*A3*A9*B3*B9*(-Q2-Q1)+A6**2*B6**2*(-Q2
3   -Q1)+2*A3*A6*B3*B6*(-Q2-Q1)+A3**2*B3**2*(-Q2-Q1)+A9**2*B7**2*
4   Q1+2*A6*A9*B4*B7*Q1+2*A3*A9*B1*B7*Q1+A6**2*B4**2*Q1+2*A3*A6*B
5   1*B4*Q1+A3**2*B1**2*Q1

```

```

Q12 = A7*A8*B8**2*Q2+A4*A8*B5*B8*Q2+A5*A7*B5*B8*Q2+A1*A8*B2*B8*
1   Q2+A2*A7*B2*B8*Q2+A4*A5*B5**2*Q2+A1*A5*B2*B5*Q2+A2*A4*B2*B5*Q
2   2+A1*A2*B2**2*Q2+A7*A8*B9**2*(-Q2-Q1)+A4*A8*B6*B9*(-Q2-Q1)+A5
3   *A7*B6*B9*(-Q2-Q1)+A1*A8*B3*B9*(-Q2-Q1)+A2*A7*B3*B9*(-Q2-Q1)+
4   A4*A5*B6**2*(-Q2-Q1)+A1*A5*B3*B6*(-Q2-Q1)+A2*A4*B3*B6*(-Q2-Q1
5   )+A1*A2*B3**2*(-Q2-Q1)+A7*A8*B7**2*Q1+A4*A8*B4*B7*Q1+A5*A7*B4
6   *B7*Q1+A1*A8*B1*B7*Q1+A2*A7*B1*B7*Q1+A4*A5*B4**2*Q1+A1*A5*B1*
7   B4*Q1+A2*A4*B1*B4*Q1+A1*A2*B1**2*Q1

```

```

Q13 = A7*A9*B8**2*Q2+A4*A9*B5*B8*Q2+A6*A7*B5*B8*Q2+A1*A9*B2*B8*
1   Q2+A3*A7*B2*B8*Q2+A4*A6*B5**2*Q2+A1*A6*B2*B5*Q2+A3*A4*B2*B5*Q
2   2+A1*A3*B2**2*Q2+A7*A9*B9**2*(-Q2-Q1)+A4*A9*B6*B9*(-Q2-Q1)+A6
3   *A7*B6*B9*(-Q2-Q1)+A1*A9*B3*B9*(-Q2-Q1)+A3*A7*B3*B9*(-Q2-Q1)+
4   A4*A6*B6**2*(-Q2-Q1)+A1*A6*B3*B6*(-Q2-Q1)+A3*A4*B3*B6*(-Q2-Q1
5   )+A1*A3*B3**2*(-Q2-Q1)+A7*A9*B7**2*Q1+A4*A9*B4*B7*Q1+A6*A7*B4
6   *B7*Q1+A1*A9*B1*B7*Q1+A3*A7*B1*B7*Q1+A4*A6*B4**2*Q1+A1*A6*B1*
7   B4*Q1+A3*A4*B1*B4*Q1+A1*A3*B1**2*Q1

```

```

Q23 = A8*A9*B8**2*Q2+A5*A9*B5*B8*Q2+A6*A8*B5*B8*Q2+A2*A9*B2*B8*
1   Q2+A3*A8*B2*B8*Q2+A5*A6*B5**2*Q2+A2*A6*B2*B5*Q2+A3*A5*B2*B5*Q

```

2       $2 + A2 * A3 * B2 ** 2 * Q2 + A8 * A9 * B9 ** 2 * (-Q2 - Q1) + A5 * A9 * B6 * B9 * (-Q2 - Q1) + A6$   
 3       $* A8 * B6 * B9 * (-Q2 - Q1) + A2 * A9 * B3 * B9 * (-Q2 - Q1) + A3 * A8 * B3 * B9 * (-Q2 - Q1) +$   
 4       $A5 * A6 * B6 ** 2 * (-Q2 - Q1) + A2 * A6 * B3 * B6 * (-Q2 - Q1) + A3 * A5 * B3 * B6 * (-Q2 - Q1)$   
 5       $) + A2 * A3 * B3 ** 2 * (-Q2 - Q1) + A8 * A9 * B7 ** 2 * Q1 + A5 * A9 * B4 * B7 * Q1 + A6 * A8 * B4$   
 6       $* B7 * Q1 + A2 * A9 * B1 * B7 * Q1 + A3 * A8 * B1 * B7 * Q1 + A5 * A6 * B4 ** 2 * Q1 + A2 * A6 * B1 *$   
 7       $B4 * Q1 + A3 * A5 * B1 * B4 * Q1 + A2 * A3 * B1 ** 2 * Q1$

D97 =  $(A33 * Q33 ** 2 * T333 ** 2 * V33 ** 2 + 4 * A33 * Q23 * Q33 * T233 * T333 * V33 ** 2 + 2$   
 1       $* A33 * Q22 * Q33 * T223 * T333 * V33 ** 2 + 4 * A33 * Q13 * Q33 * T133 * T333 * V33 ** 2 +$   
 2       $4 * A33 * Q12 * Q33 * T123 * T333 * V33 ** 2 + 2 * A33 * Q11 * Q33 * T113 * T333 * V33 ** 2$   
 3       $+ 4 * A33 * Q23 ** 2 * T233 ** 2 * V33 ** 2 + 4 * A33 * Q22 * Q23 * T223 * T233 * V33 ** 2 + 8$   
 4       $* A33 * Q13 * Q23 * T133 * T233 * V33 ** 2 + 8 * A33 * Q12 * Q23 * T123 * T233 * V33 ** 2 +$   
 5       $4 * A33 * Q11 * Q23 * T113 * T233 * V33 ** 2 + A33 * Q22 ** 2 * T223 ** 2 * V33 ** 2 + 4 * A3$   
 6       $3 * Q13 * Q22 * T133 * T223 * V33 ** 2 + 4 * A33 * Q12 * Q22 * T123 * T223 * V33 ** 2 + 2 * A$   
 7       $33 * Q11 * Q22 * T113 * T223 * V33 ** 2 + 4 * A33 * Q13 ** 2 * T133 ** 2 * V33 ** 2 + 8 * A33$   
 8       $* Q12 * Q13 * T123 * T133 * V33 ** 2 + 4 * A33 * Q11 * Q13 * T113 * T133 * V33 ** 2 + 4 * A3$   
 9       $3 * Q12 ** 2 * T123 ** 2 * V33 ** 2 + 4 * A33 * Q11 * Q12 * T113 * T123 * V33 ** 2 + A33 * Q1$   
 :       $1 ** 2 * T113 ** 2 * V33 ** 2 + A22 * Q33 ** 2 * T233 ** 2 * V22 ** 2 + 4 * A22 * Q23 * Q33 * T$   
 ;       $223 * T233 * V22 ** 2 + 2 * A22 * Q22 * Q33 * T222 * T233 * V22 ** 2 + 4 * A22 * Q13 * Q33 *$   
 <       $T123 * T233 * V22 ** 2 + 4 * A22 * Q12 * Q33 * T122 * T233 * V22 ** 2 + 2 * A22 * Q11 * Q33$   
=       $* T112 * T233 * V22 ** 2 + 4 * A22 * Q23 ** 2 * T223 ** 2 * V22 ** 2 + 4 * A22 * Q22 * Q23 * T$   
>       $222 * T223 * V22 ** 2 + 8 * A22 * Q13 * Q23 * T123 * T223 * V22 ** 2 + 8 * A22 * Q12 * Q23 *$   
?       $T122 * T223 * V22 ** 2 + 4 * A22 * Q11 * Q23 * T112 * T223 * V22 ** 2 + A22 * Q22 ** 2 * T2$   
@       $22 ** 2 * V22 ** 2 + 4 * A22 * Q13 * Q22 * T123 * T222 * V22 ** 2 + 4 * A22 * Q12 * Q22 * T12$   
1       $2 * T222 * V22 ** 2 + 2 * A22 * Q11 * Q22 * T112 * T222 * V22 ** 2 + 4 * A22 * Q13 ** 2 * T12$   
2       $3 ** 2 * V22 ** 2 + 8 * A22 * Q12 * Q13 * T122 * T123 * V22 ** 2 + 4 * A22 * Q11 * Q13 * T112$   
3       $* T123 * V22 ** 2 + 4 * A22 * Q12 ** 2 * T122 ** 2 * V22 ** 2 + 4 * A22 * Q11 * Q12 * T112 * T$   
4       $122 * V22 ** 2 + A22 * Q11 ** 2 * T112 ** 2 * V22 ** 2 + A11 * Q33 ** 2 * T133 ** 2 * V11 **$   
5       $2 + 4 * A11 * Q23 * Q33 * T123 * T133 * V11 ** 2 + 2 * A11 * Q22 * Q33 * T122 * T133 * V11 *$

```

6   *2+4*A11*Q13*Q33*T113*T133*V11**2+4*A11*Q12*Q33*T112*T133*V11
7   **2+2*A11*Q11*Q33*T111*T133*V11**2+4*A11*Q23**2*T123**2*V11**
8   2+4*A11*Q22*Q23*T122*T123*V11**2+8*A11*Q13*Q23*T113*T123*V11*
9   *2+8*A11*Q12*Q23*T112*T123*V11**2+4*A11*Q11*Q23*T111*T123*V11
:   **2+A11*Q22**2*T122**2*V11**2+4*A11*Q13*Q22*T113*T122*V11**2+
;   4*A11*Q12*Q22*T112*T122*V11**2+2*A11*Q11*Q22*T111*T122*V11**2
<   +4*A11*Q13**2*T113**2*V11**2+8*A11*Q12*Q13*T112*T113*V11**2+4
=   *A11*Q11*Q13*T111*T113*V11**2+4*A11*Q12**2*T112**2*V11**2+4*A
>   11*Q11*Q12*T111*T112*V11**2+A11*Q11**2*T111**2*V11**2)

```

```

D101 = (Q33**2*T333**2*V33**2+4*Q23*Q33*T233*T333*V33**2+2*Q22*Q3
1   3*T223*T333*V33**2+4*Q13*Q33*T133*T333*V33**2+4*Q12*Q33*T123*
2   T333*V33**2+2*Q11*Q33*T113*T333*V33**2+4*Q23**2*T233**2*V33**2
3   2+4*Q22*Q23*T223*T233*V33**2+8*Q13*Q23*T133*T233*V33**2+8*Q12
4   *Q23*T123*T233*V33**2+4*Q11*Q23*T113*T233*V33**2+Q22**2*T223*V
5   2*V33**2+4*Q13*Q22*T133*T223*V33**2+4*Q12*Q22*T123*T223*V33*V
6   *2+2*Q11*Q22*T113*T223*V33**2+4*Q13**2*T133**2*V33**2+8*Q12*Q
7   13*T123*T133*V33**2+4*Q11*Q13*T113*T133*V33**2+4*Q12**2*T123*V
8   *2*V33**2+4*Q11*Q12*T113*T123*V33**2+Q11**2*T113**2*V33**2+Q3
9   3**2*T233**2*V22**2+4*Q23*Q33*T223*T233*V22**2+2*Q22*Q33*T222
:   *T233*V22**2+4*Q13*Q33*T123*T233*V22**2+4*Q12*Q33*T122*T233*V
;   22**2+2*Q11*Q33*T112*T233*V22**2+4*Q23**2*T223**2*V22**2+4*Q2
<   2*Q23*T222*T223*V22**2+8*Q13*Q23*T123*T223*V22**2+8*Q12*Q23*T
=   122*T223*V22**2+4*Q11*Q23*T112*T223*V22**2+Q22**2*T222**2*V22
>   **2+4*Q13*Q22*T123*T222*V22**2+4*Q12*Q22*T122*T222*V22**2+2*Q
?   11*Q22*T112*T222*V22**2+4*Q13**2*T123**2*V22**2+8*Q12*Q13*T12
@   2*T123*V22**2+4*Q11*Q13*T112*T123*V22**2+4*Q12**2*T122**2*V22
1   **2+4*Q11*Q12*T112*T122*V22**2+Q11**2*T112**2*V22**2+Q33**2*T
2   133**2*V11**2+4*Q23*Q33*T123*T133*V11**2+2*Q22*Q33*T122*T133*

```

3     V11\*\*2+4\*Q13\*Q33\*T113\*T133\*V11\*\*2+4\*Q12\*Q33\*T112\*T133\*V11\*\*2+
 4     2\*Q11\*Q33\*T111\*T133\*V11\*\*2+4\*Q23\*\*2\*T123\*\*2\*V11\*\*2+4\*Q22\*Q23\*
 5     T122\*T123\*V11\*\*2+8\*Q13\*Q23\*T113\*T123\*V11\*\*2+8\*Q12\*Q23\*T112\*T1
 6     23\*V11\*\*2+4\*Q11\*Q23\*T111\*T123\*V11\*\*2+Q22\*\*2\*T122\*\*2\*V11\*\*2+4\*
 7     Q13\*Q22\*T113\*T122\*V11\*\*2+4\*Q12\*Q22\*T112\*T122\*V11\*\*2+2\*Q11\*Q22
 8     \*T111\*T122\*V11\*\*2+4\*Q13\*\*2\*T113\*\*2\*V11\*\*2+8\*Q12\*Q13\*T112\*T113
 9     \*V11\*\*2+4\*Q11\*Q13\*T111\*T113\*V11\*\*2+4\*Q12\*\*2\*T112\*\*2\*V11\*\*2+4\*
 :     Q11\*Q12\*T111\*T112\*V11\*\*2+Q11\*\*2\*T111\*\*2\*V11\*\*2)

D105 = (A33\*(-Q2-Q1)\*\*2\*T333\*\*2\*W33\*\*2+2\*A33\*(-Q2-Q1)\*Q2\*T223\*T33
 1     3\*W33\*\*2+2\*A33\*Q1\*(-Q2-Q1)\*T113\*T333\*W33\*\*2+A33\*Q2\*\*2\*T223\*\*2
 2     \*W33\*\*2+2\*A33\*Q1\*Q2\*T113\*T223\*W33\*\*2+A33\*Q1\*\*2\*T113\*\*2\*W33\*\*2
 3     +2\*A33\*(-Q2-Q1)\*\*2\*T233\*T333\*W23\*W33+2\*A33\*(-Q2-Q1)\*Q2\*T222\*T
 4     333\*W23\*W33+2\*A33\*Q1\*(-Q2-Q1)\*T112\*T333\*W23\*W33+2\*A33\*(-Q2-Q1
 5     )\*Q2\*T223\*T233\*W23\*W33+2\*A33\*Q1\*(-Q2-Q1)\*T113\*T233\*W23\*W33+2\*
 6     A33\*Q2\*\*2\*T222\*T223\*W23\*W33+2\*A33\*Q1\*Q2\*T112\*T223\*W23\*W33+2\*A
 7     33\*Q1\*Q2\*T113\*T222\*W23\*W33+2\*A33\*Q1\*\*2\*T112\*T113\*W23\*W33+2\*A3
 8     3\*(-Q2-Q1)\*\*2\*T133\*T333\*W13\*W33+2\*A33\*(-Q2-Q1)\*Q2\*T122\*T333\*W
 9     13\*W33+2\*A33\*Q1\*(-Q2-Q1)\*T111\*T333\*W13\*W33+2\*A33\*(-Q2-Q1)\*Q2\*
 :     T133\*T223\*W13\*W33+2\*A33\*Q2\*\*2\*T122\*T223\*W13\*W33+2\*A33\*Q1\*Q2\*T
 ;     111\*T223\*W13\*W33+2\*A33\*Q1\*(-Q2-Q1)\*T113\*T133\*W13\*W33+2\*A33\*Q1
 <     \*Q2\*T113\*T122\*W13\*W33+2\*A33\*Q1\*\*2\*T111\*T113\*W13\*W33+A22\*(-Q2-
 =     Q1)\*\*2\*T333\*\*2\*W23\*\*2+2\*A22\*(-Q2-Q1)\*Q2\*T223\*T333\*W23\*\*2+2\*A2
 >     2\*Q1\*(-Q2-Q1)\*T113\*T333\*W23\*\*2+A33\*(-Q2-Q1)\*\*2\*T233\*\*2\*W23\*\*2
 ?     +2\*A33\*(-Q2-Q1)\*Q2\*T222\*T233\*W23\*\*2+2\*A33\*Q1\*(-Q2-Q1)\*T112\*T2
 @     33\*W23\*\*2+A22\*Q2\*\*2\*T223\*\*2\*W23\*\*2+2\*A22\*Q1\*Q2\*T113\*T223\*W23\*
 1     \*2+A33\*Q2\*\*2\*T222\*\*2\*W23\*\*2+2\*A33\*Q1\*Q2\*T112\*T222\*W23\*\*2+A22\*
 2     Q1\*\*2\*T113\*\*2\*W23\*\*2+A33\*Q1\*\*2\*T112\*\*2\*W23\*\*2+2\*A22\*(-Q2-Q1)\*
 3     \*2\*T233\*T333\*W22\*W23+2\*A22\*(-Q2-Q1)\*Q2\*T222\*T333\*W22\*W23+2\*A2
 4     2\*Q1\*(-Q2-Q1)\*T112\*T333\*W22\*W23+2\*A22\*(-Q2-Q1)\*Q2\*T223\*T233\*W

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5   22*W23+2*A22*Q1*(-Q2-Q1)*T113*T233*W22*W23+2*A22*Q2**2*T222*T
6   223*W22*W23+2*A22*Q1*Q2*T112*T223*W22*W23+2*A22*Q1*Q2*T113*T2
7   22*W22*W23+2*A22*Q1**2*T112*T113*W22*W23+2*A33*(-Q2-Q1)**2*T1
8   33*T233*W13*W23+2*A33*(-Q2-Q1)*Q2*T122*T233*W13*W23+2*A33*Q1*
9   (-Q2-Q1)*T111*T233*W13*W23+2*A33*(-Q2-Q1)*Q2*T133*T222*W13*W2
:   3+2*A33*Q2**2*T122*T222*W13*W23+2*A33*Q1*Q2*T111*T222*W13*W23
;   +2*A33*Q1*(-Q2-Q1)*T112*T133*W13*W23+2*A33*Q1*Q2*T112*T122*W1
<   3*W23+2*A33*Q1**2*T111*T112*W13*W23+2*A22*(-Q2-Q1)**2*T133*T3
=   33*W12*W23+2*A22*(-Q2-Q1)*Q2*T122*T333*W12*W23+2*A22*Q1*(-Q2-
>   Q1)*T111*T333*W12*W23+2*A22*(-Q2-Q1)*Q2*T133*T223*W12*W23+2*A
?   22*Q2**2*T122*T223*W12*W23+2*A22*Q1*Q2*T111*T223*W12*W23+2*A2
@   2*Q1*(-Q2-Q1)*T113*T133*W12*W23+2*A22*Q1*Q2*T113*T122*W12*W23
1   +2*A22*Q1**2*T111*T113*W12*W23+A22*(-Q2-Q1)**2*T233**2*W22**2
2   +2*A22*(-Q2-Q1)*Q2*T222*T233*W22**2+2*A22*Q1*(-Q2-Q1)*T112*T2
3   33*W22**2+A22*Q2**2*T222**2*W22**2+2*A22*Q1*Q2*T112*T222*W22*
4   *2+A22*Q1**2*T112**2*W22**2+2*A22*(-Q2-Q1)**2*T133*T233*W12*W
5   22+2*A22*(-Q2-Q1)*Q2*T122*T233*W12*W22+2*A22*Q1*(-Q2-Q1)*T111
6   *T233*W12*W22+2*A22*(-Q2-Q1)*Q2*T133*T222*W12*W22+2*A22*Q2**2
7   *T122*T222*W12*W22+2*A22*Q1*Q2*T111*T222*W12*W22+2*A22*Q1*(-Q
8   2-Q1)*T112*T133*W12*W22+2*A22*Q1*Q2*T112*T122*W12*W22+2*A22*Q
9   1**2*T111*T112*W12*W22+A11*(-Q2-Q1)**2*T333**2*W13**2+2*A11*(
:   -Q2-Q1)*Q2*T223*T333*W13**2+2*A11*Q1*(-Q2-Q1)*T113*T333*W13**2
;   2+A11*Q2**2*T223**2*W13**2+2*A11*Q1*Q2*T113*T223*W13**2+A33*(-
<   -Q2-Q1)**2*T133**2*W13**2+2*A33*(-Q2-Q1)*Q2*T122*T133*W13**2+
=   2*A33*Q1*(-Q2-Q1)*T111*T133*W13**2+A33*Q2**2*T122**2*W13**2+2
>   *A33*Q1*Q2*T111*T122*W13**2+A11*Q1**2*T113**2*W13**2+A33*Q1**2
?   2*T111**2*W13**2+2*A11*(-Q2-Q1)**2*T233*T333*W12*W13+2*A11*(-
@   Q2-Q1)*Q2*T222*T333*W12*W13+2*A11*Q1*(-Q2-Q1)*T112*T333*W12*W
1   13+2*A11*(-Q2-Q1)*Q2*T223*T233*W12*W13+2*A11*Q1*(-Q2-Q1)*T113
2   *T233*W12*W13+2*A11*Q2**2*T222*T223*W12*W13+2*A11*Q1*Q2*T112*
3   T223*W12*W13+2*A11*Q1*Q2*T113*T222*W12*W13+2*A11*Q1**2*T112*T

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4   113*W12*W13+2*A11*(-Q2-Q1)**2*T133*T333*W11*W13+2*A11*(-Q2-Q1
5   )*Q2*T122*T333*W11*W13+2*A11*Q1*(-Q2-Q1)*T111*T333*W11*W13+2*
6   A11*(-Q2-Q1)*Q2*T133*T223*W11*W13+2*A11*Q2**2*T122*T223*W11*W
7   13+2*A11*Q1*Q2*T111*T223*W11*W13+2*A11*Q1*(-Q2-Q1)*T113*T133*
8   W11*W13+2*A11*Q1*Q2*T113*T122*W11*W13+2*A11*Q1**2*T111*T113*W
9   11*W13+A11*(-Q2-Q1)**2*T233**2*W12**2+2*A11*(-Q2-Q1)*Q2*T222*
:   T233*W12**2+2*A11*Q1*Q2*T112*T233*W12**2+A11*Q2**2*T222
;   **2*W12**2+2*A11*Q1*Q2*T112*T222*W12**2+A22*(-Q2-Q1)**2*T133*
<   *2*W12**2+2*A22*(-Q2-Q1)*Q2*T122*T133*W12**2+2*A22*Q1*(-Q2-Q1
=   )*T111*T133*W12**2+A22*Q2**2*T122**2*W12**2+2*A22*Q1*Q2*T111*
>   T122*W12**2+A11*Q1**2*T112**2*W12**2+A22*Q1**2*T111**2*W12**2
?   +2*A11*(-Q2-Q1)**2*T133*T233*W11*W12+2*A11*(-Q2-Q1)*Q2*T122*T
@   233*W11*W12+2*A11*Q1*(-Q2-Q1)*T111*T233*W11*W12+2*A11*(-Q2-Q1
1   )*Q2*T133*T222*W11*W12+2*A11*Q2**2*T122*T222*W11*W12+2*A11*Q1
2   *Q2*T111*T222*W11*W12+2*A11*Q1*(-Q2-Q1)*T112*T133*W11*W12+2*A
3   11*Q1*Q2*T112*T122*W11*W12+2*A11*Q1**2*T111*T112*W11*W12+A11*
4   (-Q2-Q1)**2*T133**2*W11**2+2*A11*(-Q2-Q1)*Q2*T122*T133*W11**2
5   +2*A11*Q1*(-Q2-Q1)*T111*T133*W11**2+A11*Q2**2*T122**2*W11**2+
6   2*A11*Q1*Q2*T111*T122*W11**2+A11*Q1**2*T111**2*W11**2)

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D110 =((-Q2-Q1)**2*T333**2*W33**2+2*(-Q2-Q1)*Q2*T223*T333*W33**2
1   +2*Q1*(-Q2-Q1)*T113*T333*W33**2+Q2**2*T223**2*W33**2+2*Q1*Q2*
2   T113*T223*W33**2+Q1**2*T113**2*W33**2+2*(-Q2-Q1)**2*T233*T333
3   *W23*W33+2*(-Q2-Q1)*Q2*T222*T333*W23*W33+2*Q1*(-Q2-Q1)*T112*T
4   333*W23*W33+2*(-Q2-Q1)*Q2*T223*T233*W23*W33+2*Q1*(-Q2-Q1)*T11
5   3*T233*W23*W33+2*Q2**2*T222*T223*W23*W33+2*Q1*Q2*T112*T223*W2
6   3*W33+2*Q1*Q2*T113*T222*W23*W33+2*Q1**2*T112*T113*W23*W33+2*(-
7   -Q2-Q1)**2*T133*T333*W13*W33+2*(-Q2-Q1)*Q2*T122*T333*W13*W33+
8   2*Q1*(-Q2-Q1)*T111*T333*W13*W33+2*(-Q2-Q1)*Q2*T133*T223*W13*W
9   33+2*Q2**2*T122*T223*W13*W33+2*Q1*Q2*T111*T223*W13*W33+2*Q1*(-

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:   -Q2-Q1)*T113*T133*W13*W33+2*Q1*Q2*T113*T122*W13*W33+2*Q1**2*T
;   111*T113*W13*W33+(-Q2-Q1)**2*T333**2*W23**2+2*(-Q2-Q1)*Q2*T22
<   3*T333*W23**2+2*Q1*(-Q2-Q1)*T113*T333*W23**2+(-Q2-Q1)**2*T233
=   **2*W23**2+2*(-Q2-Q1)*Q2*T222*T233*W23**2+2*Q1*(-Q2-Q1)*T112*
>   T233*W23**2+Q2**2*T223**2*W23**2+2*Q1*Q2*T113*T223*W23**2+Q2*
?   *2*T222**2*W23**2+2*Q1*Q2*T112*T222*W23**2+Q1**2*T113**2*W23*
@   *2+Q1**2*T112**2*W23**2+2*(-Q2-Q1)**2*T233*T333*W22*W23+2*(-Q
1   2-Q1)*Q2*T222*T333*W22*W23+2*Q1*(-Q2-Q1)*T112*T333*W22*W23+2*
2   (-Q2-Q1)*Q2*T223*T233*W22*W23+2*Q1*(-Q2-Q1)*T113*T233*W22*W23
3   +2*Q2**2*T222*T223*W22*W23+2*Q1*Q2*T112*T223*W22*W23+2*Q1*Q2*
4   T113*T222*W22*W23+2*Q1**2*T112*T113*W22*W23+2*(-Q2-Q1)**2*T13
5   3*T233*W13*W23+2*(-Q2-Q1)*Q2*T122*T233*W13*W23+2*Q1*(-Q2-Q1)*
6   T111*T233*W13*W23+2*(-Q2-Q1)*Q2*T133*T222*W13*W23+2*Q2**2*T12
7   2*T222*W13*W23+2*Q1*Q2*T111*T222*W13*W23+2*Q1*(-Q2-Q1)*T112*T
8   133*W13*W23+2*Q1*Q2*T112*T122*W13*W23+2*Q1**2*T111*T112*W13*W
9   23+2*(-Q2-Q1)**2*T133*T333*W12*W23+2*(-Q2-Q1)*Q2*T122*T333*W1
:   2*W23+2*Q1*(-Q2-Q1)*T111*T333*W12*W23+2*(-Q2-Q1)*Q2*T133*T223
;   *W12*W23+2*Q2**2*T122*T223*W12*W23+2*Q1*Q2*T111*T223*W12*W23+
<   2*Q1*(-Q2-Q1)*T113*T133*W12*W23+2*Q1*Q2*T113*T122*W12*W23+2*Q
=   1**2*T111*T113*W12*W23+(-Q2-Q1)**2*T233**2*W22**2+2*(-Q2-Q1)*
>   Q2*T222*T233*W22**2+2*Q1*(-Q2-Q1)*T112*T233*W22**2+Q2**2*T222
?   **2*W22**2+2*Q1*Q2*T112*T222*W22**2+Q1**2*T112**2*W22**2+2*(-
@   Q2-Q1)**2*T133*T233*W12*W22+2*(-Q2-Q1)*Q2*T122*T233*W12*W22+2
1   *Q1*(-Q2-Q1)*T111*T233*W12*W22+2*(-Q2-Q1)*Q2*T133*T222*W12*W2
2   2+2*Q2**2*T122*T222*W12*W22+2*Q1*Q2*T111*T222*W12*W22+2*Q1*(-
3   Q2-Q1)*T112*T133*W12*W22+2*Q1*Q2*T112*T122*W12*W22+2*Q1**2*T1
4   11*T112*W12*W22+(-Q2-Q1)**2*T333**2*W13**2+2*(-Q2-Q1)*Q2*T223
5   *T333*W13**2+2*Q1*(-Q2-Q1)*T113*T333*W13**2+Q2**2*T223**2*W13
6   **2+2*Q1*Q2*T113*T223*W13**2+(-Q2-Q1)**2*T133**2*W13**2+2*(-Q
7   2-Q1)*Q2*T122*T133*W13**2+2*Q1*(-Q2-Q1)*T111*T133*W13**2+Q2**2
8   *2*T122**2*W13**2+2*Q1*Q2*T111*T122*W13**2+Q1**2*T113**2*W13**2

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9   2+Q1**2*T111**2*W13**2+2*(-Q2-Q1)**2*T233*T333*W12*W13+2*(-Q2
: -Q1)*Q2*T222*T333*W12*W13+2*Q1*(-Q2-Q1)*T112*T333*W12*W13+2*(-
; -Q2-Q1)*Q2*T223*T233*W12*W13+2*Q1*(-Q2-Q1)*T113*T233*W12*W13+
< 2*Q2**2*T222*T223*W12*W13+2*Q1*Q2*T112*T223*W12*W13+2*Q1*Q2*T
= 113*T222*W12*W13+2*Q1**2*T112*T113*W12*W13+2*(-Q2-Q1)**2*T133
> *T333*W11*W13+2*(-Q2-Q1)*Q2*T122*T333*W11*W13+2*Q1*(-Q2-Q1)*T
? 111*T333*W11*W13+2*(-Q2-Q1)*Q2*T133*T223*W11*W13+2*Q2**2*T122
@ *T223*W11*W13+2*Q1*Q2*T111*T223*W11*W13+2*Q1*(-Q2-Q1)*T113*T1
1 33*W11*W13+2*Q1*Q2*T113*T122*W11*W13+2*Q1**2*T111*T113*W11*W1
2 3+(-Q2-Q1)**2*T233**2*W12**2+2*(-Q2-Q1)*Q2*T222*T233*W12**2+2
3 *Q1*(-Q2-Q1)*T112*T233*W12**2+Q2**2*T222**2*W12**2+2*Q1*Q2*T1
4 12*T222*W12**2+(-Q2-Q1)**2*T133**2*W12**2+2*(-Q2-Q1)*Q2*T122*
5 T133*W12**2+2*Q1*(-Q2-Q1)*T111*T133*W12**2+Q2**2*T122**2*W12*
6 *2+2*Q1*Q2*T111*T122*W12**2+Q1**2*T112**2*W12**2+Q1**2*T111**2
7 2*W12**2+2*(-Q2-Q1)**2*T133*T233*W11*W12+2*(-Q2-Q1)*Q2*T122*T
8 233*W11*W12+2*Q1*(-Q2-Q1)*T111*T233*W11*W12+2*(-Q2-Q1)*Q2*T13
9 3*T222*W11*W12+2*Q2**2*T122*T222*W11*W12+2*Q1*Q2*T111*T222*W1
: 1*W12+2*Q1*(-Q2-Q1)*T112*T133*W11*W12+2*Q1*Q2*T112*T122*W11*W
; 12+2*Q1**2*T111*T112*W11*W12+(-Q2-Q1)**2*T133**2*W11**2+2*(-Q
< 2-Q1)*Q2*T122*T133*W11**2+2*Q1*(-Q2-Q1)*T111*T133*W11**2+Q2**2
= 2*T122**2*W11**2+2*Q1*Q2*T111*T122*W11**2+Q1**2*T111**2*W11**2
> 2)

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D115 =(A33*(-Q2-Q1)*Q33*T333**2*V33*W33+2*A33*(-Q2-Q1)*Q23*T233*
1   T333*V33*W33+A33*Q2*Q33*T223*T333*V33*W33+A33*(-Q2-Q1)*Q22*T2
2   23*T333*V33*W33+2*A33*Q13*(-Q2-Q1)*T133*T333*V33*W33+2*A33*Q1
3   2*(-Q2-Q1)*T123*T333*V33*W33+A33*Q1*Q33*T113*T333*V33*W33+A33
4   *Q11*(-Q2-Q1)*T113*T333*V33*W33+2*A33*Q2*Q23*T223*T233*V33*W3
5   3+2*A33*Q1*Q23*T113*T233*V33*W33+A33*Q2*Q22*T223**2*V33*W33+2

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6   *A33*Q13*Q2*T133*T223*V33*W33+2*A33*Q12*Q2*T123*T223*V33*W33+
7   A33*Q1*Q22*T113*T223*V33*W33+A33*Q11*Q2*T113*T223*V33*W33+2*A
8   33*Q1*Q13*T113*T133*V33*W33+2*A33*Q1*Q12*T113*T123*V33*W33+A3
9   3*Q1*Q11*T113**2*V33*W33+A33*(-Q2-Q1)*Q33*T233*T333*V33*W23+A
:   33*Q2*Q33*T222*T333*V33*W23+A33*Q1*Q33*T112*T333*V33*W23+2*A3
;   3*(-Q2-Q1)*Q23*T233**2*V33*W23+A33*(-Q2-Q1)*Q22*T223*T233*V33
<   *W23+2*A33*Q2*Q23*T222*T233*V33*W23+2*A33*Q13*(-Q2-Q1)*T133*T
=   233*V33*W23+2*A33*Q12*(-Q2-Q1)*T123*T233*V33*W23+A33*Q11*(-Q2
>   -Q1)*T113*T233*V33*W23+2*A33*Q1*Q23*T112*T233*V33*W23+A33*Q2*
?   Q22*T222*T223*V33*W23+A33*Q1*Q22*T112*T223*V33*W23+2*A33*Q13*
@   Q2*T133*T222*V33*W23+2*A33*Q12*Q2*T123*T222*V33*W23+A33*Q11*Q
1   2*T113*T222*V33*W23+2*A33*Q1*Q13*T112*T133*V33*W23+2*A33*Q1*Q
2   12*T112*T123*V33*W23+A33*Q1*Q11*T112*T113*V33*W23+A22*(-Q2-Q1
3   )*Q33*T233*T333*V22*W23+2*A22*(-Q2-Q1)*Q23*T223*T333*V22*W23+
4   A22*(-Q2-Q1)*Q22*T222*T333*V22*W23+2*A22*Q13*(-Q2-Q1)*T123*T3
5   33*V22*W23+2*A22*Q12*(-Q2-Q1)*T122*T333*V22*W23+A22*Q11*(-Q2-
6   Q1)*T112*T333*V22*W23+A22*Q2*Q33*T223*T233*V22*W23+A22*Q1*Q33
7   *T113*T233*V22*W23+2*A22*Q2*Q23*T223**2*V22*W23+A22*Q2*Q22*T2
8   22*T223*V22*W23+2*A22*Q13*Q2*T123*T223*V22*W23+2*A22*Q12*Q2*T
9   122*T223*V22*W23+2*A22*Q1*Q23*T113*T223*V22*W23+A22*Q11*Q2*T1
:   12*T223*V22*W23+A22*Q1*Q22*T113*T222*V22*W23+2*A22*Q1*Q13*T11
;   3*T123*V22*W23+2*A22*Q1*Q12*T113*T122*V22*W23+A22*Q1*Q11*T112
<   *T113*V22*W23+A22*(-Q2-Q1)*Q33*T233**2*V22*W22+2*A22*(-Q2-Q1)
=   *Q23*T223*T233*V22*W22+A22*Q2*Q33*T222*T233*V22*W22+A22*(-Q2-
>   Q1)*Q22*T222*T233*V22*W22+2*A22*Q13*(-Q2-Q1)*T123*T233*V22*W2
?   2+2*A22*Q12*(-Q2-Q1)*T122*T233*V22*W22+A22*Q1*Q33*T112*T233*V
@   22*W22+A22*Q11*(-Q2-Q1)*T112*T233*V22*W22+2*A22*Q2*Q23*T222*T
1   223*V22*W22+2*A22*Q1*Q23*T112*T223*V22*W22+A22*Q2*Q22*T222**2
2   *V22*W22+2*A22*Q13*Q2*T123*T222*V22*W22+2*A22*Q12*Q2*T122*T22
3   2*V22*W22+A22*Q1*Q22*T112*T222*V22*W22+A22*Q11*Q2*T112*T222*V
4   22*W22+2*A22*Q1*Q13*T112*T123*V22*W22+2*A22*Q1*Q12*T112*T122*

```

5     V22\*W22+A22\*Q1\*Q11\*T112\*\*2\*V22\*W22+A33\*(-Q2-Q1)\*Q33\*T133\*T333  
 6     \*V33\*W13+A33\*Q2\*Q33\*T122\*T333\*V33\*W13+A33\*Q1\*Q33\*T111\*T333\*V3  
 7     3\*W13+2\*A33\*(-Q2-Q1)\*Q23\*T133\*T233\*V33\*W13+2\*A33\*Q2\*Q23\*T122\*  
 8     T233\*V33\*W13+2\*A33\*Q1\*Q23\*T111\*T233\*V33\*W13+A33\*(-Q2-Q1)\*Q22\*  
 9     T133\*T223\*V33\*W13+A33\*Q2\*Q22\*T122\*T223\*V33\*W13+A33\*Q1\*Q22\*T11  
 :     1\*T223\*V33\*W13+2\*A33\*Q13\*(-Q2-Q1)\*T133\*\*2\*V33\*W13+2\*A33\*Q12\*(  
 ;     -Q2-Q1)\*T123\*T133\*V33\*W13+2\*A33\*Q13\*Q2\*T122\*T133\*V33\*W13+A33\*  
 <     Q11\*(-Q2-Q1)\*T113\*T133\*V33\*W13+2\*A33\*Q1\*Q13\*T111\*T133\*V33\*W13  
=     +2\*A33\*Q12\*Q2\*T122\*T123\*V33\*W13+2\*A33\*Q1\*Q12\*T111\*T123\*V33\*W1  
>     3+A33\*Q11\*Q2\*T113\*T122\*V33\*W13+A33\*Q1\*Q11\*T111\*T113\*V33\*W13+A  
?     11\*(-Q2-Q1)\*Q33\*T133\*T333\*V11\*W13+2\*A11\*(-Q2-Q1)\*Q23\*T123\*T33  
@     3\*V11\*W13+A11\*(-Q2-Q1)\*Q22\*T122\*T333\*V11\*W13+2\*A11\*Q13\*(-Q2-Q  
1     1)\*T113\*T333\*V11\*W13+2\*A11\*Q12\*(-Q2-Q1)\*T112\*T333\*V11\*W13+A11  
2     \*Q11\*(-Q2-Q1)\*T111\*T333\*V11\*W13+A11\*Q2\*Q33\*T133\*T223\*V11\*W13+  
3     2\*A11\*Q2\*Q23\*T123\*T223\*V11\*W13+A11\*Q2\*Q22\*T122\*T223\*V11\*W13+2  
4     \*A11\*Q13\*Q2\*T113\*T223\*V11\*W13+2\*A11\*Q12\*Q2\*T112\*T223\*V11\*W13+  
5     A11\*Q11\*Q2\*T111\*T223\*V11\*W13+A11\*Q1\*Q33\*T113\*T133\*V11\*W13+2\*A  
6     11\*Q1\*Q23\*T113\*T123\*V11\*W13+A11\*Q1\*Q22\*T113\*T122\*V11\*W13+2\*A1  
7     1\*Q1\*Q13\*T113\*\*2\*V11\*W13+2\*A11\*Q1\*Q12\*T112\*T113\*V11\*W13+A11\*Q  
8     1\*Q11\*T111\*T113\*V11\*W13+A22\*(-Q2-Q1)\*Q33\*T133\*T233\*V22\*W12+A2  
9     2\*Q2\*Q33\*T122\*T233\*V22\*W12+A22\*Q1\*Q33\*T111\*T233\*V22\*W12+2\*A22  
:     \*(-Q2-Q1)\*Q23\*T133\*T223\*V22\*W12+2\*A22\*Q2\*Q23\*T122\*T223\*V22\*W1  
;     2+2\*A22\*Q1\*Q23\*T111\*T223\*V22\*W12+A22\*(-Q2-Q1)\*Q22\*T133\*T222\*V  
<     22\*W12+A22\*Q2\*Q22\*T122\*T222\*V22\*W12+A22\*Q1\*Q22\*T111\*T222\*V22\*  
=     W12+2\*A22\*Q13\*(-Q2-Q1)\*T123\*T133\*V22\*W12+2\*A22\*Q12\*(-Q2-Q1)\*T  
>     122\*T133\*V22\*W12+A22\*Q11\*(-Q2-Q1)\*T112\*T133\*V22\*W12+2\*A22\*Q13  
?     \*Q2\*T122\*T123\*V22\*W12+2\*A22\*Q1\*Q13\*T111\*T123\*V22\*W12+2\*A22\*Q1  
@     2\*Q2\*T122\*\*2\*V22\*W12+A22\*Q11\*Q2\*T112\*T122\*V22\*W12+2\*A22\*Q1\*Q1  
1     2\*T111\*T122\*V22\*W12+A22\*Q1\*Q11\*T111\*T112\*V22\*W12+A11\*(-Q2-Q1)  
2     \*Q33\*T133\*T233\*V11\*W12+2\*A11\*(-Q2-Q1)\*Q23\*T123\*T233\*V11\*W12+A  
3     11\*(-Q2-Q1)\*Q22\*T122\*T233\*V11\*W12+2\*A11\*Q13\*(-Q2-Q1)\*T113\*T23

```

4   3*V11*W12+2*A11*Q12*(-Q2-Q1)*T112*T233*V11*W12+A11*Q11*(-Q2-Q
5   1)*T111*T233*V11*W12+A11*Q2*Q33*T133*T222*V11*W12+2*A11*Q2*Q2
6   3*T123*T222*V11*W12+A11*Q2*Q22*T122*T222*V11*W12+2*A11*Q13*Q2
7   *T113*T222*V11*W12+2*A11*Q12*Q2*T112*T222*V11*W12+A11*Q11*Q2*
8   T111*T222*V11*W12+A11*Q1*Q33*T112*T133*V11*W12+2*A11*Q1*Q23*T
9   112*T123*V11*W12+A11*Q1*Q22*T112*T122*V11*W12+2*A11*Q1*Q13*T1
:   12*T113*V11*W12+2*A11*Q1*Q12*T112**2*V11*W12+A11*Q1*Q11*T111*
;   T112*V11*W12+A11*(-Q2-Q1)*Q33*T133**2*V11*W11+2*A11*(-Q2-Q1)*
<   Q23*T123*T133*V11*W11+A11*Q2*Q33*T122*T133*V11*W11+A11*(-Q2-Q
=   1)*Q22*T122*T133*V11*W11+2*A11*Q13*(-Q2-Q1)*T113*T133*V11*W11
>   +2*A11*Q12*(-Q2-Q1)*T112*T133*V11*W11+A11*Q1*Q33*T111*T133*V1
?   1*W11+A11*Q11*(-Q2-Q1)*T111*T133*V11*W11+2*A11*Q2*Q23*T122*T1
@   23*V11*W11+2*A11*Q1*Q23*T111*T123*V11*W11+A11*Q2*Q22*T122**2*
1   V11*W11+2*A11*Q13*Q2*T113*T122*V11*W11+2*A11*Q12*Q2*T112*T122
2   *V11*W11+A11*Q1*Q22*T111*T122*V11*W11+A11*Q11*Q2*T111*T122*V1
3   1*W11+2*A11*Q1*Q13*T111*T113*V11*W11+2*A11*Q1*Q12*T111*T112*V
4   11*W11+A11*Q1*Q11*T111**2*V11*W11)

```

```

D119 =((-Q2-Q1)*Q33*T333**2*V33*W33+2*(-Q2-Q1)*Q23*T233*T333*V33
1   *W33+Q2*Q33*T223*T333*V33*W33+(-Q2-Q1)*Q22*T223*T333*V33*W33+
2   2*Q13*(-Q2-Q1)*T133*T333*V33*W33+2*Q12*(-Q2-Q1)*T123*T333*V33
3   *W33+Q1*Q33*T113*T333*V33*W33+Q11*(-Q2-Q1)*T113*T333*V33*W33+
4   2*Q2*Q23*T223*T233*V33*W33+2*Q1*Q23*T113*T233*V33*W33+Q2*Q22*
5   T223**2*V33*W33+2*Q13*Q2*T133*T223*V33*W33+2*Q12*Q2*T123*T223
6   *V33*W33+Q1*Q22*T113*T223*V33*W33+Q11*Q2*T113*T223*V33*W33+2*
7   Q1*Q13*T113*T133*V33*W33+2*Q1*Q12*T113*T123*V33*W33+Q1*Q11*T1
8   13**2*V33*W33+(-Q2-Q1)*Q33*T233*T333*V33*W23+Q2*Q33*T222*T333
9   *V33*W23+Q1*Q33*T112*T333*V33*W23+2*(-Q2-Q1)*Q23*T233**2*V33*
:   W23+(-Q2-Q1)*Q22*T223*T233*V33*W23+2*Q2*Q23*T222*T233*V33*W23
;   +2*Q13*(-Q2-Q1)*T133*T233*V33*W23+2*Q12*(-Q2-Q1)*T123*T233*V3

```

<  $3*W23+Q11*(-Q2-Q1)*T113*T233*V33*W23+2*Q1*Q23*T112*T233*V33*W$   
 =  $23+Q2*Q22*T222*T223*V33*W23+Q1*Q22*T112*T223*V33*W23+2*Q13*Q2$   
 >  $*T133*T222*V33*W23+2*Q12*Q2*T123*T222*V33*W23+Q11*Q2*T113*T22$   
 ?  $2*V33*W23+2*Q1*Q13*T112*T133*V33*W23+2*Q1*Q12*T112*T123*V33*W$   
 @  $23+Q1*Q11*T112*T113*V33*W23+(-Q2-Q1)*Q33*T233*T333*V22*W23+2*$   
 1  $(-Q2-Q1)*Q23*T223*T333*V22*W23+(-Q2-Q1)*Q22*T222*T333*V22*W23$   
 2  $+2*Q13*(-Q2-Q1)*T123*T333*V22*W23+2*Q12*(-Q2-Q1)*T122*T333*V2$   
 3  $2*W23+Q11*(-Q2-Q1)*T112*T333*V22*W23+Q2*Q33*T223*T233*V22*W23$   
 4  $+Q1*Q33*T113*T233*V22*W23+2*Q2*Q23*T223**2*V22*W23+Q2*Q22*T22$   
 5  $2*T223*V22*W23+2*Q13*Q2*T123*T223*V22*W23+2*Q12*Q2*T122*T223*$   
 6  $V22*W23+2*Q1*Q23*T113*T223*V22*W23+Q11*Q2*T112*T223*V22*W23+Q$   
 7  $1*Q22*T113*T222*V22*W23+2*Q1*Q13*T113*T123*V22*W23+2*Q1*Q12*T$   
 8  $113*T122*V22*W23+Q1*Q11*T112*T113*V22*W23+(-Q2-Q1)*Q33*T233**$   
 9  $2*V22*W22+2*(-Q2-Q1)*Q23*T223*T233*V22*W22+Q2*Q33*T222*T233*V$   
 :  $22*W22+(-Q2-Q1)*Q22*T222*T233*V22*W22+2*Q13*(-Q2-Q1)*T123*T23$   
 ;  $3*V22*W22+2*Q12*(-Q2-Q1)*T122*T233*V22*W22+Q1*Q33*T112*T233*V$   
 <  $22*W22+Q11*(-Q2-Q1)*T112*T233*V22*W22+2*Q2*Q23*T222*T223*V22*$   
 =  $W22+2*Q1*Q23*T112*T223*V22*W22+Q2*Q22*T222**2*V22*W22+2*Q13*Q$   
 >  $2*T123*T222*V22*W22+2*Q12*Q2*T122*T222*V22*W22+Q1*Q22*T112*T2$   
 ?  $22*V22*W22+Q11*Q2*T112*T222*V22*W22+2*Q1*Q13*T112*T123*V22*W2$   
 @  $2+2*Q1*Q12*T112*T122*V22*W22+Q1*Q11*T112**2*V22*W22+(-Q2-Q1)*$   
 1  $Q33*T133*T333*V33*W13+Q2*Q33*T122*T333*V33*W13+Q1*Q33*T111*T3$   
 2  $33*V33*W13+2*(-Q2-Q1)*Q23*T133*T233*V33*W13+2*Q2*Q23*T122*T23$   
 3  $3*V33*W13+2*Q1*Q23*T111*T233*V33*W13+(-Q2-Q1)*Q22*T133*T223*V$   
 4  $33*W13+Q2*Q22*T122*T223*V33*W13+Q1*Q22*T111*T223*V33*W13+2*Q1$   
 5  $3*(-Q2-Q1)*T133**2*V33*W13+2*Q12*(-Q2-Q1)*T123*T133*V33*W13+2$   
 6  $*Q13*Q2*T122*T133*V33*W13+Q11*(-Q2-Q1)*T113*T133*V33*W13+2*Q1$   
 7  $*Q13*T111*T133*V33*W13+2*Q12*Q2*T122*T123*V33*W13+2*Q1*Q12*T1$   
 8  $11*T123*V33*W13+Q11*Q2*T113*T122*V33*W13+Q1*Q11*T111*T113*V33$   
 9  $*W13+(-Q2-Q1)*Q33*T133*T333*V11*W13+2*(-Q2-Q1)*Q23*T123*T333*$   
 :  $V11*W13+(-Q2-Q1)*Q22*T122*T333*V11*W13+2*Q13*(-Q2-Q1)*T113*T3$

```

;      33*V11*W13+2*Q12*(-Q2-Q1)*T112*T333*V11*W13+Q11*(-Q2-Q1)*T111
<      *T333*V11*W13+Q2*Q33*T133*T223*V11*W13+2*Q2*Q23*T123*T223*V11
=      *W13+Q2*Q22*T122*T223*V11*W13+2*Q13*Q2*T113*T223*V11*W13+2*Q1
>      2*Q2*T112*T223*V11*W13+Q11*Q2*T111*T223*V11*W13+Q1*Q33*T113*T
?      133*V11*W13+2*Q1*Q23*T113*T123*V11*W13+Q1*Q22*T113*T122*V11*W
@      13+2*Q1*Q13*T113**2*V11*W13+2*Q1*Q12*T112*T113*V11*W13+Q1*Q11
1      *T111*T113*V11*W13+(-Q2-Q1)*Q33*T133*T233*V22*W12+Q2*Q33*T122
2      *T233*V22*W12+Q1*Q33*T111*T233*V22*W12+2*(-Q2-Q1)*Q23*T133*T2
3      23*V22*W12+2*Q2*Q23*T122*T223*V22*W12+2*Q1*Q23*T111*T223*V22*
4      W12+(-Q2-Q1)*Q22*T133*T222*V22*W12+Q2*Q22*T122*T222*V22*W12+Q
5      1*Q22*T111*T222*V22*W12+2*Q13*(-Q2-Q1)*T123*T133*V22*W12+2*Q1
6      2*(-Q2-Q1)*T122*T133*V22*W12+Q11*(-Q2-Q1)*T112*T133*V22*W12+2*
7      *Q13*Q2*T122*T123*V22*W12+2*Q1*Q13*T111*T123*V22*W12+2*Q12*Q2
8      *T122**2*V22*W12+Q11*Q2*T112*T122*V22*W12+2*Q1*Q12*T111*T122*
9      V22*W12+Q1*Q11*T111*T112*V22*W12+(-Q2-Q1)*Q33*T133*T233*V11*W
:      12+2*(-Q2-Q1)*Q23*T123*T233*V11*W12+(-Q2-Q1)*Q22*T122*T233*V1
;      1*W12+2*Q13*(-Q2-Q1)*T113*T233*V11*W12+2*Q12*(-Q2-Q1)*T112*T2
<      33*V11*W12+Q11*(-Q2-Q1)*T111*T233*V11*W12+Q2*Q33*T133*T222*V1
=      1*W12+2*Q2*Q23*T123*T222*V11*W12+Q2*Q22*T122*T222*V11*W12+2*Q
>      13*Q2*T113*T222*V11*W12+2*Q12*Q2*T112*T222*V11*W12+Q11*Q2*T11
?      1*T222*V11*W12+Q1*Q33*T112*T133*V11*W12+2*Q1*Q23*T112*T123*V1
@      1*W12+Q1*Q22*T112*T122*V11*W12+2*Q1*Q13*T112*T113*V11*W12+2*Q
1      1*Q12*T112**2*V11*W12+Q1*Q11*T111*T112*V11*W12+(-Q2-Q1)*Q33*T
2      133**2*V11*W11+2*(-Q2-Q1)*Q23*T123*T133*V11*W11+Q2*Q33*T122*T
3      133*V11*W11+(-Q2-Q1)*Q22*T122*T133*V11*W11+2*Q13*(-Q2-Q1)*T11
4      3*T133*V11*W11+2*Q12*(-Q2-Q1)*T112*T133*V11*W11+Q1*Q33*T111*T
5      133*V11*W11+Q11*(-Q2-Q1)*T111*T133*V11*W11+2*Q2*Q23*T122*T123
6      *V11*W11+2*Q1*Q23*T111*T123*V11*W11+Q2*Q22*T122**2*V11*W11+2*
7      Q13*Q2*T113*T122*V11*W11+2*Q12*Q2*T112*T122*V11*W11+Q1*Q22*T1
8      11*T122*V11*W11+Q11*Q2*T111*T122*V11*W11+2*Q1*Q13*T111*T113*V
9      11*W11+2*Q1*Q12*T111*T112*V11*W11+Q1*Q11*T111**2*V11*W11)

```

TERM=(D97-ALDYN\*D101+D105-ALDYN\*D110+2.\*D115-2.\*ALDYN\*D119)

FI(X2,X3,X4,X5,X6)=(1/(1080.\*3.14159265358979323846\*\*2))\*(SI  
+ N(BE1(X3))\*SIN(BE2(X6)))\*TERM

C

C CALCULATION OF THE SHAPE POTENTIAL:

C

G1(X3,X4,X6)=4.\*PARAM2\*1.380622E-23\*R\*\*12\*(SHAPE1\*(3.\*COS(BE1(X3)  
+ )\*\*2+3.\*COS(BE2(X6))\*\*2-2.)+SHAPE2\*(3.\*COS(GA1(X4))\*\*2\*SIN(BE1(X3  
+ ))\*\*2+3.\*COS(GA2(X7))\*\*2\*SIN(BE2(X6))\*\*2-2.))

80 CONTINUE

70 CONTINUE

60 CONTINUE

50 CONTINUE

c WRITE(4,1444)term

c1444 FORMAT(1X,'term IS',E15.7)

```
40      CONTINUE
```

```
C
```

```
C THE INTEGRAL IS CALCULATED:
```

```
C
```

```
SS6=0.00
```

```
DO 940 X6=1,16
```

```
C      WRITE(6,1911)X6
```

```
c1911  FORMAT (1X, 'sub-index (in range 1 to 16) is currently ',I2 )
```

```
SS5=0.00
```

```
DO 950 X5=1,16
```

```
SS4=0.00
```

```
DO 960 X4=1,16
```

```
SS3=0.00
```

```
DO 970 X3=1,16
```

```
SS2=0.00
```

```
DO 980 X2=1,16
```

```
SS1=0.00
```

```
DO 990 X1=1,64
```

```
C
```

```
C SUMMATION OF THE ENERGY TERMS WITH SUBSEQUENT DIVISION BY (-kT):
```

```
C
```

```
G3=-1.*(D1(X1)+E1(X2,X3,X4,X5,X6)/SE5(X1)+F1(X2,X3,X4,X5,X6)/SE8(
+ X1)+G1(X3,X4,X6)/SE12(X1)+DDP(X2,X3,X4,X5,X6)/SE3(X1)+DIDP(X2,X3,
+ X4,X5,X6)/SE6(X1)+DQP(X2,X3,X4,X5,X6)/SE4(X1))/TEMPK
```

```
IF(G3.LT.-85) GO TO 5000
G4=2.71828**G3
GO TO 5010
5000 G4=0
5010 SS1=SS1+(FI(X2,X3,X4,X5,X6)/(SEP(X1)**6))*G4*COEF2(X1,2)
990      CONTINUE
SS2=SS2+SS1*COEF1(X2,2)
C
C
980      CONTINUE
SS3=SS3+SS2*COEF1(X3,2)
C
C
970      CONTINUE
SS4=SS4+SS3*COEF1(X4,2)
C
C
960      CONTINUE
SS5=SS5+SS4*COEF1(X5,2)
C
C
950      CONTINUE
SS6=SS6+SS5*COEF1(X6,2)
C
C
940      CONTINUE
SS7=SS7+SS6*COEF1(X7,2)

C
C
939      CONTINUE
```

```
ANS=SS7*SEP1*AL11*BE11*GA11*AL21*BE21*GA21*6.022169**2*
+ 8.987552**3*1E-36/(TEMP*1.380622)**2

C
C THE INTEGRAL IS PRINTED TOGETHER WITH MOLECULAR DATA USED
C

      WRITE(4,2266)
2266  FORMAT(1X,'THE Q2A3 TERM CONTRIBUTION TO B(Kerr) FOR ETHENE:')
      WRITE(4,2267)
2267  FORMAT(1X,'    ')
      WRITE(4,2269)
2269  FORMAT(1X,'    ')
      WRITE(4,1140)ANS
1140  FORMAT(1X,'THE INTEGRAL IS',E15.7)
      WRITE(4,2150)
2150  FORMAT(1X,'INPUT DATA:')
      WRITE(4,2155)TEMP
2155  FORMAT(1X,'TEMPERATURE:      ',F10.5)
      WRITE(4,9260)ALDYN
9260  FORMAT(1X,'MEAN DYNAMIC ALPHA:',F10.5)
      WRITE(4,9261)A11
9261  FORMAT(1X,'DYNAMIC ALPHA11:   ',F10.5)
      WRITE(4,9262)A22
9262  FORMAT(1X,'DYNAMIC ALPHA22:   ',F10.5)
      WRITE(4,9263)A33
9263  FORMAT(1X,'DYNAMIC ALPHA33:   ',F10.5)
      WRITE(4,9264)ALSTAT
9264  FORMAT(1X,'MEAN STATIC ALPHA: ',F10.5)
      WRITE(4,9961)V11
9961  FORMAT(1X,'STATIC ALPHA11:   ',F10.5)
```

```
      WRITE(4,9962)V22
9962  FORMAT(1X,'STATIC ALPHA22:      ',F10.5)
      WRITE(4,9963)V33
9963  FORMAT(1X,'STATIC ALPHA33:      ',F10.5)
      WRITE(4,2190)Q1
2190  FORMAT(1X,'THETA11:           ',F10.5)
      WRITE(4,2241)Q2
2241  FORMAT(1X,'THETA22:           ',F10.5)
      WRITE(4,2210)R
2210  FORMAT(1X,'R(0):             ',F6.5)
      WRITE(4,2220)SHAPE1
2220  FORMAT(1X,'SHAPE FACTOR 1:    ',F10.5)
      WRITE(4,2221)SHAPE2
2221  FORMAT(1X,'SHAPE FACTOR 2:    ',F10.5)
      WRITE(4,2230)PARAM2
2230  FORMAT(1X,'E/K:              ',F9.5)
      WRITE(4,2235)AMIN1,AMAX1
2235  FORMAT(1X,'MIN AND MAX POINTS OF RANGE (64 INTERVALS):',2(F10.5,3
+ X))
      WRITE(4,2240)
2240  FORMAT(1X,'END BT')
      WRITE(4,2261)
2261  FORMAT(1X,'   ')
      WRITE(4,2262)
2262  FORMAT(1X,'   ')
      WRITE(4,2263)
2263  FORMAT(1X,'   ')
      WRITE(4,2264)
2264  FORMAT(1X,'   ')
      WRITE(4,2265)
2265  FORMAT(1X,'   ')
```

```
close(unit=4)
```

```
END
```

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