

APPENDIX 2

Rovibrational **G** tensor for penta-atomic amine-like molecules

To illustrate our method, we derive the rovibrational **G** tensor of the simplest amine molecule of a type NH₂OH. It is a prototype of other amines of the first class because more complex molecules can be constructed including additional bonds to this penta-atomic core.

For this molecule the internuclear vectors are chosen according to Figure 1. The determination of the mass coefficients is elementary and gives

$$\left[\frac{1}{m_{i,j}} \right] = \begin{bmatrix} \frac{1}{m_0} + \frac{1}{m_1} & \frac{1}{m_0} & \frac{1}{m_0} & -\frac{1}{m_1} \\ \frac{1}{m_0} & \frac{1}{m_0} + \frac{1}{m_2} & \frac{1}{m_0} & 0 \\ \frac{1}{m_0} & \frac{1}{m_0} & \frac{1}{m_0} + \frac{1}{m_3} & 0 \\ -\frac{1}{m_1} & 0 & 0 & \frac{1}{m_1} + \frac{1}{m_4} \end{bmatrix}.$$

The components of the **G** tensor are simply the dot products of the **s** and **Ω** vectors, given by Eqs. (11-13).

The rotation, vibration and Coriolis subtensors of the frame can be considered as the **G** tensor for ammonia-like molecules determined in Ref.(16). As the top part is not included in the construction of the rotating MSA, it contributes only to the vibration and Coriolis tensor elements. The total **G** tensor derived by hands is reported below. It has been checked numerically by the method as described in Ref. (10).

A. 1. The vibrational G tensor of the frame

$$g^{r_1, r_1} = \frac{1}{m_{1,1}}, \quad g^{r_1, r_2} = \frac{\cos^2 \alpha + \sin^2 \alpha \cos \tau_2}{m_0}, \quad g^{r_1, r_3} = \frac{\cos^2 \alpha + \sin^2 \alpha \cos \tau_3}{m_0},$$

$$g^{r_2, r_2} = \frac{1}{m_{2,2}}, \quad g^{r_2, r_3} = \frac{\cos^2 \alpha + \sin^2 \alpha \cos \tau_1}{m_0}, \quad g^{r_3, r_3} = \frac{1}{m_{3,3}},$$

$$g^{r_1, \alpha} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_2} S_{1,2} + \frac{1 - \cos \tau_3}{m_0 r_3} S_{1,3} \right),$$

$$g^{r_2, \alpha} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_1} (S_{1,1} - 1) + \frac{1 - \cos \tau_1}{m_0 r_3} S_{1,3} \right),$$

$$g^{r_3, \alpha} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_3}{m_0 r_1} (S_{1,1} - 1) + \frac{1 - \cos \tau_1}{m_0 r_3} S_{1,2} \right),$$

$$g^{r_1, \tau_2} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_2} T_{2,2} + \frac{1 - \cos \tau_3}{m_0 r_3} T_{2,3} \right) - \frac{\sin \tau_2}{m_0 r_2},$$

$$g^{r_1, \tau_3} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_2} T_{3,2} + \frac{1 - \cos \tau_3}{m_0 r_3} T_{3,3} \right) - \frac{\sin \tau_3}{m_0 r_3},$$

$$g^{r_2, \tau_2} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_1} T_{2,1} + \frac{1 - \cos \tau_1}{m_0 r_3} T_{2,3} \right) - \frac{\sin \tau_2}{m_0 r_1},$$

$$g^{r_2, \tau_3} = -\sin^2 \alpha \left(\frac{\sin \tau_2}{m_0 r_1} + \frac{\sin \tau_1}{m_0 r_3} \right),$$

$$g^{r_3, \tau_2} = -\sin^2 \alpha \left(\frac{\sin \tau_3}{m_0 r_1} - \frac{\sin \tau_1}{m_0 r_2} \right),$$

$$g^{r_3, \tau_3} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_3}{m_0 r_1} T_{3,1} + \frac{1 - \cos \tau_1}{m_0 r_2} T_{3,2} \right) - \frac{\sin \tau_3}{m_0 r_1},$$

$$g^{\alpha, \alpha} = \frac{(S_{1,1} - 1)^2}{m_{1,1} r_1^2} + \frac{S_{1,2}^2}{m_{2,2} r_2^2} + \frac{S_{1,3}^2}{m_{3,3} r_3^2} + 2 \frac{(S_{1,1} - 1) S_{1,2}}{m_0 r_1 r_2} f(\tau_2) + 2 \frac{(S_{1,1} - 1) S_{1,3}}{m_0 r_1 r_3} f(\tau_3) + 2 \frac{S_{1,2} S_{1,3}}{m_0 r_2 r_3} f(\tau_1),$$

$$\begin{aligned}
g^{\alpha, \tau_2} &= \frac{(S_{1,1}-1)T_{2,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}T_{2,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}T_{2,3}}{m_{3,3}r_3^2} \\
&+ \frac{(S_{1,1}-1)[\cot\alpha\sin\tau_2 + f(\tau_2)T_{2,2}] + S_{1,2}[\cot\alpha\sin\tau_2 + f(\tau_2)T_{2,1}]}{m_0r_1r_2} \\
&+ \frac{(S_{1,1}-1)T_{2,3}f(\tau_3) + S_{1,3}T_{2,1}\chi(\tau_3)}{m_0r_1r_3} + \frac{S_{1,2}T_{2,3}f(\tau_1) + S_{1,3}T_{2,2}\chi(\tau_1)}{m_0r_2r_3}, \\
g^{\alpha, \tau_3} &= \frac{(S_{1,1}-1)T_{3,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}T_{3,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}T_{3,3}}{m_{3,3}r_3^2} + \frac{(S_{1,1}-1)T_{3,2}f(\tau_2) + S_{1,2}T_{3,1}\chi(\tau_2)}{m_0r_1r_2} \\
&+ \frac{(S_{1,1}-1)[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,3}] + S_{1,3}[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,1}]}{m_0r_1r_3} \\
&+ \frac{S_{1,3}T_{3,2}f(\tau_1) + S_{1,2}T_{3,3}\chi(\tau_1)}{m_0r_2r_3}, \\
g^{\tau_2, \tau_2} &= \frac{T_{2,1}^2 + 1 + \cot^2\alpha}{m_{1,1}r_1^2} + \frac{T_{2,2}^2 + 1 + \cot^2\alpha}{m_{2,2}r_2^2} + \frac{T_{2,3}^2}{m_{3,3}r_3^2} + 2\frac{T_{2,1}T_{2,2}\chi(\tau_2) - \psi(\tau_2)}{m_0r_1r_2} \\
&+ 2\frac{T_{2,1}T_{2,3}\chi(\tau_3)}{m_0r_1r_3} + 2\frac{T_{2,2}T_{2,3}\chi(\tau_1)}{m_0r_2r_3}, \\
g^{\tau_3, \tau_3} &= \frac{T_{3,1}^2 + 1 + \cot^2\alpha}{m_{1,1}r_1^2} + \frac{T_{3,2}^2}{m_{2,2}r_2^2} + \frac{T_{3,3}^2 + 1 + \cot^2\alpha}{m_{3,3}r_3^2} + 2\frac{T_{3,1}T_{3,2}\chi(\tau_2)}{m_0r_1r_2} \\
&+ 2\frac{T_{3,1}T_{3,3}\chi(\tau_3) - \psi(\tau_3)}{m_0r_1r_3} + 2\frac{T_{3,2}T_{3,3}\chi(\tau_1)}{m_0r_2r_3}, \\
g^{\tau_2, \tau_3} &= \frac{T_{2,1}T_{3,1} + 1 + \cot^2\alpha}{m_{1,1}r_1^2} + \frac{T_{2,2}T_{3,2}}{m_{2,2}r_2^2} + \frac{T_{2,3}T_{3,3}}{m_{3,3}r_3^2} + \frac{(T_{2,1}T_{3,2} + T_{2,2}T_{3,1})\chi(\tau_2) - \psi(\tau_2)}{m_0r_1r_2} \\
&+ \frac{(T_{2,1}T_{3,3} + T_{2,3}T_{3,1})\chi(\tau_3) - \psi(\tau_3)}{m_0r_1r_3} + \frac{(T_{2,2}T_{3,3} + T_{2,3}T_{3,2})\chi(\tau_1) + \psi(\tau_1)}{m_0r_2r_3}.
\end{aligned}$$

A. 2. The Coriolis tensor of the frame

$$C_x^{r_i} = \sin\alpha\cos\alpha\left(\frac{1-\cos\tau_2}{m_0r_2}S_{2,2} + \frac{1-\cos\tau_3}{m_0r_3}S_{2,3}\right),$$

$$C_y^{r_i} = -\sin\alpha\cos\alpha\left(\frac{1-\cos\tau_2}{m_0r_2}S_{1,2} + \frac{1-\cos\tau_3}{m_0r_3}S_{1,3}\right),$$

$$C_z^{r_i} = \cot\alpha C_x^{r_i},$$

$$C_x^{r_2} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_1} S_{2,1} + \frac{1 - \cos \tau_1}{m_0 r_3} S_{2,3} \right),$$

$$C_y^{r_2} = -\sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_2}{m_0 r_1} S_{1,1} + \frac{1 - \cos \tau_1}{m_0 r_3} S_{1,3} \right),$$

$$C_z^{r_2} = \frac{\sin \tau_2}{m_0 r_1} + \cot \alpha C_x^{r_2},$$

$$C_x^{r_3} = \sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_3}{m_0 r_1} S_{2,1} + \frac{1 - \cos \tau_1}{m_0 r_2} S_{2,2} \right),$$

$$C_y^{r_3} = -\sin \alpha \cos \alpha \left(\frac{1 - \cos \tau_3}{m_0 r_1} S_{1,1} + \frac{1 - \cos \tau_1}{m_0 r_2} S_{1,2} \right),$$

$$C_z^{r_3} = \frac{\sin \tau_3}{m_0 r_1} + \cot \alpha C_x^{r_3}.$$

$$\begin{aligned} C_x^\alpha &= \frac{(S_{1,1} - 1)S_{2,1}}{m_{1,1} r_1^2} + \frac{S_{1,2}S_{2,2}}{m_{2,2} r_2^2} + \frac{S_{1,3}S_{2,3}}{m_{3,3} r_3^2} + \frac{(S_{1,1} - 1)S_{2,2} + S_{1,2}S_{2,1}}{m_0 r_1 r_2} f(\tau_2) \\ &\quad + \frac{(S_{1,1} - 1)S_{2,3} + S_{1,3}S_{2,1}}{m_0 r_1 r_3} f(\tau_3) + \frac{S_{1,2}S_{2,3} + S_{1,3}S_{2,2}}{m_0 r_2 r_3} f(\tau_1), \end{aligned}$$

$$\begin{aligned} C_y^\alpha &= - \left[\frac{(S_{1,1} - 1)S_{1,1}}{m_{1,1} r_1^2} + \frac{S_{1,2}^2}{m_{2,2} r_2^2} + \frac{S_{1,3}^2}{m_{3,3} r_3^2} + \frac{(S_{1,1} - 1)S_{1,2} + S_{1,2}S_{1,1}}{m_0 r_1 r_2} f(\tau_2) \right. \\ &\quad \left. + \frac{(S_{1,1} - 1)S_{1,3} + S_{1,3}S_{1,1}}{m_0 r_1 r_3} f(\tau_3) + \frac{S_{1,2}S_{1,3} + S_{1,3}S_{1,2}}{m_0 r_2 r_3} f(\tau_1) \right], \end{aligned}$$

$$C_z^\alpha = \cot \alpha \left(C_x^\alpha - \frac{\sin \tau_2}{m_0 r_1 r_2} S_{1,2} - \frac{\sin \tau_3}{m_0 r_1 r_3} S_{1,3} \right),$$

$$\begin{aligned} C_x^{\tau_2} &= \frac{S_{2,1}T_{2,1}}{m_{1,1} r_1^2} + \frac{S_{2,2}T_{2,2}}{m_{2,2} r_2^2} + \frac{S_{2,3}T_{2,3}}{m_{3,3} r_3^2} \\ &\quad + \frac{S_{2,1}[\cot \alpha \sin \tau_2 + f(\tau_2)T_{2,2}] + S_{2,2}[\cot \alpha \sin \tau_2 + f(\tau_2)T_{2,1}]}{m_0 r_1 r_2} \\ &\quad + \frac{S_{2,1}T_{2,3}f(\tau_3) + S_{2,3}T_{2,1}\chi(\tau_3)}{m_0 r_1 r_3} + \frac{S_{2,2}T_{2,3}f(\tau_1) + S_{2,3}T_{2,2}\chi(\tau_1)}{m_0 r_2 r_3}, \end{aligned}$$

$$C_y^{\tau_2} = - \left[\frac{S_{1,1}T_{2,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}T_{2,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}T_{2,3}}{m_{3,3}r_3^2} \right. \\ \left. + \frac{S_{1,1}[\cot\alpha\sin\tau_2 + f(\tau_2)T_{2,2}] + S_{1,2}[\cot\alpha\sin\tau_2 + f(\tau_2)T_{2,1}]}{m_0r_1r_2} \right. \\ \left. + \frac{S_{1,1}T_{2,3}f(\tau_3) + S_{1,3}T_{2,1}\chi(\tau_3)}{m_0r_1r_3} + \frac{S_{1,2}T_{2,3}f(\tau_1) + S_{1,3}T_{2,2}\chi(\tau_1)}{m_0r_2r_3} \right],$$

$$C_z^{\tau_2} = - \frac{1}{\sin^2\alpha m_{1,1}r_1^2} + \frac{(1+\cot^2\alpha)\cos\tau_2}{m_0r_1r_2} + \cot\alpha \left(C_x^{\tau_2} - \frac{\sin\tau_2}{m_0r_1r_2} T_{2,2} - \frac{\sin\tau_3}{m_0r_1r_3} T_{2,3} \right),$$

$$C_x^{\tau_3} = \frac{S_{2,1}T_{3,1}}{m_{1,1}r_1^2} + \frac{S_{2,2}T_{3,2}}{m_{2,2}r_2^2} + \frac{S_{2,3}T_{3,3}}{m_{3,3}r_3^2} + \frac{S_{2,1}T_{3,2}f(\tau_2) + S_{2,2}T_{3,1}\chi(\tau_2)}{m_0r_1r_2} \\ + \frac{S_{2,1}[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,3}] + S_{2,3}[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,1}]}{m_0r_1r_3} \\ + \frac{S_{2,3}T_{3,2}f(\tau_1) + S_{2,2}T_{3,3}\chi(\tau_1)}{m_0r_2r_3},$$

$$C_y^{\tau_3} = - \left[\frac{S_{1,1}T_{3,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}T_{3,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}T_{3,3}}{m_{3,3}r_3^2} + \frac{S_{1,1}T_{3,2}f(\tau_2) + S_{1,2}T_{3,1}\chi(\tau_2)}{m_0r_1r_2} \right. \\ \left. + \frac{S_{1,1}[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,3}] + S_{1,3}[\cot\alpha\sin\tau_3 + f(\tau_3)T_{3,1}]}{m_0r_1r_3} \right. \\ \left. + \frac{S_{1,3}T_{3,2}f(\tau_1) + S_{1,2}T_{3,3}\chi(\tau_1)}{m_0r_2r_3} \right],$$

$$C_z^{\tau_3} = - \frac{1}{\sin^2\alpha m_{1,1}r_1^2} + \frac{(1+\cot^2\alpha)\cos\tau_3}{m_0r_1r_3} + \cot\alpha \left(C_x^{\tau_3} - \frac{\sin\tau_2}{m_0r_1r_2} T_{3,2} - \frac{\sin\tau_3}{m_0r_1r_3} T_{3,3} \right),$$

A. 3. The rotatrorial μ tensor

$$\mu_{xx} = \frac{S_{2,1}^2}{m_{1,1}r_1^2} + \frac{S_{2,2}^2}{m_{2,2}r_2^2} + \frac{S_{2,3}^2}{m_{3,3}r_3^2} + 2\frac{S_{2,1}S_{2,2}f(\tau_2)}{m_0r_1r_2} + 2\frac{S_{2,1}S_{2,3}f(\tau_3)}{m_0r_1r_3} + 2\frac{S_{2,2}S_{2,3}f(\tau_1)}{m_0r_2r_3},$$

$$\mu_{yy} = \frac{S_{1,1}^2}{m_{1,1}r_1^2} + \frac{S_{1,2}^2}{m_{2,2}r_2^2} + \frac{S_{1,3}^2}{m_{3,3}r_3^2} + 2\frac{S_{1,1}S_{1,2}f(\tau_2)}{m_0r_1r_2} + 2\frac{S_{1,1}S_{1,3}f(\tau_3)}{m_0r_1r_3} + 2\frac{S_{1,2}S_{1,3}f(\tau_1)}{m_0r_2r_3},$$

$$\mu_{xy} = - \left[\frac{S_{1,1}S_{2,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}S_{2,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}S_{2,3}}{m_{3,3}r_3^2} + \frac{S_{1,2}S_{2,1} + S_{1,1}S_{2,2}}{m_0r_1r_2} f(\tau_2) \right. \\ \left. + \frac{S_{1,1}S_{2,3} + S_{2,1}S_{1,3}}{m_0r_1r_3} f(\tau_3) + \frac{S_{2,2}S_{1,3} + S_{1,2}S_{2,3}}{m_0r_2r_3} f(\tau_1) \right],$$

$$\mu_{xz} = \cot\alpha \left(\mu_{xx} - \frac{\sin\tau_2}{m_0r_1r_2} S_{2,2} - \frac{\sin\tau_3}{m_0r_1r_3} S_{2,3} \right),$$

$$\mu_{yz} = \cot\alpha \left(\mu_{xy} + \frac{\sin\tau_2}{m_0r_1r_2} S_{1,2} + \frac{\sin\tau_3}{m_0r_1r_3} S_{1,3} \right),$$

$$\mu_{zz} = \frac{1}{\sin^2\alpha m_{1,1}r_1^2} + \cot^2\alpha \left(\mu_{xx} - 2\frac{\sin\tau_2}{m_0r_1r_2} S_{2,2} - 2\frac{\sin\tau_3}{m_0r_1r_3} S_{2,3} \right).$$

A. 4. The vibrational G tensor involving the top coordinates

$$g^{r_4, r_1} = \frac{\cos\theta}{m_1}, \quad g^{r_4, r_2} = 0, \quad g^{r_4, r_3} = 0, \quad g^{r_4, r_4} = \frac{1}{m_1} + \frac{1}{m_4},$$

$$g^{r_4, \alpha} = -\frac{(S_{1,1}-1)\sin\theta\cos\phi}{m_1r_1},$$

$$g^{r_4, \tau_2} = -\frac{(T_{2,1}\sin\alpha\cos\phi - \sin\phi)\sin\theta}{m_1r_1\sin\alpha},$$

$$g^{r_4, \tau_3} = -\frac{(T_{3,1}\sin\alpha\cos\phi - \sin\phi)\sin\theta}{m_1r_1\sin\alpha},$$

$$g^{\theta, r_1} = -\frac{\sin\theta}{m_1r_4}, \quad g^{\theta, r_2} = \frac{\sin\alpha[\cos\alpha\cos\phi(\cos\tau_2-1) + \sin\phi\sin\tau_2]}{m_0r_1}, \\ g^{\theta, r_4} = -\frac{\sin\theta}{m_1r_1}, \quad g^{\theta, r_3} = \frac{\sin\alpha[\cos\alpha\cos\phi(\cos\tau_3-1) + \sin\phi\sin\tau_3]}{m_0r_1},$$

$$\begin{aligned}
g^{\theta,\alpha} &= \frac{\cos\phi(S_{1,1}-1)}{m_{1,1}r_1^2} + \frac{S_{1,2}[\cos\phi f(\tau_2)-\cos\alpha\sin\phi\sin\tau_2]}{m_0r_1r_2} \\
&\quad + \frac{S_{1,3}[\cos\phi f(\tau_3)-\cos\alpha\sin\phi\sin\tau_3]}{m_0r_1r_3} - \frac{(S_{1,1}-1)\cos\theta\cos\phi}{m_1r_1r_4}, \\
g^{\theta,\tau_2} &= \frac{T_{2,1}\sin\alpha\cos\phi-\sin\phi}{m_{1,1}r_1^2} + \frac{T_{2,2}[\cos\phi f(\tau_2)-\cos\alpha\sin\phi\sin\tau_2]}{m_0r_1r_2} \\
&\quad + \frac{T_{2,3}[\cos\phi f(\tau_3)-\cos\alpha\sin\phi\sin\tau_3]}{m_0r_1r_3} - \frac{\cos\theta(T_{2,1}\sin\alpha\cos\phi-\sin\phi)}{m_1r_1r_4\sin\alpha} \\
&\quad + \frac{\cos\alpha\cos\phi\sin\tau_2+\sin\phi\cos\tau_2}{m_0r_1r_2\sin\alpha}, \\
g^{\theta,\tau_3} &= \frac{T_{3,1}\sin\alpha\cos\phi-\sin\phi}{m_{1,1}r_1^2} + \frac{T_{3,2}[\cos\phi f(\tau_2)-\cos\alpha\sin\phi\sin\tau_2]}{m_0r_1r_2} \\
&\quad + \frac{T_{3,3}[\cos\phi f(\tau_3)-\cos\alpha\sin\phi\sin\tau_3]}{m_0r_1r_3} - \frac{\cos\theta(T_{3,1}\sin\alpha\cos\phi-\sin\phi)}{m_1r_1r_4\sin\alpha} \\
&\quad + \frac{\cos\alpha\cos\phi\sin\tau_2+\sin\phi\cos\tau_3}{m_0r_1r_3\sin\alpha}, \\
g^{\theta,\theta} &= \frac{1}{m_{1,1}r_1^2} + \frac{1}{m_{4,4}r_4^2} - \frac{2\cos\theta}{m_1r_1r_4}, \\
g^{\theta,\phi} &= \frac{1}{\sin\alpha} \left[\frac{(S_{2,1}\cos\phi+\cos\alpha\sin\phi)}{m_{1,1}r_1^2} + \frac{S_{2,2}[\cos\phi f(\tau_2)-\cos\alpha\sin\phi\sin\tau_2]}{m_0r_1r_2} \right. \\
&\quad \left. + \frac{S_{2,3}[\cos\phi f(\tau_3)-\cos\alpha\sin\phi\sin\tau_3]}{m_0r_1r_3} - \frac{\cos\theta(S_{2,1}\cos\phi+\cos\alpha\sin\phi)}{m_1r_1r_4} \right], \\
g^{\phi,r_1} &= \cos\alpha \left(\frac{1-\cos\tau_2}{m_0r_2} S_{2,2} + \frac{1-\cos\tau_3}{m_0r_3} S_{2,3} \right), \\
g^{\phi,r_2} &= \cos\alpha \left(\frac{1-\cos\tau_2}{m_0r_2} S_{2,1} + \frac{1-\cos\tau_1}{m_0r_3} S_{2,3} \right) \\
&\quad - \frac{\cos\alpha\sin\alpha\cos\theta\sin\phi(1-\cos\tau_2)-(\cos\alpha\sin\theta+\sin\alpha\cos\theta\cos\phi)\sin\tau_2}{m_0r_1\sin\theta}, \\
g^{\phi,r_3} &= \cos\alpha \left(\frac{1-\cos\tau_3}{m_0r_1} S_{2,1} + \frac{1-\cos\tau_1}{m_0r_2} S_{2,2} \right) \\
&\quad - \frac{\cos\alpha\sin\alpha\cos\theta\sin\phi(1-\cos\tau_3)-(\cos\alpha\sin\theta+\sin\alpha\cos\theta\cos\phi)\sin\tau_3}{m_0r_1\sin\theta}, \\
g^{\phi,r_4} &= -\frac{\sin\theta(S_{2,1}\cos\phi+\cos\alpha\sin\phi)}{m_1r_1\sin\alpha},
\end{aligned}$$

$$\begin{aligned}
g^{\phi,\alpha} = & \frac{1}{\sin \alpha} \left[\frac{(S_{1,1}-1)S_{2,1}}{m_{1,1}r_1^2} + \frac{S_{1,2}S_{2,2}}{m_{2,2}r_2^2} + \frac{S_{1,3}S_{2,3}}{m_{3,3}r_3^2} + \frac{(S_{1,1}-1)S_{2,2} + S_{1,2}S_{2,1}}{m_0r_1r_2} f(\tau_2) \right. \\
& \left. + \frac{(S_{1,1}-1)S_{2,3} + S_{1,3}S_{2,1}}{m_0r_1r_3} f(\tau_3) + \frac{S_{1,2}S_{2,3} + S_{1,3}S_{2,2}}{m_0r_2r_3} f(\tau_1) \right] \\
& - \frac{1}{\sin \theta} \left[\frac{(S_{1,1}-1)\cos \theta \sin \phi}{m_{1,1}r_1^2} + \frac{S_{1,2}[\cos \theta \sin \phi f(\tau_2) + \cot \alpha \sin \tau_2 (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta)]}{m_0r_1r_2} \right. \\
& \left. + \frac{S_{1,3}[\cos \theta \sin \phi f(\tau_3) + \cot \alpha \sin \tau_3 (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta)]}{m_0r_1r_3} - \frac{(S_{1,1}-1)\sin \phi}{m_1r_1r_4} \right],
\end{aligned}$$

$$\begin{aligned}
g^{\phi,\tau_2} = & \frac{1}{\sin \alpha} \left[\frac{S_{2,1}T_{2,1}}{m_{1,1}r_1^2} + \frac{S_{2,2}T_{2,2}}{m_{2,2}r_2^2} + \frac{S_{2,3}T_{2,3}}{m_{3,3}r_3^2} + \frac{S_{2,1}T_{2,2} + S_{2,2}T_{2,1}}{m_0r_1r_2} f(\tau_2) \right. \\
& \left. + \frac{S_{2,1}T_{2,3} + S_{2,3}T_{2,1}}{m_0r_1r_3} f(\tau_3) + \frac{S_{2,2}T_{2,3} + S_{2,3}T_{2,2}}{m_0r_2r_3} f(\tau_1) \right] - \frac{\cos \theta \sin \phi}{\sin \theta} \left[\frac{T_{2,1}}{m_{1,1}r_1^2} + \frac{T_{2,2}f(\tau_2)}{m_0r_1r_2} + \frac{T_{2,3}f(\tau_3)}{m_0r_1r_3} \right] \\
& - \frac{1}{\sin \alpha \sin \theta} \left[\frac{\cos \alpha \sin \tau_2 (T_{2,2} (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta) + \cos \theta \sin \phi)}{m_0r_1r_2} \right. \\
& \left. + \frac{T_{2,3} \cos \alpha \sin \tau_3 (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta)}{m_0r_1r_3} - \frac{\cos \phi + \sin \alpha \sin \phi T_{2,1}}{m_1r_1r_4} \right] \\
& - \frac{S_{2,3} \cos \alpha}{\sin^2 \alpha} \left[\frac{\sin \tau_2}{m_0r_1r_2} - \frac{\sin \tau_3}{m_0r_1r_3} + \frac{\sin \tau_1}{m_0r_2r_3} \right] - \frac{\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta}{\sin^2 \alpha \sin \theta} \left(\frac{1}{m_{1,1}r_1^2} - \frac{\cos \tau_2}{m_0r_1r_2} \right),
\end{aligned}$$

$$\begin{aligned}
g^{\phi,\tau_3} = & \frac{1}{\sin \alpha} \left[\frac{S_{2,1}T_{3,1}}{m_{1,1}r_1^2} + \frac{S_{2,2}T_{3,2}}{m_{2,2}r_2^2} + \frac{S_{2,3}T_{3,3}}{m_{3,3}r_3^2} + \frac{S_{2,1}T_{3,2} + S_{2,2}T_{3,1}}{m_0r_1r_2} f(\tau_2) \right. \\
& \left. + \frac{S_{2,1}T_{3,3} + S_{2,3}T_{3,1}}{m_0r_1r_3} f(\tau_3) + \frac{S_{2,2}T_{3,3} + S_{2,3}T_{3,2}}{m_0r_2r_3} f(\tau_1) \right] - \frac{\cos \theta \sin \phi}{\sin \theta} \left[\frac{T_{3,1}}{m_{1,1}r_1^2} + \frac{T_{3,2}f(\tau_2)}{m_0r_1r_2} + \frac{T_{3,3}f(\tau_3)}{m_0r_1r_3} \right] \\
& - \frac{1}{\sin \alpha \sin \theta} \left[\frac{T_{3,2} \cos \alpha \sin \tau_2 (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta)}{m_0r_1r_2} \right. \\
& \left. + \frac{\cos \alpha \sin \tau_3 (T_{3,3} (\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta) + \cos \theta \sin \phi)}{m_0r_1r_3} - \frac{\cos \phi + \sin \alpha \sin \phi T_{3,1}}{m_1r_1r_4} \right] \\
& + \frac{S_{2,2} \cos \alpha}{\sin^2 \alpha} \left[\frac{\sin \tau_2}{m_0r_1r_2} - \frac{\sin \tau_3}{m_0r_1r_3} + \frac{\sin \tau_1}{m_0r_2r_3} \right] - \frac{\sin \alpha \cos \theta \cos \phi + \cos \alpha \sin \theta}{\sin^2 \alpha \sin \theta} \left(\frac{1}{m_{1,1}r_1^2} - \frac{\cos \tau_3}{m_0r_1r_3} \right),
\end{aligned}$$

$$\begin{aligned}
g^{\phi,\phi} = & \frac{1}{\sin^2 \alpha} \left(\frac{S_{2,1}^2}{m_{1,1}r_1^2} + \frac{S_{2,2}^2}{m_{2,2}r_2^2} + \frac{S_{2,3}^2}{m_{3,3}r_3^2} + 2 \frac{S_{2,1}S_{2,2}f(\tau_2)}{m_0r_1r_2} + 2 \frac{S_{2,1}S_{2,3}f(\tau_3)}{m_0r_1r_3} + 2 \frac{S_{2,2}S_{2,3}f(\tau_1)}{m_0r_2r_3} \right) \\
& + \frac{1}{\sin^2 \theta m_{4,4}r_4^2} - \frac{2 \cot \theta \sin \phi}{\sin \alpha} \left(\frac{S_{2,1}}{m_{1,1}r_1^2} + \frac{S_{2,2}f(\tau_2)}{m_0r_1r_2} + \frac{S_{2,3}f(\tau_3)}{m_0r_1r_3} \right) \\
& + \left[\frac{\cot^2 \alpha + \cot^2 \theta + 2 \cot \alpha \cot \theta \cos \phi}{m_{1,1}r_1^2} - 2(\cot \alpha \cot \theta \cos \phi + \cot^2 \alpha) \left(\frac{S_{2,2} \sin \tau_2}{m_0r_1r_2} + \frac{S_{2,3} \sin \tau_3}{m_0r_1r_3} \right) \right] \\
& + \frac{2}{m_1r_1r_4 \sin \theta} \left(\frac{S_{2,1} \sin \phi}{\sin \alpha} - \cot \theta - \cot \alpha \cos \phi \right).
\end{aligned}$$

A. 5. The Coriolis tensor involving the top coordinates

$$\begin{aligned}
C_x^{r_4} = & -\frac{S_{2,1} \sin \theta \cos \phi}{m_1r_1}, \quad C_y^{r_4} = \frac{S_{1,1} \sin \theta \cos \phi}{m_1r_1}, \quad C_z^{r_4} = -\frac{(S_{2,1} \cos \alpha \cos \phi + \sin \phi) \sin \theta}{m_1r_1 \sin \alpha}, \\
C_x^\theta = & \frac{S_{2,1} \cos \phi}{m_{1,1}r_1^2} - \frac{S_{2,1} \cos \theta \cos \phi}{m_1r_1r_4} + \frac{S_{2,2} [\cos \phi f(\tau_2) - \cos \alpha \sin \phi \sin \tau_2]}{m_0r_1r_2} \\
& + \frac{S_{2,3} [\cos \phi f(\tau_3) - \cos \alpha \sin \phi \sin \tau_3]}{m_0r_1r_3}, \\
C_y^\theta = & -\frac{S_{1,1} \cos \phi}{m_{1,1}r_1^2} + \frac{S_{1,1} \cos \theta \cos \phi}{m_1r_1r_4} - \frac{S_{1,2} [\cos \phi f(\tau_2) - \cos \alpha \sin \phi \sin \tau_2]}{m_0r_1r_2} \\
& - \frac{S_{1,3} [\cos \phi f(\tau_3) - \cos \alpha \sin \phi \sin \tau_3]}{m_0r_1r_3}, \\
C_z^\theta = & \frac{1}{\sin \alpha} \left[\frac{S_{2,1} \cos \alpha \cos \phi + \sin \phi}{m_{1,1}r_1^2} + \frac{S_{2,2} [\cos \phi f(\tau_2) - \cos \alpha \sin \phi \sin \tau_2] \cos \alpha}{m_0r_1r_2} \right. \\
& \left. + \frac{S_{2,3} [\cos \phi f(\tau_3) - \cos \alpha \sin \phi \sin \tau_3] \cos \alpha}{m_0r_1r_3} - \frac{(S_{2,1} \cos \alpha \cos \phi + \sin \phi) \cos \theta}{m_1r_1r_4} \right], \\
C_x^\phi = & \frac{1}{\sin \alpha} \left(\frac{S_{2,1}^2}{m_{1,1}r_1^2} + \frac{S_{2,2}^2}{m_{2,2}r_2^2} + \frac{S_{2,3}^2}{m_{3,3}r_3^2} + 2 \frac{S_{2,1}S_{2,2}f(\tau_2)}{m_0r_1r_2} + 2 \frac{S_{2,1}S_{2,3}f(\tau_3)}{m_0r_1r_3} + 2 \frac{S_{2,2}S_{2,3}f(\tau_1)}{m_0r_2r_3} \right) \\
& - \frac{\cos^2 \alpha}{\sin \alpha} \left(\frac{S_{2,2} \sin \tau_2}{m_0r_1r_2} + \frac{S_{2,3} \sin \tau_3}{m_0r_1r_3} \right) + \frac{S_{2,1} \sin \phi}{m_1r_1r_4 \sin \theta} \\
& - \frac{\cos \theta}{\sin \theta} \left(\frac{S_{2,1} \sin \phi}{m_{1,1}r_1^2} + \frac{S_{2,2} [\sin \phi f(\tau_2) + \cos \alpha \cos \phi \sin \tau_2]}{m_0r_1r_2} + \frac{S_{2,3} [\sin \phi f(\tau_3) + \cos \alpha \cos \phi \sin \tau_3]}{m_0r_1r_3} \right),
\end{aligned}$$

$$\begin{aligned}
C_y^\phi = & -\frac{1}{\sin \alpha} \left(\frac{S_{2,1}S_{1,1}}{m_{1,1}r_1^2} + \frac{S_{2,2}S_{1,2}}{m_{2,2}r_2^2} + \frac{S_{2,3}S_{1,3}}{m_{3,3}r_3^2} + \frac{S_{2,1}S_{1,2} + S_{1,1}S_{2,2}}{m_0r_1r_2} f(\tau_2) + \frac{S_{1,1}S_{2,3} + S_{2,1}S_{1,3}}{m_0r_1r_3} f(\tau_3) \right. \\
& \left. + \frac{S_{2,2}S_{1,3} + S_{1,2}S_{2,3}}{m_0r_2r_3} f(\tau_1) \right) + \frac{\cos^2 \alpha}{\sin \alpha} \left(\frac{S_{1,2}\sin \tau_2}{m_0r_1r_2} + \frac{S_{1,3}\sin \tau_3}{m_0r_1r_3} \right) - \frac{S_{1,1}\sin \phi}{m_1r_1r_4 \sin \theta} \\
& + \frac{\cos \theta}{\sin \theta} \left(\frac{S_{1,1}\sin \phi}{m_{1,1}r_1^2} + \frac{S_{1,2}[\sin \phi f(\tau_2) + \cos \alpha \cos \phi \sin \tau_2]}{m_0r_1r_2} + \frac{S_{1,3}[\sin \phi f(\tau_3) + \cos \alpha \cos \phi \sin \tau_3]}{m_0r_1r_3} \right), \\
C_z^\phi = & \frac{\cos \alpha}{\sin^2 \alpha} \left(\frac{S_{2,1}^2 + 1}{m_{1,1}r_1^2} + \frac{S_{2,2}^2}{m_{2,2}r_2^2} + \frac{S_{2,3}^2}{m_{3,3}r_3^2} + 2 \frac{S_{2,1}S_{2,2}f(\tau_2)}{m_0r_1r_2} + 2 \frac{S_{2,1}S_{2,3}f(\tau_3)}{m_0r_1r_3} + 2 \frac{S_{2,2}S_{2,3}f(\tau_1)}{m_0r_2r_3} \right) \\
& - \frac{\cos \alpha (1 + \cos^2 \alpha)}{\sin^2 \alpha} \left(\frac{S_{2,2}\sin \tau_2}{m_0r_1r_2} + \frac{S_{2,3}\sin \tau_3}{m_0r_1r_3} \right) + \frac{1}{\sin \alpha \sin \theta} \left(\frac{\cos \theta \cos \phi}{m_{1,1}r_1^2} + \frac{S_{2,1}\cos \alpha \sin \phi - \cos \phi}{m_1r_1r_4} \right) \\
& - \frac{\cos \alpha \cos \theta}{\sin \alpha \sin \theta} \left(\frac{S_{2,1}\sin \phi}{m_{1,1}r_1^2} + \frac{S_{2,2}[\sin \phi f(\tau_2) + \cos \alpha \cos \phi \sin \tau_2]}{m_0r_1r_2} + \frac{S_{2,3}[\sin \phi f(\tau_3) + \cos \alpha \cos \phi \sin \tau_3]}{m_0r_1r_3} \right).
\end{aligned}$$

Here, the functions $f(\tau_i), \chi(\tau_i), \psi(\tau_i)$ are defined for $i=1,2,3$ as follows

$$f(\tau_i) = \sin^2 \alpha + \cos^2 \alpha \cos \tau_i,$$

$$\chi(\tau_i) = 1 - \cos \tau_i + f(\tau_i),$$

$$\psi(\tau_i) = \cot^2 \alpha + \cos \tau_i.$$