

```
In[50]:= ClearAll[E01, E02, E03, F1, F2, F3, F4, F5, F6, F7, F8, F9, Fi1, Fi2, Fi3, Fi4,
    Fi5, Fi6, Fi7, Fi8, Fi9, d, r01, r02, r03, r04, r05, r06, r07, r08, r09]
```

```
(*DEFINICIONES*)
```

```
(*Definicion de matrices de primeros vecinos*)
```

```
Fi1 = Array[F1, {3, 3}];
```

```
Fi2 = Array[F2, {3, 3}];
```

```
Fi3 = Array[F3, {3, 3}];
```

```
(*Definicion de matrices de segundos vecinos*)
```

```
Fi4 = Array[F4, {3, 3}];
```

```
Fi5 = Array[F5, {3, 3}];
```

```
Fi6 = Array[F6, {3, 3}];
```

```
Fi7 = Array[F7, {3, 3}];
```

```
Fi8 = Array[F8, {3, 3}];
```

```
Fi9 = Array[F9, {3, 3}];
```

```
(*Definicion de matrices de rotación de 120° y -120°=240°*)
```

```
Q60 = RotationMatrix[60 Degree, {0, 0, 1}];
```

```
Q90 = RotationMatrix[90 Degree, {0, 0, 1}];
```

```
Q120 = RotationMatrix[120 Degree, {0, 0, 1}];
```

```
Q240 = RotationMatrix[240 Degree, {0, 0, 1}];
```

```
(*Definición de matriz de reflexión en el plano XY:z→-z*)
```

```
Rz = {{1, 0, 0}, {0, 1, 0}, {0, 0, -1}};
```

```
(*Definición de matriz de reflexión en el plano XZ:y→-y*)
```

```
Ry = {{1, 0, 0}, {0, -1, 0}, {0, 0, 1}};
```

```
(*RESOLUCIÓN DE LAS ECUACIONES*)
```

```
(*PRIMEROS VECINOS*)
```

```
(*reflexiones z→-z, y→-y, primer vecino: F1,
reflejado en YZ ha de coincidir consigo mismo, ídem reflejado en XY*)
```

```
Fi1 = Fi1 /. Flatten[Solve[Fi1 == Rz.Fi1.(Transpose[Rz])]];]
```

```
Fi1 = Fi1 /. Flatten[Solve[Fi1 == Ry.Fi1.(Transpose[Ry])]];]
```

```
(* giros, primeros vecinos*)
```

```
Fi2 = Fi2 /. Flatten[Solve[Fi2 == Q240.Fi1.(Transpose[Q240]), {F2[1, 1], F2[1, 2],
    F2[1, 3], F2[2, 1], F2[2, 2], F2[2, 3], F2[3, 1], F2[3, 2], F2[3, 3]}]];]
```

```
Fi3 = Fi3 /. Flatten[Solve[Fi3 == Q120.Fi1.(Transpose[Q120]), {F3[1, 1], F3[1, 2],
    F3[1, 3], F3[2, 1], F3[2, 2], F3[2, 3], F3[3, 1], F3[3, 2], F3[3, 3]}]];]
```

```
TextCell["Fi1="]
```

```
Fi1 // MatrixForm
```

```
TextCell["Fi2="]
```

```
Fi2 // MatrixForm
```

```
TextCell["Fi3="]
```

```
Fi3 // MatrixForm
```

```
(*SEGUNDOS VECINOS*)
```

```
(*En primer lugar, hallamos la expresión general de Fi4*)
```

```
Fi4 = Fi4 /. Flatten[Solve[Fi4 == Rz.Fi4.(Transpose[Rz])]]];
```

```
Fi6 = Fi6 /. Flatten[Solve[Fi6 == Q120.Fi4.(Transpose[Q120]), {F6[1, 1], F6[1, 2],  
F6[1, 3], F6[2, 1], F6[2, 2], F6[2, 3], F6[3, 1], F6[3, 2], F6[3, 3]}]]];
```

```
Fi5 = Fi5 /. Flatten[Solve[Fi5 == Ry.Fi6.(Transpose[Ry]), {F5[1, 1], F5[1, 2],  
F5[1, 3], F5[2, 1], F5[2, 2], F5[2, 3], F5[3, 1], F5[3, 2], F5[3, 3]}]]];
```

```
Fi7 = Fi7 /. Flatten[Solve[Fi7 == Q120.Fi5.(Transpose[Q120]), {F7[1, 1], F7[1, 2],  
F7[1, 3], F7[2, 1], F7[2, 2], F7[2, 3], F7[3, 1], F7[3, 2], F7[3, 3]}]]];
```

```
(*Esta última operación proporciona que  $F7[1,2] = -F4[1,2]$  y  $F7[2,1] = F4[2,1]$   
y como  $F7[1,2] = F4[2,1]$  y  $F7[2,1] = F4[1,2]$  tenemos que  $F4[2,1] = -F4[1,2]$ *)
```

```
Fi4 = Fi4 /. Flatten[F4[2, 1] → -F4[1, 2]]];
```

```
TextCell[" La forma general de Fi4, aplicadas todas las simetrías y condiciones es"]
```

```
TextCell["Fi4="]
```

```
Fi4 // MatrixForm
```

```
(* con lo que ya tenemos Fi7:*)
```

```
Fi7 = Fi7 /. Flatten[F4[2, 1] → -F4[1, 2]]];
```

```
TextCell["Fi7="]
```

```
Fi7 // MatrixForm
```

```
(*Fi6 y Fi8 se hallan aplicando a Fi4 un giro de 120° y -  
120° (alrededor del eje Z) respectivamente:*)
```

```
Fi6 = Fi6 /. Flatten[Solve[Fi6 == Q120.Fi4.(Transpose[Q120]), {F6[1, 1], F6[1, 2],  
F6[1, 3], F6[2, 1], F6[2, 2], F6[2, 3], F6[3, 1], F6[3, 2], F6[3, 3]}]]];
```

```
TextCell["Fi6="]
```

```
Fi6 // MatrixForm
```

```
Fi8 = Fi8 /. Flatten[Solve[Fi8 == Q240.Fi4.(Transpose[Q240]), {F8[1, 1], F8[1, 2],  
F8[1, 3], F8[2, 1], F8[2, 2], F8[2, 3], F8[3, 1], F8[3, 2], F8[3, 3]}]]];
```

```
TextCell["Fi8="]
```

```
Fi8 // MatrixForm
```

```
(*Fi5 y Fi9 se halla haciendo un giro de 120° y -  
120° respectivamente al ya hallado Fi7*)
```

```
Fi5 = Fi5 /. Flatten[Solve[Fi5 == Q240.Fi7.(Transpose[Q240]), {F5[1, 1], F5[1, 2],  
F5[1, 3], F5[2, 1], F5[2, 2], F5[2, 3], F5[3, 1], F5[3, 2], F5[3, 3]}]]];
```

```
TextCell["Fi5="]
```

```
Fi5 // MatrixForm
```

```
Fi9 = Fi9 /. Flatten[Solve[Fi9 == Q120.Fi7.(Transpose[Q120]), {F9[1, 1], F9[1, 2],  
F9[1, 3], F9[2, 1], F9[2, 2], F9[2, 3], F9[3, 1], F9[3, 2], F9[3, 3]}]]];
```

```
TextCell["Fi9="]
```

```
Fi9 // MatrixForm
```

Out[70]= **Fi1=**

Out[71]/MatrixForm=

$$\begin{pmatrix} F1[1, 1] & 0 & 0 \\ 0 & F1[2, 2] & 0 \\ 0 & 0 & F1[3, 3] \end{pmatrix}$$

Out[72]= **Fi2=**

Out[73]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F1[1, 1] + 3 F1[2, 2]) & \frac{1}{4} (\sqrt{3} F1[1, 1] - \sqrt{3} F1[2, 2]) & 0 \\ \frac{1}{4} (\sqrt{3} F1[1, 1] - \sqrt{3} F1[2, 2]) & \frac{1}{4} (3 F1[1, 1] + F1[2, 2]) & 0 \\ 0 & 0 & F1[3, 3] \end{pmatrix}$$

Out[74]= **Fi3=**

Out[75]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F1[1, 1] + 3 F1[2, 2]) & \frac{1}{4} (-\sqrt{3} F1[1, 1] + \sqrt{3} F1[2, 2]) & 0 \\ \frac{1}{4} (-\sqrt{3} F1[1, 1] + \sqrt{3} F1[2, 2]) & \frac{1}{4} (3 F1[1, 1] + F1[2, 2]) & 0 \\ 0 & 0 & F1[3, 3] \end{pmatrix}$$

Out[81]= La forma general de **Fi4**, aplicadas todas las simetrías y condiciones es

Out[82]= **Fi4=**

Out[83]/MatrixForm=

$$\begin{pmatrix} F4[1, 1] & F4[1, 2] & 0 \\ -F4[1, 2] & F4[2, 2] & 0 \\ 0 & 0 & F4[3, 3] \end{pmatrix}$$

Out[85]= **Fi7=**

Out[86]/MatrixForm=

$$\begin{pmatrix} F4[1, 1] & -F4[1, 2] & 0 \\ F4[1, 2] & F4[2, 2] & 0 \\ 0 & 0 & F4[3, 3] \end{pmatrix}$$

Out[88]= **Fi6=**

Out[89]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F4[1, 1] + \sqrt{3} F4[1, 2] + \sqrt{3} F4[2, 1] + 3 F4[2, 2]) & \frac{1}{4} (-\sqrt{3} F4[1, 1] + F4[1, 2] - 3 F4[2, 1]) + \\ \frac{1}{4} (-\sqrt{3} F4[1, 1] - 3 F4[1, 2] + F4[2, 1] + \sqrt{3} F4[2, 2]) & \frac{1}{4} (3 F4[1, 1] - \sqrt{3} F4[1, 2] - \sqrt{3} F4[2, 1] \\ 0 & 0 \end{pmatrix}$$

Out[90]=  $\left\{ \left\{ \frac{1}{4} (F4[1, 1] + 3 F4[2, 2]), \frac{1}{4} (\sqrt{3} F4[1, 1] + 4 F4[1, 2] - \sqrt{3} F4[2, 2]), 0 \right\}, \right.$

$\left. \left\{ \frac{1}{4} (\sqrt{3} F4[1, 1] - 4 F4[1, 2] - \sqrt{3} F4[2, 2]), \frac{1}{4} (3 F4[1, 1] + F4[2, 2]), 0 \right\}, \{0, 0, F4[3, 3]\} \right\}$

Out[91]= **Fi8=**

Out[92]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F4[1, 1] + 3 F4[2, 2]) & \frac{1}{4} (\sqrt{3} F4[1, 1] + 4 F4[1, 2] - \sqrt{3} F4[2, 2]) & 0 \\ \frac{1}{4} (\sqrt{3} F4[1, 1] - 4 F4[1, 2] - \sqrt{3} F4[2, 2]) & \frac{1}{4} (3 F4[1, 1] + F4[2, 2]) & 0 \\ 0 & 0 & F4[3, 3] \end{pmatrix}$$

Out[94]= **Fi5=**

Out[95]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F4[1, 1] + \sqrt{3} F4[1, 2] + \sqrt{3} F4[2, 1] + 3 F4[2, 2]) & \frac{1}{4} (\sqrt{3} F4[1, 1] - F4[1, 2] + 3 F4[2, 1] - \sqrt{3} F4[2, 2]) \\ \frac{1}{4} (\sqrt{3} F4[1, 1] + 3 F4[1, 2] - F4[2, 1] - \sqrt{3} F4[2, 2]) & \frac{1}{4} (3 F4[1, 1] - \sqrt{3} F4[1, 2] - \sqrt{3} F4[2, 1] - F4[2, 2]) \\ 0 & 0 \end{pmatrix}$$

Out[97]= Fi9=

Out[98]/MatrixForm=

$$\begin{pmatrix} \frac{1}{4} (F4[1, 1] + 3 F4[2, 2]) & \frac{1}{4} (-\sqrt{3} F4[1, 1] - 4 F4[1, 2] + \sqrt{3} F4[2, 2]) & 0 \\ \frac{1}{4} (-\sqrt{3} F4[1, 1] + 4 F4[1, 2] + \sqrt{3} F4[2, 2]) & \frac{1}{4} (3 F4[1, 1] + F4[2, 2]) & 0 \\ 0 & 0 & F4[3, 3] \end{pmatrix}$$

In[962]:=

```

ClearAll[d, r01, r02, r03, r04, r05, r06, r07, r08, r09,
  r12, r23, r31, r98, r76, r54, e1, e2, e3, a1, a2, γ1, γ2, δ, θ1, θ2]
(*Definición de matrices de rotación de 120° y -120°=240°*)
Q60 = RotationMatrix[60 Degree, {0, 0, 1}];
Q90 = RotationMatrix[90 Degree, {0, 0, 1}];
Q120 = RotationMatrix[120 Degree, {0, 0, 1}]; T120 = Transpose[Q120];
Q240 = RotationMatrix[240 Degree, {0, 0, 1}];
(*Definición de vectores posición de átomos*)
(*primeros vecinos*)
r01 = {d, 0, 0};
r02 = Q240.r01;
r03 = Q120.r01;
(*segundos vecinos*)
r04 = {0, d √3, 0};
r05 = Q60.r04;
r06 = Q60.r05;
r07 = Q60.r06;
r08 = Q60.r07;
r09 = Q60.r08;

r12 = r02 - r01;
r23 = r03 - r02;
r31 = r01 - r03;
r98 = r08 - r09;
r76 = r06 - r07;
r54 = r04 - r05;
r19 = -r02;
r18 = -r03;
r27 = -r03;
r26 = -r01;
r35 = -r01;
r34 = -r02;

(*primeros vecinos, p.ej.:Eprimeros[r01]*)

Eprimeros = (a1 / (d^2)) Outer[Times, #, #] &;

(*segundos vecinos, p.ej.:Esegundos[r12]*)
Esegundos = (a2 / (3 d^2)) (Outer[Times, #, #]) &;
TEsegundos = (a2 / (3 d^2)) Transpose[(Outer[Times, #, #])] &;

(*angulos en el plano xy, p.ej.: Eangulos[r01,r02]*)
Eangulos = (γ1 / (d^4)) Q90.(Outer[Times, #1, #2]).Transpose[Q90] &;

```

```

TEangulos = ( $\gamma_1 / (d^4)$ ) Transpose[Q90.(Outer[Times, #1, #2]).Transpose[Q90]] &;

(*flexión fuera del plano*)
Eflexion = ( $\gamma_2 / (d^2)$ ) {{0, 0, 0}, {0, 0, 0}, {0, 0, 1}};

(*torsión*)
Etorsion = ( $\delta / (3 * d^2)$ ) {{0, 0, 0}, {0, 0, 0}, {0, 0, 1}};

(*sumamos cada contribución a su matriz psi correspondiente*)

psi[0, 1, 1] =
  Eprimeros[r01] + Esegundos[r12] + Esegundos[r31] + Esegundos[r54] + Esegundos[r76] +
  2 * Eangulos[r01, r01] + Eangulos[r35, r35] + Eangulos[r26, r26] + Eflexion + 4 * Etorsion;
psi[0, 2, 2] = Eprimeros[r02] + Esegundos[r12] + Esegundos[r23] +
  Esegundos[r98] + Esegundos[r54] + 2 * Eangulos[r02, r02] +
  Eangulos[r19, r19] + Eangulos[r34, r34] + Eflexion + 4 * Etorsion;
psi[0, 3, 3] = Eprimeros[r03] + Esegundos[r31] + Esegundos[r23] +
  Esegundos[r98] + Esegundos[r76] + 2 * Eangulos[r03, r03] +
  Eangulos[r18, r18] + Eangulos[r27, r27] + Eflexion + 4 * Etorsion;

psi[0, 1, 2] = -Esegundos[r12] - Eangulos[r01, r02] + Eflexion - Etorsion;
psi[0, 2, 1] = -Esegundos[r12] - TEangulos[r01, r02] + Eflexion - Etorsion;
psi[0, 1, 3] = -Esegundos[r31] - TEangulos[r03, r01] + Eflexion - Etorsion;
psi[0, 3, 1] = -Esegundos[r31] - Eangulos[r03, r01] + Eflexion - Etorsion;
psi[0, 2, 3] = -Esegundos[r23] - Eangulos[r02, r03] + Eflexion - Etorsion;
psi[0, 3, 2] = -Esegundos[r23] - TEangulos[r02, r03] + Eflexion - Etorsion;

psi[-e3, 2, 3] = -Esegundos[r98] - Eangulos[r19, r18] - Etorsion;
psi[e3, 3, 2] = -Esegundos[r98] - TEangulos[r19, r18] - Etorsion;
psi[e2, 1, 2] = -Esegundos[r54] - Eangulos[r35, r34] - Etorsion;
psi[-e2, 2, 1] = -Esegundos[r54] - TEangulos[r35, r34] - Etorsion;
psi[e1, 1, 3] = -Esegundos[r76] - TEangulos[r27, r26] - Etorsion;
psi[-e1, 3, 1] = -Esegundos[r76] - Eangulos[r27, r26] - Etorsion;

psi[-e2, 2, 3] = Etorsion;
psi[e2, 3, 2] = Etorsion;
psi[e2, 1, 3] = Etorsion;
psi[-e2, 3, 1] = Etorsion;
psi[-e1, 3, 2] = Etorsion;
psi[e1, 2, 3] = Etorsion;
psi[e1, 1, 2] = Etorsion;
psi[-e1, 2, 1] = Etorsion;
psi[e3, 1, 2] = Etorsion;
psi[-e3, 2, 1] = Etorsion;
psi[-e3, 1, 3] = Etorsion;
psi[e3, 3, 1] = Etorsion;

psi[e2, 2, 2] = -Etorsion;
psi[-e2, 2, 2] = -Etorsion;
psi[e1, 3, 3] = -Etorsion;
psi[-e1, 3, 3] = -Etorsion;
psi[e1, 1, 1] = -Etorsion;
psi[-e1, 1, 1] = -Etorsion;
psi[e3, 2, 2] = -Etorsion;
psi[-e3, 2, 2] = -Etorsion;
psi[e3, 3, 3] = -Etorsion;
psi[-e3, 3, 3] = -Etorsion;

```

```

psi[e2, 1, 1] = -Etorsion;
psi[-e2, 1, 1] = -Etorsion;

theta = {theta1, theta2};
cero = {0, 0};
e1 = {1, 0};
e2 = {0, 1};
e3 = {-1, 1};
f1 = Exp[-I*theta.#] &;

(*montamos las transformadas de las psi*)

Fpsi11 = psi[0, 1, 1] f1[cero] + psi[e1, 1, 1] f1[e1] +
  psi[-e1, 1, 1] f1[-e1] + psi[e2, 1, 1] f1[e2] + psi[-e2, 1, 1] f1[-e2];

Fpsi22 = psi[0, 2, 2] f1[cero] + psi[e2, 2, 2] f1[e2] +
  psi[-e2, 2, 2] f1[-e2] + psi[e3, 2, 2] f1[e3] + psi[-e3, 2, 2] f1[-e3];

Fpsi33 = psi[0, 3, 3] f1[cero] + psi[e3, 3, 3] f1[e3] +
  psi[-e3, 3, 3] f1[-e3] + psi[e1, 3, 3] f1[e1] + psi[-e1, 3, 3] f1[-e1];

Fpsi12 =
  psi[0, 1, 2] f1[cero] + psi[e2, 1, 2] f1[e2] + psi[e1, 1, 2] f1[e1] + psi[e3, 1, 2] f1[e3];

Fpsi21 = psi[0, 2, 1] f1[cero] +
  psi[-e2, 2, 1] f1[-e2] + psi[-e1, 2, 1] f1[-e1] + psi[-e3, 2, 1] f1[-e3];

Fpsi13 =
  psi[0, 1, 3] f1[cero] + psi[e1, 1, 3] f1[e1] + psi[e2, 1, 3] f1[e2] + psi[-e3, 1, 3] f1[-e3];

Fpsi31 = psi[0, 3, 1] f1[cero] +
  psi[-e1, 3, 1] f1[-e1] + psi[-e2, 3, 1] f1[-e2] + psi[e3, 3, 1] f1[e3];

Fpsi23 = psi[0, 2, 3] f1[cero] +
  psi[-e3, 2, 3] f1[-e3] + psi[-e2, 2, 3] f1[-e2] + psi[e1, 2, 3] f1[e1];

Fpsi32 =
  psi[0, 3, 2] f1[cero] + psi[e3, 3, 2] f1[e3] + psi[e2, 3, 2] f1[e2] + psi[-e1, 3, 2] f1[-e1];

(*montamos la matriz con las transformadas de las psi, Fpsi*)
Fpsi = {{Fpsi11, Fpsi12, Fpsi13}, {Fpsi21, Fpsi22, Fpsi23}, {Fpsi31, Fpsi32, Fpsi33}};

Q = {{1, 1, 1}, {-e^{i theta2}, -1, -e^{i (theta2 - theta1)}}};
(*Definimos CQ como la conjugada de Q*)
CQ = {{1, 1, 1}, {-e^{-i theta2}, -1, -e^{-i (theta2 - theta1)}}};
TCQ = Transpose[CQ];

Ffi11 = Sum[Q[[1, i]] * Fpsi[[i, j]] * TCQ[[j, 1]], {i, 1, 3}, {j, 1, 3}];
Ffi12 = Sum[Q[[1, i]] * Fpsi[[i, j]] * TCQ[[j, 2]], {i, 1, 3}, {j, 1, 3}];
Ffi21 = Sum[Q[[2, i]] * Fpsi[[i, j]] * TCQ[[j, 1]], {i, 1, 3}, {j, 1, 3}];
Ffi22 = Sum[Q[[2, i]] * Fpsi[[i, j]] * TCQ[[j, 2]], {i, 1, 3}, {j, 1, 3}];

(*Deshacemos la transformación para hallar las Fi*)

```

```

f2 = Exp[I * {θ1, θ2}.#] &;
(*primeros vecinos*)
Fi01 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi12 * f2[e2], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi02 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi12 * f2[e3], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi03 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi12 * f2[{0, 0}], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
(*segundos vecinos*)
Fi04 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[e3], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi05 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[-e1], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi06 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[-e2], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi07 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[-e3], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi08 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[e1], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];
Fi09 = (1 / (2 * Pi) ^ 2) * Integrate[Ffi11 * f2[e2], {θ1, -Pi, Pi}, {θ2, -Pi, Pi}];

Simplify[Fi01] // MatrixForm
Simplify[Fi02] // MatrixForm
Simplify[Fi03] // MatrixForm

Fi04 // MatrixForm
Fi05 // MatrixForm
Fi06 // MatrixForm
Fi07 // MatrixForm
Fi08 // MatrixForm
Fi09 // MatrixForm

```

Out[1067]//MatrixForm=

$$\begin{pmatrix} -\alpha_1 & 0 & 0 \\ 0 & -\frac{6\gamma_1}{d^2} & 0 \\ 0 & 0 & -\frac{3\gamma_2}{d^2} \end{pmatrix}$$

Out[1068]//MatrixForm=

$$\begin{pmatrix} -\frac{\alpha_1}{4} - \frac{9\gamma_1}{2d^2} & \frac{\sqrt{3}(d^2\alpha_1 - 6\gamma_1)}{4d^2} & 0 \\ \frac{\sqrt{3}(d^2\alpha_1 - 6\gamma_1)}{4d^2} & \frac{3}{4}\left(-\alpha_1 - \frac{2\gamma_1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{3\gamma_2}{d^2} \end{pmatrix}$$

Out[1069]//MatrixForm=

$$\begin{pmatrix} -\frac{\alpha_1}{4} - \frac{9\gamma_1}{2d^2} & -\frac{\sqrt{3}(d^2\alpha_1 - 6\gamma_1)}{4d^2} & 0 \\ -\frac{\sqrt{3}(d^2\alpha_1 - 6\gamma_1)}{4d^2} & -\frac{3\alpha_1}{4} - \frac{3\gamma_1}{2d^2} & 0 \\ 0 & 0 & -\frac{3\gamma_2}{d^2} \end{pmatrix}$$

Out[1070]//MatrixForm=

$$\begin{pmatrix} \frac{3\gamma_1}{4d^2} & -\frac{\sqrt{3}\gamma_1}{4d^2} & 0 \\ \frac{\sqrt{3}\gamma_1}{4d^2} & -\frac{4d^2\alpha_2 + \gamma_1}{4d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1071]//MatrixForm=

$$\begin{pmatrix} -\frac{3\alpha_2}{4} & \frac{\sqrt{3}(d^2\alpha_2 + 2\gamma_1)}{4d^2} & 0 \\ \frac{\sqrt{3}\alpha_2}{4} & \frac{1}{4}\left(-\alpha_2 + \frac{2\gamma_1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1072]//MatrixForm=

$$\begin{pmatrix} -\frac{3\alpha 2}{4} & -\frac{\sqrt{3}(d^2\alpha 2+2\gamma 1)}{4d^2} & 0 \\ -\frac{\sqrt{3}\alpha 2}{4} & \frac{1}{4}\left(-\alpha 2+\frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1073]//MatrixForm=

$$\begin{pmatrix} \frac{3\gamma 1}{4d^2} & \frac{\sqrt{3}\gamma 1}{4d^2} & 0 \\ -\frac{\sqrt{3}\gamma 1}{4d^2} & -\frac{4d^2\alpha 2+\gamma 1}{4d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1074]//MatrixForm=

$$\begin{pmatrix} -\frac{3\alpha 2}{4} & \frac{\sqrt{3}\alpha 2}{4} & 0 \\ \frac{\sqrt{3}(d^2\alpha 2+2\gamma 1)}{4d^2} & \frac{1}{4}\left(-\alpha 2+\frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1075]//MatrixForm=

$$\begin{pmatrix} -\frac{3\alpha 2}{4} & -\frac{\sqrt{3}\alpha 2}{4} & 0 \\ -\frac{\sqrt{3}(d^2\alpha 2+2\gamma 1)}{4d^2} & \frac{1}{4}\left(-\alpha 2+\frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

In[868]:= **Fi00 = Simplify[-(Fi01 + Fi02 + Fi03 + Fi04 + Fi05 + Fi06 + Fi07 + Fi08 + Fi09)] // MatrixForm**

Out[868]//MatrixForm=

$$\begin{pmatrix} \frac{3}{2}\left(\alpha 1+2\alpha 2+\frac{5\gamma 1}{d^2}\right) & 0 & 0 \\ 0 & \frac{3}{2}\left(\alpha 1+2\alpha 2+\frac{5\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & \frac{9\gamma 2+2\delta}{d^2} \end{pmatrix}$$

In[1076]:=

```

TextCell["psi[0,1,1]="]
psi[0, 1, 1] // MatrixForm
TextCell["psi[0,2,2]="]
psi[0, 2, 2] // MatrixForm
TextCell["psi[0,3,3]="]
psi[0, 3, 3] // MatrixForm
TextCell["psi[0,1,2]="]
psi[0, 1, 2] // MatrixForm
TextCell["psi[0,2,1]="]
psi[0, 2, 1] // MatrixForm
TextCell["psi[0,1,3]="]
psi[0, 1, 3] // MatrixForm
TextCell["psi[0,3,1]="]
psi[0, 3, 1] // MatrixForm;
TextCell["psi[0,2,3]="]
psi[0, 2, 3] // MatrixForm
TextCell["psi[0,3,2]="]
psi[0, 3, 2] // MatrixForm
TextCell["psi[0,3,2]="]
psi[-ε3, 2, 3] // MatrixForm
TextCell["psi[-ε3,2,3]="]
psi[ε3, 3, 2] // MatrixForm
TextCell["psi[ε2,1,2]="]

```



```

psi[e2, 1, 2] // MatrixForm
TextCell["psi[-e2,2,1]="]
psi[-e2, 2, 1] // MatrixForm
TextCell["psi[e1,1,3]="]
psi[e1, 1, 3] // MatrixForm
TextCell["psi[-e1,3,1]="]
psi[-e1, 3, 1] // MatrixForm
TextCell["psi[-e2,2,3]="]
psi[-e2, 2, 3] // MatrixForm
TextCell["psi[e2,3,2]="]
psi[e2, 3, 2] // MatrixForm
TextCell["psi[e2,1,3]="]
psi[e2, 1, 3] // MatrixForm
TextCell["psi[-e2,3,1]="]
psi[-e2, 3, 1] // MatrixForm
TextCell["psi[-e1,3,2]="]
psi[-e1, 3, 2] // MatrixForm
TextCell["psi[e1,2,3]="]
psi[e1, 2, 3] // MatrixForm
TextCell["psi[e1,1,2]="]
psi[e1, 1, 2] // MatrixForm
TextCell["psi[-e1,2,1]="]
psi[-e1, 2, 1] // MatrixForm
TextCell["psi[e3,1,2]9="]
psi[e3, 1, 2] // MatrixForm
TextCell["[-e3,2,1]="]
psi[-e3, 2, 1] // MatrixForm
TextCell["psi[-e3,1,3]="]
psi[-e3, 1, 3] // MatrixForm;
TextCell["psi[e3,3,1]="]
psi[e3, 3, 1] // MatrixForm
TextCell["psi[e2,2,2]="]
psi[e2, 2, 2] // MatrixForm
TextCell["psi[-e2,2,2]="]
psi[-e2, 2, 2] // MatrixForm
TextCell["psi[e1,3,3]="]
psi[e1, 3, 3] // MatrixForm
TextCell["psi[-e1,3,3]="]
psi[-e1, 3, 3] // MatrixForm
TextCell["psi[e1,1,1]="]
psi[e1, 1, 1] // MatrixForm
TextCell["psi[-e1,1,1]="]
psi[-e1, 1, 1] // MatrixForm
TextCell["psi[e3,2,2]="]
psi[e3, 2, 2] // MatrixForm
TextCell["si[-e3,2,2]="]
psi[-e3, 2, 2] // MatrixForm
TextCell["psi[e3,3,3]="]
psi[e3, 3, 3] // MatrixForm
TextCell["psi[-e3,3,3]="]
psi[-e3, 3, 3] // MatrixForm
TextCell["psi[e2,1,1]="]
psi[e2, 1, 1] // MatrixForm
TextCell["psi[-e2,1,1]="]
psi[-e2, 1, 1] // MatrixForm

```

Out[1076]= psi[0,1,1]=

Out[1077]//MatrixForm=

$$\begin{pmatrix} \alpha 1 + 3 \alpha 2 & 0 & 0 \\ 0 & \alpha 2 + \frac{4 \gamma 1}{d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} + \frac{4 \delta}{3 d^2} \end{pmatrix}$$

Out[1078]= **psi**[0,2,2]=

Out[1079]//MatrixForm=

$$\begin{pmatrix} \frac{\alpha 1}{4} + \frac{3 \alpha 2}{2} + \frac{3 \gamma 1}{d^2} & \frac{\sqrt{3} \alpha 1}{4} + \frac{\sqrt{3} \alpha 2}{2} - \frac{\sqrt{3} \gamma 1}{d^2} & 0 \\ \frac{\sqrt{3} \alpha 1}{4} + \frac{\sqrt{3} \alpha 2}{2} - \frac{\sqrt{3} \gamma 1}{d^2} & \frac{3 \alpha 1}{4} + \frac{5 \alpha 2}{2} + \frac{\gamma 1}{d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} + \frac{4 \delta}{3 d^2} \end{pmatrix}$$

Out[1080]= **psi**[0,3,3]=

Out[1081]//MatrixForm=

$$\begin{pmatrix} \frac{\alpha 1}{4} + \frac{3 \alpha 2}{2} + \frac{3 \gamma 1}{d^2} & -\frac{\sqrt{3} \alpha 1}{4} - \frac{\sqrt{3} \alpha 2}{2} + \frac{\sqrt{3} \gamma 1}{d^2} & 0 \\ -\frac{\sqrt{3} \alpha 1}{4} - \frac{\sqrt{3} \alpha 2}{2} + \frac{\sqrt{3} \gamma 1}{d^2} & \frac{3 \alpha 1}{4} + \frac{5 \alpha 2}{2} + \frac{\gamma 1}{d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} + \frac{4 \delta}{3 d^2} \end{pmatrix}$$

Out[1082]= **psi**[0,1,2]=

Out[1083]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha 2}{4} & -\frac{\sqrt{3} \alpha 2}{4} & 0 \\ -\frac{\sqrt{3} \alpha 2}{4} - \frac{\sqrt{3} \gamma 1}{2 d^2} & -\frac{\alpha 2}{4} + \frac{\gamma 1}{2 d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} - \frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1084]= **psi**[0,2,1]=

Out[1085]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha 2}{4} & -\frac{\sqrt{3} \alpha 2}{4} - \frac{\sqrt{3} \gamma 1}{2 d^2} & 0 \\ -\frac{\sqrt{3} \alpha 2}{4} - \frac{\alpha 2}{4} + \frac{\gamma 1}{2 d^2} & 0 & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} - \frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1086]= **psi**[0,1,3]=

Out[1087]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha 2}{4} & \frac{\sqrt{3} \alpha 2}{4} & 0 \\ \frac{\sqrt{3} \alpha 2}{4} + \frac{\sqrt{3} \gamma 1}{2 d^2} & -\frac{\alpha 2}{4} + \frac{\gamma 1}{2 d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} - \frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1088]= **psi**[0,3,1]=Out[1090]= **psi**[0,2,3]=

Out[1091]//MatrixForm=

$$\begin{pmatrix} \frac{3 \gamma 1}{4 d^2} & \frac{\sqrt{3} \gamma 1}{4 d^2} & 0 \\ -\frac{\sqrt{3} \gamma 1}{4 d^2} & -\alpha 2 - \frac{\gamma 1}{4 d^2} & 0 \\ 0 & 0 & \frac{\gamma 2}{d^2} - \frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1092]= **psi**[0,3,2]=

Out[1093]//MatrixForm=

$$\begin{pmatrix} \frac{3 \gamma_1}{4 d^2} & -\frac{\sqrt{3} \gamma_1}{4 d^2} & 0 \\ \frac{\sqrt{3} \gamma_1}{4 d^2} & -\alpha_2 - \frac{\gamma_1}{4 d^2} & 0 \\ 0 & 0 & \frac{\gamma_2}{d^2} - \frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1094]= **psi**[0,3,2]=

Out[1095]//MatrixForm=

$$\begin{pmatrix} \frac{3 \gamma_1}{4 d^2} & \frac{\sqrt{3} \gamma_1}{4 d^2} & 0 \\ -\frac{\sqrt{3} \gamma_1}{4 d^2} & -\alpha_2 - \frac{\gamma_1}{4 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1096]= **psi**[-ε3,2,3]=

Out[1097]//MatrixForm=

$$\begin{pmatrix} \frac{3 \gamma_1}{4 d^2} & -\frac{\sqrt{3} \gamma_1}{4 d^2} & 0 \\ \frac{\sqrt{3} \gamma_1}{4 d^2} & -\alpha_2 - \frac{\gamma_1}{4 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1098]= **psi**[ε2,1,2]=

Out[1099]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha_2}{4} & -\frac{\sqrt{3} \alpha_2}{4} & 0 \\ -\frac{\sqrt{3} \alpha_2}{4} - \frac{\sqrt{3} \gamma_1}{2 d^2} & -\frac{\alpha_2}{4} + \frac{\gamma_1}{2 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1100]= **psi**[-ε2,2,1]=

Out[1101]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha_2}{4} & -\frac{\sqrt{3} \alpha_2}{4} - \frac{\sqrt{3} \gamma_1}{2 d^2} & 0 \\ -\frac{\sqrt{3} \alpha_2}{4} & -\frac{\alpha_2}{4} + \frac{\gamma_1}{2 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1102]= **psi**[ε1,1,3]=

Out[1103]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha_2}{4} & \frac{\sqrt{3} \alpha_2}{4} & 0 \\ \frac{\sqrt{3} \alpha_2}{4} + \frac{\sqrt{3} \gamma_1}{2 d^2} & -\frac{\alpha_2}{4} + \frac{\gamma_1}{2 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1104]= **psi**[-ε1,3,1]=

Out[1105]//MatrixForm=

$$\begin{pmatrix} -\frac{3 \alpha_2}{4} & \frac{\sqrt{3} \alpha_2}{4} + \frac{\sqrt{3} \gamma_1}{2 d^2} & 0 \\ \frac{\sqrt{3} \alpha_2}{4} & -\frac{\alpha_2}{4} + \frac{\gamma_1}{2 d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3 d^2} \end{pmatrix}$$

Out[1106]= **psi**[-ε2,2,3]=

Out[1107]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1108]= **psi** [€2, 3, 2] =

Out[1109]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1110]= **psi** [€2, 1, 3] =

Out[1111]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1112]= **psi** [-€2, 3, 1] =

Out[1113]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1114]= **psi** [-€1, 3, 2] =

Out[1115]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1116]= **psi** [€1, 2, 3] =

Out[1117]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1118]= **psi** [€1, 1, 2] =

Out[1119]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1120]= **psi** [-€1, 2, 1] =

Out[1121]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1122]= **psi** [€3, 1, 2] 9=

Out[1123]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3a^2} \end{pmatrix}$$

Out[1124]=  $[-\epsilon 3, 2, 1] =$

Out[1125]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3d^2} \end{pmatrix}$$

Out[1126]=  $\text{psi}[-\epsilon 3, 1, 3] =$

Out[1128]=  $\text{psi}[\epsilon 3, 3, 1] =$

Out[1129]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\delta}{3d^2} \end{pmatrix}$$

Out[1130]=  $\text{psi}[\epsilon 2, 2, 2] =$

Out[1131]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1132]=  $\text{psi}[-\epsilon 2, 2, 2] =$

Out[1133]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1134]=  $\text{psi}[\epsilon 1, 3, 3] =$

Out[1135]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1136]=  $\text{psi}[-\epsilon 1, 3, 3] =$

Out[1137]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1138]=  $\text{psi}[\epsilon 1, 1, 1] =$

Out[1139]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1140]=  $\text{psi}[-\epsilon 1, 1, 1] =$

Out[1141]/MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix}$$

Out[1142]=  $\text{psi}[\epsilon 3, 2, 2] =$

Out[1143]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

Out[1144]= **si** [- $\epsilon$ 3, 2, 2] =

Out[1145]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

Out[1146]= **psi** [ $\epsilon$ 3, 3, 3] =

Out[1147]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

Out[1148]= **psi** [- $\epsilon$ 3, 3, 3] =

Out[1149]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

Out[1150]= **psi** [ $\epsilon$ 2, 1, 1] =

Out[1151]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

Out[1152]= **psi** [- $\epsilon$ 2, 1, 1] =

Out[1153]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\delta}{3a^2} \end{pmatrix}$$

In[869]:=

```
(*distancia interatómica en grafeno*)
d = 1.42 * 10^(-10);
(*constantes de Aizawa en el sistema métrico*)
 $\alpha$ 1 = 7.28 * 10^6;
 $\alpha$ 2 = 1.24 * 10^6;
 $\gamma$ 1 = 8.31 * 10^(-19);
 $\gamma$ 2 = 3.38 * 10^(-19);
 $\delta$  = 3.17 * 10^(-19);
```

Simplify[Fi01] // MatrixForm

Simplify[Fi02] // MatrixForm

Simplify[Fi03] // MatrixForm

Fi04 // MatrixForm

Fi05 // MatrixForm

Fi06 // MatrixForm

Fi07 // MatrixForm

Fi08 // MatrixForm

Fi09 // MatrixForm

Out[875]//MatrixForm=

$$\begin{pmatrix} -7.28 \times 10^6 & 0 & 0 \\ 0 & -247.272 & 0 \\ 0 & 0 & -50.2876 \end{pmatrix}$$

Out[876]//MatrixForm=

$$\begin{pmatrix} -1.82019 \times 10^6 & 3.15223 \times 10^6 & 0 \\ 3.15223 \times 10^6 & -5.46006 \times 10^6 & 0 \\ 0 & 0 & -50.2876 \end{pmatrix}$$

Out[877]//MatrixForm=

$$\begin{pmatrix} -1.82019 \times 10^6 & -3.15223 \times 10^6 & 0 \\ -3.15223 \times 10^6 & -5.46006 \times 10^6 & 0 \\ 0 & 0 & -50.2876 \end{pmatrix}$$

Out[878]//MatrixForm=

$$\begin{pmatrix} 30.909 & -17.8453 & 0 \\ 17.8453 & -1.24001 \times 10^6 & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$

Out[879]//MatrixForm=

$$\begin{pmatrix} -930\,000. & 536\,971. & 0 \\ 536\,936. & -309\,979. & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$

Out[880]//MatrixForm=

$$\begin{pmatrix} -930\,000. & -536\,971. & 0 \\ -536\,936. & -309\,979. & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$

Out[881]//MatrixForm=

$$\begin{pmatrix} 30.909 & 17.8453 & 0 \\ -17.8453 & -1.24001 \times 10^6 & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$

Out[882]//MatrixForm=

$$\begin{pmatrix} -930\,000. & 536\,936. & 0 \\ 536\,971. & -309\,979. & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$

Out[883]//MatrixForm=

$$\begin{pmatrix} -930\,000. & -536\,936. & 0 \\ -536\,971. & -309\,979. & 0 \\ 0 & 0 & -5.24036 \end{pmatrix}$$