Figures and calculations to the paper *Rigorously proven chaos in chemical kinetics* by M. Susits and J. Tóth

Preparations

In[198]:=
```
SetDirectory[NotebookDirectory[]];
SetOptions[#, AxesStyle → Arrowheads[Automatic]] & /@
  {ContourPlot, DateListPlot, Plot, ListLinePlot, ListPlot,
   ListLogPlot, LogLinearPlot, LogPlot, ParametricPlot, Plot3D,
   RegionPlot, ComplexListPlot, ComplexPlot, DateListPlot};
SetOptions[GraphPlot, DirectedEdges → True, VertexLabels → All];
Get["FormalReactionKinetics/src/ReactionKinetics.wl"];
```

```
ReactionKinetics Version 1.0 [July 13, 2018] using
  Mathematica Version 13.0.0 for Microsoft Windows (64-bit) (December 3,
  2021) (Version 13., Release 0) loaded 02 March 2024 at 15:43 TimeZone
GNU General Public License (GPLv3) Terms Apply.
```

```
Please report any issues, comments, complaint related to ReactionKinetics at
jtoth@math.bme.hu, nagyal@math.bme.hu or dpapp@iems.northwestern.edu
```

Set: Symbol $ReactionKineticsPackageLoaded is Protected.

General: Further output of Set::wrsym will be suppressed during this calculation.

In[202]:=
```
ClearAll[cm, figurexp, gl, H, extent];
cm = 72 / 2.54 ;
(*figurexp[filename_,picturename_]:=Export[
  "d:\\Kollegak\\GasparVilmos\\Chaos\\Figures\\"<>filename<>".png",picturename]*)
figurexp[filename_, picturename_] := Export["Figures\\" <> filename <> ".pdf",
   Show[picturename, ImageSize → 10 cm], ImageResolution → 300];
gl = {"BipartiteEmbedding", "CircularEmbedding", "CircularMultipartiteEmbedding",
   "DiscreteSpiralEmbedding", "GridEmbedding", "LinearEmbedding",
   "MultipartiteEmbedding", "SpiralEmbedding", "StarEmbedding", "BalloonEmbedding",
   "RadialEmbedding", "LayeredDigraphEmbedding", "LayeredEmbedding",
   "HighDimensionalEmbedding", "PlanarEmbedding", "SpectralEmbedding",
   "SpringElectricalEmbedding", "SpringEmbedding", "TutteEmbedding"};
```

In[206]:=
```
sheq[rhs_, shift_, vars_] := rhs /. Thread[vars → vars - shift];
shini[orig_, sh_] := Thread[First /@ orig == ((Last /@ orig) + sh)];
sami[orig_, mult_ : x[t] × y[t] × z[t]] :=
  Expand[Thread[First /@ orig == ((Last /@ orig) mult)]];
mester[param_, orig_, ini_, name_, shift_ : {0, 0, 0}, Tlow_ : 0, Tup_ : 120, h_ : 0.01,
   pr_ : All, PP_ : 244, imp_ : {{30, 30}, {30, 30}}] := Module[{nds, transformed},
   Column[{param, orig, ini}];
   nds = NDSolveValue[equ = Join[orig, ini] /. param, {x[t], y[t], z[t]}, {t, Tlow, Tup},
     Method → {"StiffnessSwitching", Method → {"ExplicitRungeKutta", Automatic}},
     AccuracyGoal → 5, PrecisionGoal → 4];
   traj = ParametricPlot3D[nds, {t, Tlow, Tup}, PlotPoints → PP,
     Boxed → False, AxesLabel → {x, y, z}, PlotRange → pr];
   sol = Plot[Evaluate[nds], {t, 0, Tup}, PlotPoints → Round[PP / 10], AxesLabel →
      {t, "X,Y,Z"}, AxesOrigin → {0, 0}, PlotLabels → {X, Y, Z}, ImagePadding → imp];
   sol1 = Plot[Evaluate[nds[[1]]], {t, Tlow, Tup}, PlotPoints → Round[PP / 10],
     AxesLabel → {t, "X"}, PlotLabels → {X}, ImagePadding → imp];
   fm = Quiet[FindMinimum[#, {t, 0, Tup}] & /@ nds];
nm = (*Quiet[NMinimize[{#,Tlow≤t<Tup},t]&/@nds]*)
    NMinimize[{#, Tlow ≤ t < Tup}, t] & /@ nds;
   min = Flatten[MinimalBy[Table[{t, #}, {t, Tlow, Tup, h}], Last] & /@ nds, 1];
   results = Grid[
     {{traj, sol, sol1}, {figurexp[name <> "traj", traj], figurexp[name <> "sol", sol],
       figurexp[name <> "sol1", sol1]}, min, Join[orig, ini] /. param}]];
```

I. Introduction

II. Chaos in chemical kinetic experiments and models

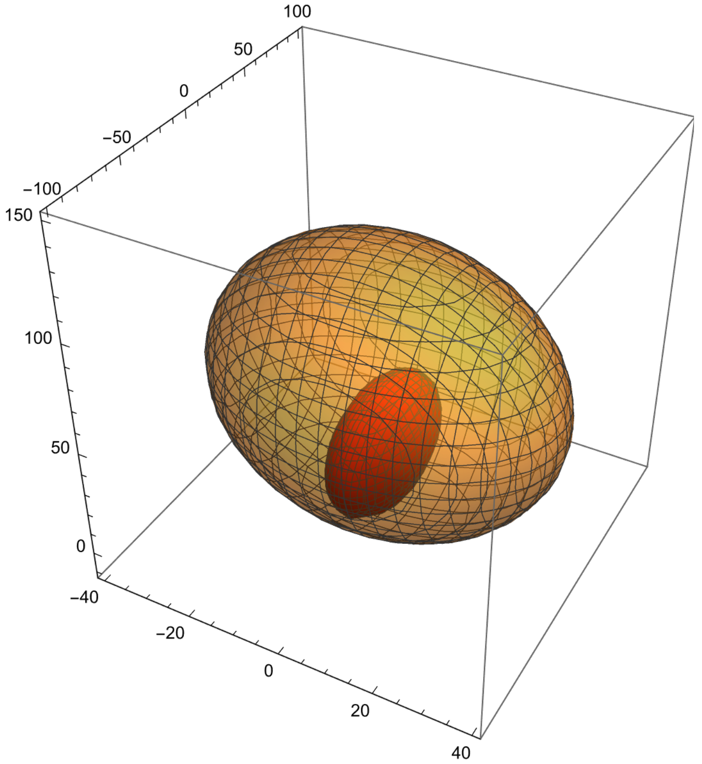
III. Rigorously proven chaos in formal kinetic models

A. The Lorenz System

1. Trapping region of the Lorenz system

In[210]:=
```
param = {σ → 10, ρ → 28, β → 8 / 3};
eD = y^2 + β (z - ρ)^2 + x^2 ρ == β ρ^2 /. param;
eE = x^2 ρ + y^2 σ + (z - 2 ρ)^2 σ /. param;
d = ContourPlot3D[28 x^2 + y^2 + 8/3 (-28 + z)^2 == 6272/3,
    {x, -40, 40}, {y, -100, 100}, {z, -10, 150}, ContourStyle → Red];
e = ContourPlot3D[28 x^2 + 10 y^2 + 10 (-56 + z)^2 == 200^2, {x, -40, 40},
    {y, -100, 100}, {z, -10, 150}, ContourStyle → Opacity[0.5]];
Show[d, e]
```

Out[215]=

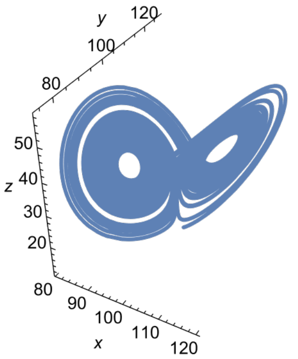


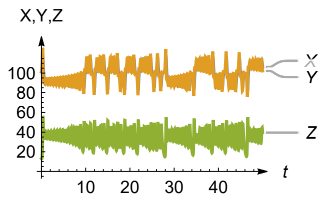
2. Transforming the Lorenz system

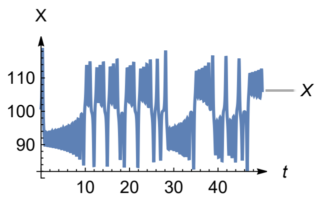
Original and shifted trajectories

In[216]:=
```
param = {σ → 10, ρ → 28, β → 8 / 3};
orig =
  {x'[t] == σ (y[t] - x[t]), y'[t] == x[t] (ρ - z[t]) - y[t], z'[t] == x[t] × y[t] - β z[t]};
shift = {100, 100, 10};
ini = {x[0] == 1, y[0] == 2, z[0] == 3};
mester[param, sheq[orig, shift, {x[t], y[t], z[t]}],
 shini[ini, shift], "LorenzShifted", shift, 0, 50]
```

Out[220]=





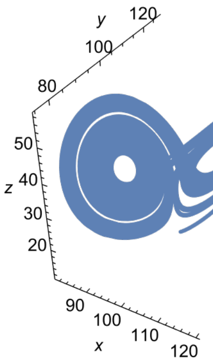


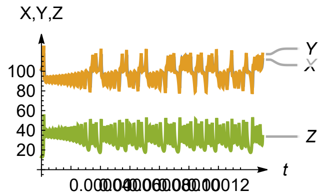

```
Figures\LorenzShiftedtraj.pdf    Figures\LorenzShiftedsol.pdf    Figures\LorenzShiftedsol1.pdf
{46.6, 81.8289}                  {46.55, 75.5208}                {0.06, 12.7884}
```

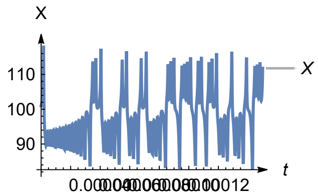
$x'[t] == 10\,(-x[t] + y[t])$ $\quad$ $y'[t] == 100 - y[t] + (-100 + x[t])\,(38 - z[t])$ $\quad$ $z'[t] == (-100 + x[t])\,(-100 + y[t]) - \frac{8}{3}\,(-10 + z[t])$ $\quad$ $x[0] == 101$

Shifted and multiplied trajectories

In[221]:=
```
mester[param, sami[sheq[orig, shift, {x[t], y[t], z[t]}], x[t] × y[t] × z[t]],
 shini[ini, shift], "LorenzMultiplied", shift, 0, 0.00015]
```







Out[221]=

Figures\LorenzMultipliedtraj.pdf	Figures\LorenzMultipliedsol.pdf	Figures\LorenzMultipliedsol1.pdf
{0., 101.}	{0., 102.}	{0., 13.}

$$x'[t] == -10\, x[t]^2\, y[t] \times z[t] + 10\, x[t]\, y[t]^2\, z[t]$$

$$y'[t] == -3700\, x[t] \times y[t] \times z[t] + 38\, x[t]^2\, y[t] \times z[t] - x[t]\, y[t]^2\, z[t] + 100\, x[t] \times y[t]\, z[t]^2 - x[t]^2\, y[t]\, z[t]^2$$

$$z'[t] == \frac{30080}{3}\, x[t] \times y[t] \times z[t] - 100\, x[t]^2\, y[t] \times z[t] - 100\, x[t]\, y[t]^2\, z[t] + x[t]^2\, y[t]^2\, z[t] - \frac{8}{3}\, x[t] \times y[t]\, z[t]^2$$

$$x[0] == 101$$

3. A realization of the transformed Lorenz system

In[222]:=
```
lrhs = (#[[2]] & /@ sheq[orig, shift, {x[t], y[t], z[t]}]);
lrhs2 = lrhs /. param /. {x[t] → x, y[t] → y, z[t] → z};
lrhs3 = y z # & /@ lrhs2;
lorenzCanonic = CanonicReaction[lrhs3, {x, y, z}];
lorenzCanonic // MatrixForm
```

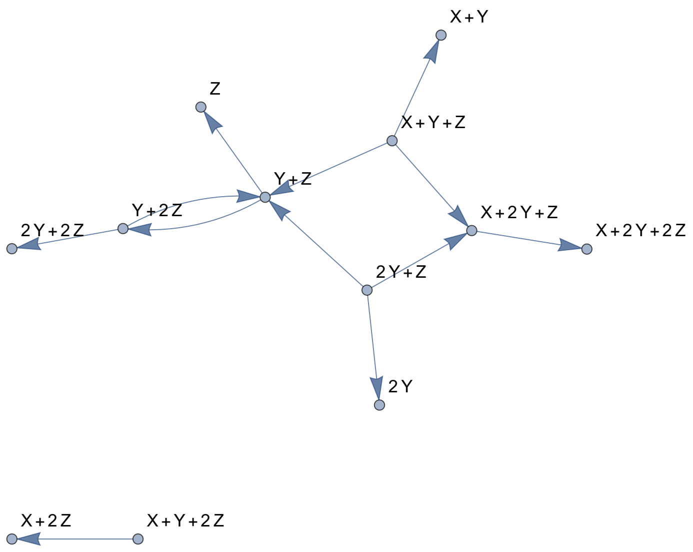
Out[226]//MatrixForm=

$$\begin{pmatrix} 2Y+Z \to X+2Y+Z & 10 \\ X+Y+Z \to Y+Z & 10 \\ X+Y+Z \to X+2Y+Z & 38 \\ Y+2Z \to 2Y+2Z & 100 \\ X+Y+2Z \to X+2Z & 1 \\ 2Y+Z \to Y+Z & 1 \\ Y+Z \to Z & 3700 \\ X+2Y+Z \to X+2Y+2Z & 1 \\ Y+Z \to Y+2Z & \frac{30080}{3} \\ X+Y+Z \to X+Y & 100 \\ 2Y+Z \to 2Y & 100 \\ Y+2Z \to Y+Z & \frac{8}{3} \end{pmatrix}$$

The FHJ graph of the Lorenz reaction

In[227]:=
```
lorenzCanonicReactions = First /@ lorenzCanonic;
GraphPlot[FHJGraph[lorenzCanonicReactions], VertexLabels → "Name"]
```

Out[228]=



B. The Chen System

1. Trapping region of the Chen system

In[229]:=

$$\text{ChenA}[a\_ : 35, b\_ : 3, c\_ : 28] := \frac{a}{b}$$

$$\text{ChenB}[a\_ : 35, b\_ : 3, c\_ : 28] := \frac{a - c}{b} - 1$$

$$\text{ChenC}[a\_ : 35, b\_ : 3, c\_ : 28] := \frac{c + b}{a}$$

$$\text{ChenD}[a\_ : 35, b\_ : 3, c\_ : 28] := 1 + 2\frac{c}{b} - \frac{c + b}{a}$$

```
In[233]:= ChenU0[z0_, a_ : 35, b_ : 3, c_ : 28] :=
  ((ChenA[a, b, c] × ChenB[a, b, c] - ChenA[a, b, c] - ChenB[a, b, c] z0) /
      (ChenA[a, b, c] × ChenC[a, b, c]))^2 / 2
ChenU0Min[z0_, a_ : 35, b_ : 3, c_ : 28] := (ChenD[a, b, c] - z0)^2 / 2
ChenStep[zu_, a_ : 35, b_ : 3, c_ : 28] := Block[{zi = zu[[1]], ui = zu[[2]], zn, un},
   zn = zi (1 + ChenB[a, b, c] / (ChenA[a, b, c] × ChenC[a, b, c])) - (ChenB[a, b, c] - 1) / ChenC[a, b, c];
   un = (ChenA[a, b, c] - zn) / (ChenA[a, b, c] - zi) (ui - (zi - zn)^2 / 2);
   {zn, un}];
ZiUi[z0_, u0times_ : 0, a_ : 35, b_ : 3, c_ : 28] :=
 NestWhileList[ChenStep[#, a, b, c] &, {z0, ChenU0Min[z0, a, b, c] * (1 + u0times)},
  #[[2]] > 1/2 ((ChenB[a, b, c] - 1) / ChenC[a, b, c] - #[[1]] ChenB[a, b, c] / (ChenA[a, b, c] × ChenC[a, b, c]))^2 &]

In[237]:= EiEquation[zi_, u_, a_ : 35, b_ : 3, c_ : 28] := 2 u == (ChenA[a, b, c] - zi) / ChenA[a, b, c] x^2 + y^2 + (z - zi)^2;
EiEquations[z0_, u0times_ : 0, a_ : 35, b_ : 3, c_ : 28] :=
  EiEquation[#[[1]], #[[2]], a, b, c] & /@ ZiUi[z0, u0times, a, b, c];
PlotEllipsoids[z0_, u0times_ : 0, a_ : 35, b_ : 3, c_ : 28] :=
  Module[{equations, ellipsoids},
   equations = EiEquations[z0, u0times, a, b, c];
   ellipsoids = ContourPlot3D[Evaluate[#], {x, -50, 50},
       {y, -100, 100}, {z, -300, 30}, ContourStyle → Opacity[0.5],
       PlotPoints → 100, Mesh → None, Boxed → False, Axes → False] & /@ equations;
   Show@ellipsoids
  ];
```

In[240]:=
```
PlotEllipsoids[0]
```

Out[240]=

2. The transformed Chen system and its realization

Sufficient shift

In[241]:=
```
ZUToCoordianteRanges[z_, u_, a_ : 35, b_ : 3, c_ : 28] :=
  {{-Sqrt[ChenA[a, b, c] / (ChenA[a, b, c] - z) 2 u], Sqrt[ChenA[a, b, c] / (ChenA[a, b, c] - z) 2 u]},
   {-Sqrt[2 u], Sqrt[2 u]}, {-Sqrt[2 u] + z, Sqrt[2 u] + z}}
ChenRectangle[z0_, u0times_ : 0, a_ : 35, b_ : 3, c_ : 28] :=
  Min /@ (((Min /@ ZUToCoordianteRanges[#[[1]], #[[2]], a, b, c] &) /@
       ZiUi[z0, u0times, a, b, c]) // Transpose)
```

In[243]:=
```
N[ChenRectangle[0]]
```

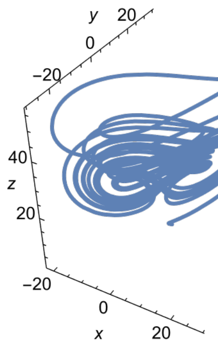
Out[243]= {-18.781, -48.1914, -271.508}

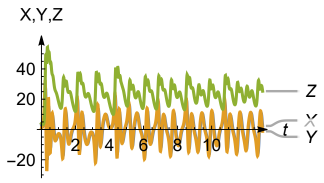
Trajectories

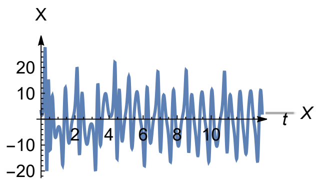
Original

In[244]:=
```
ClearAll[oaram, orig, ini];
param = {a → 35, b → 3, c → 28};
orig = {x'[t] == a (y[t] - x[t]),
   y'[t] == (c - a) x[t] + c y[t] - x[t] × z[t], z'[t] == x[t] × y[t] - b z[t]};
ini = {x[0] == 3, y[0] == 1, z[0] == 4};
ini2 = {x[0] == 10, y[0] == 10, z[0] == 0.1};
mester[param, orig, ini, "Chen", , 0, 13]
```

Out[249]=





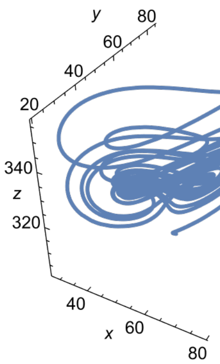


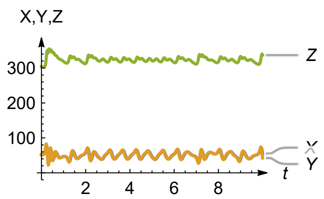
Figures\Chentraj.pdf	Figures\Chensol.pdf	Figures\Chensol1.pdf
{0.34, -20.024}	{0.32, -27.2664}	{0.1, 3.29023}
x′[t] == 35 (-x[t] + y[t])	y′[t] == -7 x[t] + 28 y[t] - x[t] × z[t]	z′[t] == x[t] × y[t] - 3 z[t] x[0] == 3 y

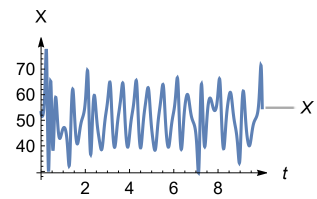
Shifted

In[250]:=
```
shift = {50, 50, 300};
mester[param, sheq[orig, shift, {x[t], y[t], z[t]}],
 shini[ini, shift], "ChenShifted", shift, 0, 10]
```

Out[251]=





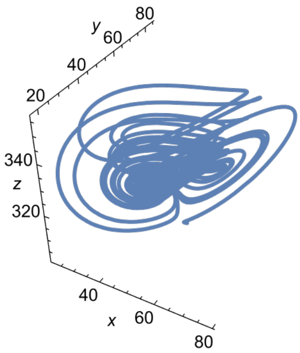


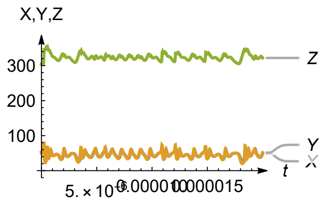
Figures\ChenShiftedtraj.pdf	Figures\ChenShiftedsol.pdf	Figures\ChenShiftedsol1.pdf	
{7.12, 29.5284}	{0.32, 22.7253}	{0.1, 303.283}	
x′[t] == 35 (-x[t] + y[t])	y′[t] == -7 (-50 + x[t]) + 28 (-50 + y[t]) - (-50 + x[t]) (-300 + z[t])	z′[t] == (-50 + x[t]) (-50 + y[t]) - 3 (-300 + z[t])	x[0] == 53 y

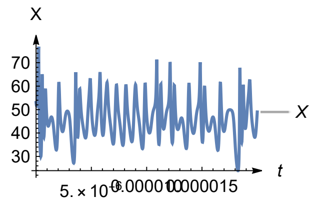
Shifted and multiplied

In[252]:=
```
mester[param, sami[sheq[orig, shift, {x[t], y[t], z[t]}]],
 shini[ini, shift], "ChenMultiplied", shift, 0.00, 0.00002]
```

Out[252]=







Figures\ChenMultipliedtraj.pdf {0., 53.}

Figures\ChenMultipliedsol.pdf {0., 51.}

Figures\ChenMultipliedsol1.pdf {0., 304.}

$x'[t] == -35\, x[t]^2\, y[t]\, z[t] + 35\, x[t]\, y[t]^2\, z[t]$

$y'[t] == -16050\, x[t]\, y[t]\, z[t] + 293\, x[t]^2\, y[t]\, z[t] + 28\, x[t]\, y[t]^2\, z[t] + 50\, x[t]\, y[t]\, z[t]^2 - x[t]^2\, y[t]\, z[t]^2$

$z'[t] == 3400\, x[t]\, y[t]\, z[t] - 50\, x[t]^2\, y[t]\, z[t] - 50\, x[t]\, y[t]^2\, z[t] + x[t]^2\, y[t]^2\, z[t] - 3\, x[t]\, y[t]\, z[t]^2$

$x[0] == 53$ ꞌ

Reaction

In[253]:=
```
crhs = (#[[2]] & /@ sheq[orig, shift, {x[t], y[t], z[t]}]);
crhs2 = crhs /. param /. {x[t] → x, y[t] → y, z[t] → z};
crhs3 = y z # & /@ crhs2;
chenCanonic = CanonicReaction[crhs3, {x, y, z}];
chenCanonic // MatrixForm
```

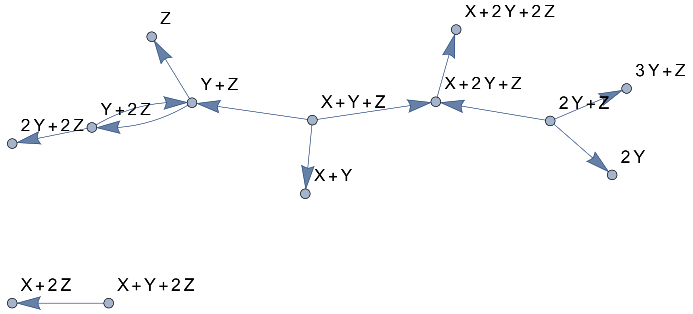
Out[257]//MatrixForm=

2 Y + Z → X + 2 Y + Z	35
X + Y + Z → Y + Z	35
X + Y + Z → X + 2 Y + Z	293
2 Y + Z → 3 Y + Z	28
Y + 2 Z → 2 Y + 2 Z	50
X + Y + 2 Z → X + 2 Z	1
Y + Z → Z	16 050
X + 2 Y + Z → X + 2 Y + 2 Z	1
Y + Z → Y + 2 Z	3400
X + Y + Z → X + Y	50
2 Y + Z → 2 Y	50
Y + 2 Z → Y + Z	3

FHJ-graph

In[258]:=
```
chenCanonicReactions = First /@ chenCanonic;
GraphPlot[FHJGraph[chenCanonicReactions], VertexLabels → "Name"]
```

Out[259]=



IV. Discussion and outlook