CHW Example 6.1

Loads the chemJac command file, which contains all commands used below

```
(* SetDirectory["C:\CHEMmma"] *) (* Put in path to chemJac.m *)
<< "chemJac.m"
```

```
C:\CHEMmma
```

```
chemJac is loading...
```

```
chemJac has loaded
```

Inputting the stoichiometric matrix S

```
S = {{-1, 0, 2}, {-1, -1, 0}, {0, -1, -1}, {1, 0, 0}, {0, 1, 0}}
(*stoichiometric matrix*); S // MatrixForm
```

$$\begin{pmatrix} -1 & 0 & 2 \\ -1 & -1 & 0 \\ 0 & -1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Making the mass-action flux vector 'monomials' and the list of species concentrations 'vars' automatically from S

```
monomials = makeMonomial[S]
```

```
{a[1] a[2] k[1], a[2] a[3] k[2], a[3] k[3]}
```

```
vars = svars[S]
```

```
{a[1], a[2], a[3], a[4], a[5]}
```

'S.monomials' is the right hand side of the ODE

```
S.monomials
```

```
{-a[1] a[2] k[1] + 2 a[3] k[3], -a[1] a[2] k[1] - a[2] a[3] k[2],
 -a[2] a[3] k[2] - a[3] k[3], a[1] a[2] k[1], a[2] a[3] k[2]}
```

The Jacobian of the RHS of the ODE, and its Craciun-Feinberg determinant

```
j = jac[S.monomials, vars];
j // MatrixForm
```

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

```
det = cfDet[j]
```

```
-1 - a[1] k[1] - a[2] k[1] - a[2] k[2] - a[3] k[2] - a[1] a[2] k[1] k[2] - a[2]^2 k[1] k[2] -
 a[2] a[3] k[1] k[2] - k[3] - a[1] k[1] k[3] - a[2] k[1] k[3] - a[3] k[2] k[3] + a[2] a[3] k[1] k[2] k[3]
```

```
coeffs[det]
```

The number of terms in the det expansion is 13,

and (a,b) says that the number of terms with coef a is b:

```
{{-1, 12}, {1, 1}}
```

```
Collect[det, a[2] a[3]]
```

```
-1 - a[1] k[1] - a[2] k[1] - a[2] k[2] - a[3] k[2] - a[1] a[2] k[1] k[2] - a[2]^2 k[1] k[2] - k[3] -
 a[1] k[1] k[3] - a[2] k[1] k[3] - a[3] k[2] k[3] + a[2] a[3] (-k[1] k[2] + k[1] k[2] k[3])
```

Core Determinant of the Jacobian of the RHS of the ODE

```
core = coreDet[j, S]
```

```
a[2] a[3] k[1] k[2] k[3]
```

```
coeffs[core]
```

The number of terms in the det expansion is 1,

and (a,b) says that the number of terms with coef a is b:

```
{{1, 1}}
```