# Documentation prototype for mathscout package

May 28, 2007

## 1 Embedding text

The MATHSCOUT statement `embedExtracts[inRoot, outRoot]` reads the LaTeX file `inRoot.tex` that contains lines of the forms

1. \\!!*externalFileName*!!\\,
2. \\!!*externalFileName*, *startLineNumber*!!\\,
3. \\!!*externalFileName*, *startKey*!!\\,
4. \\!!*externalFileName*, *startLineNumber*, *lineCount*!!\\,
5. \\!!*externalFileName*, *startKey*, *lineCount*!!\\,
6. \\!!*externalFileName*, *startKey*, *offset*, *lineCount*!!\\,
7. \\!!*externalFileName*, *n*[*startKey*]!!\\,
8. \\!!*externalFileName*, *n*[*startKey*], *lineCount*!!\\,
9. \\!!*externalFileName*, *n*[*startKey*], *offset*, *lineCount*!!\\.

Each of these lines is replaced by

```
\small\begin{verbatim}
⋮
\end{verbatim}\normalsize
```

where the ... stand for lines extracted from the specified external file for the five cases as follows:

1. the entire file,
2. from the starting line number to the end of the file,
3. from the first line that begins with the specified key to the end of the file,
4. the specified number of lines beginning at the specified line number,
5. the specified number of lines beginning at the specified offset from the first line which starts with the specified key,
6. the specified number of lines beginning at the specified offset from the $n$'th line which starts with the specified key.

You are reading a file called `docDemo.pdf`. It was created by:

1. typing a file called `docDemoRaw.tex` that alternates standard LaTeX coding of the text with `\\!!...!!\\` lines for the displays,

2. executing `embedExtracts["embedDemo", "embeddedDemo"]`; this produces `embeddedDemo.tex` by inserting the appropriate extracts, and then runs LaTeX and `dvips` in succession.

3. running Adobe Acrobat on the result.

The `\\!!...!!\\` lines conform to LaTeX syntax. The alternation of standard LaTeX with these lines can be seen, accordingly, by processing `embedDemo.tex` through LaTeX, `dvips` and Acrobat.

Case 1 is illustrated by the line `\\!!"forThermal"!!\\` which follows the present line.

```
{Thermal correction to Energy = 0.024185,
Thermal correction to Enthalpy = 0.025129,
Thermal correction to Gibbs Free Energy = 0.003701,
Sum of electronic and zero-point Energies = -76.427488,
Sum of electronic and thermal Energies = -76.424653,
Sum of electronic and thermal Enthalpies = -76.423709,
Sum of electronic and thermal Free Energies = -76.445137}
```

Case 2 is illustrated by the line `\\!!"forThermal", 6!!\\` which follows the present line.

```
Sum of electronic and thermal Enthalpies = -76.423709,
Sum of electronic and thermal Free Energies = -76.445137}
```

Case 3 is illustrated by the line `\\!!"forThermal", "Sum"!!\\` which follows the present line.

```
Sum of electronic and zero-point Energies = -76.427488,
Sum of electronic and thermal Energies = -76.424653,
Sum of electronic and thermal Enthalpies = -76.423709,
Sum of electronic and thermal Free Energies = -76.445137}
```

Case 4 is illustrated by the line `\\!!"forThermal", 3, 2!!\\` which follows the present line.

```
Thermal correction to Gibbs Free Energy = 0.003701,
Sum of electronic and zero-point Energies = -76.427488,
```

Case 5 is illustrated by the line `\\!!"forThermal", "Sum", 1!!\\` which follows the present line.

```
Sum of electronic and zero-point Energies = -76.427488,
```

Case 6 is illustrated by the line `\\!!"forThermal", "Sum", 1, 2!!\\` which follows the present line .

```
Sum of electronic and thermal Energies = -76.424653,
Sum of electronic and thermal Enthalpies = -76.423709,
```

and, for negative offset, by the line `\\!!"forThermal", "Sum", -1, 2!!\\` which follows the present line.

```
Thermal correction to Gibbs Free Energy = 0.003701,
Sum of electronic and zero-point Energies = -76.427488,
```

The subsidiary case of a null item implying zero offset is illustrated by the line `\\!!"forThermal", "Sum", , 2!!\\` which follows the present line.

```
Sum of electronic and zero-point Energies = -76.427488,
Sum of electronic and thermal Energies = -76.424653,
```

Case 7 is illustrated by the line `\\!!"forThermal", 2["Sum"]!!\\` which follows the present line.

```
Sum of electronic and thermal Energies = -76.424653,
Sum of electronic and thermal Enthalpies = -76.423709,
Sum of electronic and thermal Free Energies = -76.445137}
```

Case 8 is illustrated by the line `\\!!"forThermal", 2["Sum"], 2!!\\` which follows the present line.

```
Sum of electronic and thermal Energies = -76.424653,
Sum of electronic and thermal Enthalpies = -76.423709,
```

Case 9 is illustrated by the line `\\!!"forThermal", 2["Sum"], 1, 2!!\\` which follows the present line.

```
Sum of electronic and thermal Enthalpies = -76.423709,
Sum of electronic and thermal Free Energies = -76.445137}
```

The diagnostic for a request containing too many commas is triggered by
!!"water.log", "(5D, 7F)", 1, 3!!
The diagnostic for an embed request containing a MATHEMATICA syntax error is triggered by
!!"forThermal", 2["Sum], 2!!
The diagnostic for an embed request containing a file that is not found is triggered by
!!"ForThermal"!!
The diagnostic for an embed request containing a key that is not found is triggered by
!!"forThermal", "vibrational"!!
The diagnostic for an embed request specifying the $n$th occurrence of a key with invalid $n$ is triggered by
!!"forThermal", 7["Sum"], 2!!
and for negative $n$ by
!!"forThermal", -3["Sum"], 2!!
The diagnostic for an embed request with second argument neither integer nor string is triggered by
!!"forThermal", Sum, 2!!
The diagnostic for a request with positive offset out of range is triggered by
!!"forThermal", "Sum", 7, 1!!
The diagnostic for an embed request excessively negative offset is triggered by
!!"forThermal", "Sum", -7, 1!!

## 2 Embedding a diagram

The plot of energy against internuclear distance for the nitrogen molecule is incorporated in the tutorial by

```
\psfig{figure=nitrogen01.ps,bbllx=72bp,bburx=540bp,bblly=252bp,bbury=540bp,width=4in,clip=}
```

Hence:

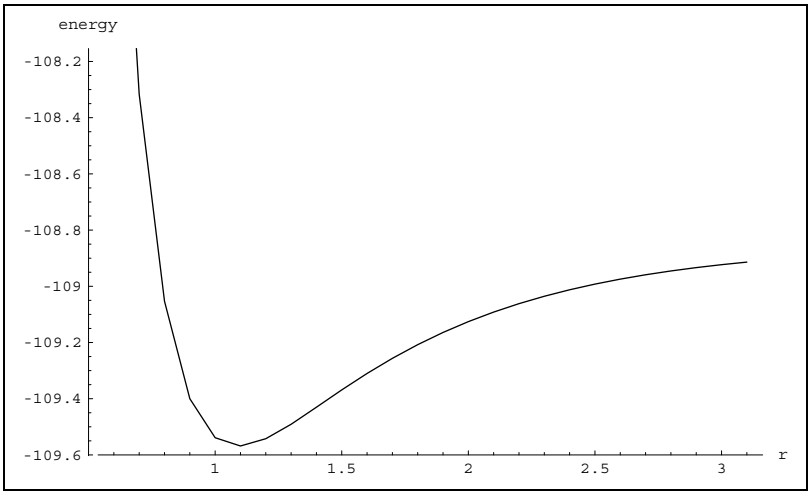


Figure 1. Energy *vs* internuclear distance in $N_2$.

## 3 Embedding a table

The plot that shows the geometry and dipole moments of some cyclobutanes is incorporated in the CPC paper, and here, by `\input{table01.tex}`. Hence

| | $d_{12}$ | $d_{23}$ | $d_{34}$ | $d_{14}$ | $t_1$ | $t_2$ | $t_3$ | $t_4$ | $\phi_{12}$ | $\phi_{23}$ | $\mu$ D |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CB | 1.55 | 1.55 | 1.55 | 1.55 | 88.57 | 88.57 | 88.57 | 88.57 | 25.48 | 25.48 | 0.00 |
| *cis*1,3-$Cl_2$CB | 1.54 | 1.54 | 1.54 | 1.54 | 86.78 | 89.70 | 86.78 | 89.70 | 27.94 | 28.65 | 2.07 |
| *trans*1,3-$Cl_2$CB | 1.54 | 1.55 | 1.55 | 1.54 | 88.11 | 89.27 | 88.11 | 89.67 | 23.33 | 23.60 | 1.14 |
| *cis*1,3-$Br_2$CB | 1.54 | 1.54 | 1.54 | 1.54 | 86.33 | 89.90 | 86.33 | 89.90 | 28.78 | 29.68 | 1.96 |
| *trans*1,3-$Br_2$CB | 1.54 | 1.55 | 1.55 | 1.54 | 87.85 | 89.32 | 87.85 | 89.81 | 24.09 | 24.45 | 1.15 |
| silaCB | 2.38 | 2.38 | 2.38 | 2.38 | 87.72 | 87.72 | 87.72 | 87.72 | 32.09 | 32.09 | 0.00 |
| *cis*1,3-$Cl_2$silaCB | 2.38 | 2.38 | 2.38 | 2.38 | 87.89 | 89.80 | 87.89 | 89.80 | 22.74 | 23.11 | 2.69 |
| *trans*1,3-$Cl_2$silaCB | 2.38 | 2.38 | 2.38 | 2.38 | 86.26 | 89.53 | 86.26 | 89.62 | 30.28 | 31.15 | 0.84 |
| azetane | 1.49 | 1.55 | 1.55 | 1.49 | 88.85 | 86.01 | 88.85 | 90.43 | 25.87 | 25.75 | 1.22 |
| phosphetane | 1.90 | 1.54 | 1.54 | 1.90 | 90.95 | 96.91 | 90.95 | 74.99 | 26.85 | 26.18 | 1.34 |
| oxetane | 1.45 | 1.54 | 1.54 | 1.45 | 91.81 | 84.76 | 91.80 | 91.64 | 0.11 | 0.11 | 1.87 |
| thietane | 1.86 | 1.54 | 1.54 | 1.86 | 91.28 | 96.83 | 91.27 | 76.58 | 21.70 | 21.18 | 2.03 |

Table 1. Geometry and dipole moments of cyclobutanes.