Reference manuals

CBS

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Extrapolation to CBS

Extrapolation

$$E(x) = E_{CBS} + Ae^{-Bx}$$

Because we have four input energies (for x=2, 3, 4, and 5) and only three unknowns (E_{CBS}, A and B) we must use the least squares method. The aim of the method is to find the value of the parameters E_{CBS}, A and B so that the purpose (error) function is minimal.

$$f(E_{CBS}, A, B) = \sum_{x=2}^{5} \left[E(x, E_{CBS}, A, B) - E_{HF}(x) \right]^2 = \min!$$

We can use the **fit** method from the program **gnuplot** to find the optimal parameters.

See original documentation gnuplot or:
http://www.root.cz/clanky/gnuplot-prikaz-fit/

Procedure

- Prepare a text file **data.txt**, which will contain two columns: the cardinal number of the base (2, 3, 4, ...) and the energy calculated by the HF method.

- Run the program gnuplot and display the energy profile from the file **data.txt**:

```
gnuplot> plot './data.txt' using 1:2 with points
```

- Define a function for extrapolation:

```
gnuplot> E(x) = Ecbs + A * exp(-B*x)
```

- Set the default values of the parameter for optimization:

```
gnuplot> A = 1
gnuplot> B = 1
gnuplot> Ecbs= -80 # lower than the smallest calculated energy
```

- Perform pre-optimization of the parameters E_{CBS} and A and then final optimization of all parameters:

```
gnuplot> fit E(x) "./data.txt" via Ecbs, A
gnuplot> fit E(x) "./data.txt" via Ecbs, A, B
```

Procedure, *cont.*

- Display the input data, E(x) function and the value of E_{CBS}. Perform a visual inspection of the obtained results. The E(x) function must pass through all points and approach the found value of E as a CBS limit.

```
gnuplot> set xrange[2:7]
gnuplot> plot './data.txt' using 1:2 with points, E(x), Ecbs
```

- Print the exact value of E_{CBS}

```
gnuplot> print Ecbs
```